The Impact of Climate Change on Wine Quality



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Declaration

I declare that this thesis was composed by myself and that the work contained herein is my own except where explicitly stated in the text. The work has not been submitted for any degree or professional qualification except as specified.

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Here's to the Georgians, who say they invented it,
Burying the stuff in big clay pots;
To the French, and Italians, who further fermented it,
Made appellations, and drank lots and lots.

Here's to the boozers, the vintners and sellers,
Who offer us stuff we could never afford,
And here's to the keepers of cavernous cellars,
Whose bottles are dusty, and heavily insured.

Here's to Our Lord, who made it from water,
And here's to producers who make it from grapes.
We drink to the health of the tolerant porter
Who lets us ship booze to the lodge by the crate.

And here's to the Bacchants, from way back when,
Who frolicked and drank by the light of the moon;
And their modern successors, on Little Clarendon Street
Who drink from the bottle, and spurn the spittoon.

Here's to the Club – long may it persist;
And here's to us all – may we not get too pissed.
To Bacchus!

Patrick Hudson

Publications and Contributions

The following publications have arisen from this thesis.

Chapter 2

- **Wood, A.**, Gascoigne, S. J. L., Gambetta, G. A., Jeffers, E. S., & Coulson, T. (2023). Seasonal weather impacts wine quality in Bordeaux. iScience (Vol. 26, Issue 10, p. 107954). Elsevier BV. https://doi.org/10.1016/j.isci.2023.107954

A.W. and S.G. conceived the main ideas and initial methodology; all authors contributed improvements to ideas and the methodology; A.W. collected the data and A.W. and S.G. analysed the data; A.W. led the writing of the manuscript, with edits from all authors. All authors contributed critically to the drafts and gave final approval for publication.

The following manuscripts have arisen from this thesis, and are presented in chapters 3, 4, and 5:

Chapter 3

- **Wood, A*,** Vargas Soto, S., Gambetta, G., Schober, D., Jeffers, E., Coulson, T., Modelling the Climate Changing Concentrations of Key Red-Grape Quality Molecules Using a Flexible Modelling Approach (In Prep)

AW conceived the project with additional input from SVS and DS, then performed all the analyses with input from TC, EJ and SVS. AW created all the figures and wrote the complete first draft. AW led the writing of the manuscript, with edits from all authors. All authors contributed critically to the drafts and gave final approval for publication.

Chapter 4

- **Wood, A.***, Shiaelis, N., Jeffers, E., Gambetta, G., Coulson, T. Determining the Optimal Temporal Resolution of Temperature as a Predictor of Grape Harvest Dates (In Prep)

AW conceived the project with NS, then performed all the analyses, created all the figures, and wrote the first draft. AW led the writing of the manuscript, with edits from all authors. All authors contributed critically to the drafts and gave final approval for publication.

Chapter 5

- **Wood, A.*,** Jeffers, E., Gambetta, G., Miles, J., Neder, A., Coulson, T. Wine on the Move: Mapping the Shifting Terrains of Global Wine with Distribution Models (In Prep)

AW conceived the project, AN and JM assisted with data preparation. AW performed all the analyses, created all the figures, and wrote the first draft. AW led the writing of the manuscript, with edits from all authors. All authors contributed critically to the drafts and gave final approval for publication.

Abstract

This thesis seeks to explore the impact of changing weather and climate on the quality of wine. It does this through utilising multiple metrics to examine the changes in different aspects of high-quality wine. These metrics include wine critics scores (Chapter 1), metabolic indicators of quality (Chapter 2), the harvest dates (Chapter 3), and finally wine price (Chapter 4). Each measure reveals a different facet of the story, with temperature and rainfall playing key roles, but the suite of factors that make up terroir playing their part too. The first half of the thesis uses classical frequentist statistics in the form of generalised linear models and coupled linear models (to form a path model) to seek to understand the drivers of wine quality. The second half of the thesis uses machine learning techniques to attempt to understand the predictability of wine harvests and global spatial distributions. In doing so, this thesis endeavours to make predictions both on the future of wine, but also to understand the predictability of harvest dates. In achieving these aims this thesis seeks to navigate the complex interplay between climate dynamics and wine. Each chapter adds a dimension to this understanding of quality. After an introduction to wine quality in the first chapter, the second chapter explores the impact of changes in weather during the calendar year on wine critics scores. It finds that weather impacts the wine throughout the year, but with the best wines being made in years with higher winter rainfall, warmer temperatures (particularly during the summer) and earlier, shorter seasons. The third chapter finds that climate change is predicted to create bigger, bolder, red wines with higher concentrations of metabolic markers of quality. The fourth chapter explores the timing of the optimal harvest of wine. It finds that optimal harvest timings are advancing, but also that weather resolution depends on changeability of harvest date (more stable harvest weekly weather is best, and monthly in more variable

environments). The fifth chapter explores the changing distribution of wine, finding that it is context dependent. For each region a shift, contraction, and expansion (including persistence *in situ*) of the wine producing range is possible, but also that this is quality level dependent too – each quality band moves differently. Combined, these chapters suggest that wine quality will vary with global climate change, with cooler areas producing stronger, richer, wines which are generally perceived as higher in quality. The risk is that in warmer areas these changes will be too great for the grapevines to cope with, and thus each chapter also provides applied climate change mitigation strategies to help maximise the quality of wines in years to come.

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1

Introduction

Number of words in Chapter: 3872

Wine is a complex biological product. It is produced by the fermentation of grapes from the common grapevine, *Vitis vinifera* L. Variation in the quality of grapes and wine is a multifaceted issue which can often lead to debates from vineyard to critic, and from academic journals to the dining table. This is because perceived quality is difficult to quantify, has many metrics and approaches possible, and can also be incredibly personal. The quality of wine and wine grapes is also incredibly important, as quality determines the price of the crop and final product and by doing so it determines the added value of the production much more so than yield. Therefore, determining any impacts of weather on quality of wine, or indeed the prospects of wine quality with climate change, requires a multi-faceted exploration of quality via different measures of quality in wine-grapes and the wine that comes from them. This thesis seeks to explore the impact of weather and climate on quality in wine and wine grapes. In doing so it endeavours to explore the impact of changes of weather and climate on the quality of future wines.

Vitis vinifera is a woody perennial crop species, renowned for growing throughout the spring and summer, and producing berries during the autumn. There is high genetic variation within grapevines, with 10,000 registered varieties globally. The four major stages in the grapevine lifecycle are: budburst, flowering, veraison, and harvest of the

grape berries. Grapevine flowers are monoecious, and plants can be self-pollinating, wind-pollinated, or pollinated through bees. Berries that grow start off highly acidic with a strong bitter taste due to a high concentration of tannins that make them unpalatable by animals during ripening. As the season progresses the grapes become more neutral in pH, sweeter, more complex in aromas, and during ripening they change colour from green to dark red or black as the pips (seeds) mature. These changes all evolved in pre-domesticated grapevines to allow for the attraction and enticement of birds and mammals that disperse the seeds. The main diseases of grapevines are fungal – powdery (*Erysiphe necator*) and downy mildew (*Plasmopara viticola*), as well as grey fruit rot (*Botrytis cinerea*). Some pathogens are nematodes (most notably root-knot nematode, *Meloidogyne incognita*), others are caused by insects, most notably Phylloxera (*Daktulosphaira vitifoliae*).

Part of the problem of defining wine quality results from the diversity in modern wine growing regions. Such regions range from the cooler climates of Germany and the United Kingdom to the much hotter and arid areas of Australia and Argentina[1]. The adage is that wine is grown between 30 and 50 degrees in both the Northern and Southern hemispheres, however this knowledge is now being challenged with tropical and wines being grown since the 20th century[2], and wine spreading outside of the

latitudinal range (into regions such as the UK). As well as temperature ranges, there are also differences in the macroclimate (for example light, precipitation, humidity, and salinity as well as temperature) between regions used to grow wine grapes[3]. For instance, there is evident difference between maritime wines, such as Bordeaux, and the alpine wines of Switzerland and Northern Italy[1]. The macroclimatic differences between regions are suggested to lead to the variation in wine styles which exist, from the hot and intense wines of Australia (most notably in red wines like Shiraz) to the lighter wines of Northern Europe (a Mosel Riesling or an English sparkling wine for example)[4]. It has therefore been suggested that the intensity of wine is on a scale[4], with flavours starting lighter with vegetal style (green grass and floral notes) and ending up heavier with cooked fruit style (fruits in alcohol and oxidised prunes)[4]. This scale is thought to correlate with climate, with hotter and drier climates generally leading to stronger and more powerful wines[4].

This evidence is more than anecdotal, and climate has long been cited as one of the major factors that affects the quality of wine. The impact of atmospheric conditions on core metabolic quality parameters has been repeatedly examined experimentally in isolated conditions and in individual regions[5–7]. Such potential effects on different grape and wine quality parameters have been collated in review papers on this topic[5,7,8].

Each of these studies detail the interannual effects of changes in the weather to changes in the grape. When taken as a group, they suggest generally that higher sugar and lower acidity occurs at higher temperatures and lower rainfalls. The trend of the relationship between weather and aromatic compounds is more irregular, but often is the inverse for phenolics, berry weight, and anthocyanins[5–8]. These relationships are found to be noisy, varying in magnitude, and hence the precise impact of weather on these aspects of wine is varying or unknown[5–8]. Such relationships have also not been widely studied across space and time, leading to issues when forecasting the potential impacts of climate on future compositions.

Anthropomorphic climate change has been caused by the increase in greenhouse gas concentrations in the atmosphere, most notably CO_2. These increased concentrations have led to a warming of the global atmosphere[9]. This increased warming has led to several predicted, and more commonly realised, impacts of climate change on wine growing regions[10]. The variation in the wine growing regions of the world can be attested to the impacts of these macroclimatic changes. It is theorised that as the average temperature increases the length and intensity of growing seasons will also increase. This increase in temperature also changes the phenology of the growing seasons with growing seasons starting earlier, and earlier budbreak and flowering leading to longer potential seasons[10–13]. There are also changes to precipitation, with lower average rainfall leading to higher water scarcity[13]. Combined, it is expected that there will also be changes in cloud cover and consequential light intensity, however this is currently an area of uncertainty in the climate change modelling areas[14–16, 88,89]. As these impacts of climate change occur globally, they also occur outside of wine growing regions, making them suitable for the growth of wine, as is seen in the south of the United

Kingdom. Thus, some areas may become more suitable for the growth of wine, and others less suitable for the growth of wine, or perhaps only possible with a change in style.

Increases in the mean temperature are not the only predicted changes in future climates of wine growing regions. The other major predicted difference is the increase in the number of extreme events, which can be considered as a change in the variability of the climate[13,17–21]. Accordingly, there will be more heatwaves, more droughts, but also more colder periods during ripening, and higher numbers of frost events post-bud burst[13,17–21], although this last one is controversial[90]. This leads to the potential for increasing impacts of extreme events on the yields and quality of harvested grapes. It also increases the need to understand these linkages as much as possible.

To understand the complexity in researching quality in wine requires an understanding of the history of wine quality. This is because wine has been drunk since antiquity and has, to a varying extent, been cited as responsible for shaping global civilisation[22–25]. *Vitis vinifera* L. is one of 83 recognised species within the genus Vitis[26], a genus that phylogenetically split from its closest relatives about 30 million years ago and grew in North America[27–30].

When grapes were first domesticated quality was not an issue that was considered. It is thought that the ancient grapevine, *Vitis vinifera subsp. sylvestris* L., was domesticated in the Caucus mountains between the Black Sea and Iran[30], with wild relatives growing in the lands surrounding what is now the Mediterranean, Black, and Caspian Seas. During the domestication process humans selected for attributes which increased quality of the grapes. The resulting changes were increase in berry size, sugar content,

and the ability to self-pollinate. This was thought to happen around 8000 years ago, with the oldest archaeological records of domesticated grapes in the hill-top towns of Shulaveri and Imiri, in Georgia[23,24,31]. The first written records of grapes and wine can be found in the Epic of Gilgamesh, the Sumerian text from approximately 2100BC[32]. These records do not mention the quality of the wine, nor the climate in which they were produced, only that Gilgamesh should "fill his belly with good things"[33].

This early wine was produced to be a safe to drink form of water, and little thought was put into making it a quality product that could be exported and sold. Bunches of grapes were fermented whole, and thus the mixture of grape skins and seeds, which make up the must (grape juice) and pulp (fruit flesh) of the wine, were all present in the wine as it was made.

The first considerations of quality and climate in wine seems to be during the Roman period. After the Phoenicians and Greeks had transported wine across the seas, the Romans dominated the maritime wine trade, and it was also transported with the Centurions when they travelled. When the Centurions settled in various parts of Europe, they took wine with them and planted their own vines. There is some evidence that the Celts were already making wine[22], but due to the Romanisation of Europe there was a large increase in wine demand and large vineyards were planted in France and Spain, and smaller vineyards in other parts of the Empire, including the UK[34]. This Roman wine making marked the beginning of innovation in both grape growing (viticulture) and in winemaking (viniculture) in terms of quality.

Most of what we know about Roman viti- and viniculture, as well as consumption, comes from the writings of Columella, in his 12-volume agricultural treatise "De Re

Rustica" (On Agriculture)[34]. Two of the volumes were written on vines, and most aspects of viticulture were talked about: from aspect and slope of vineyard to variety of grape, training of vines, exposure to sunshine, and soil composition. This is the first recorded instance of the discussion of wine quality, with aspects of the treatise focusing on quantity versus quality of wine being produced[35]. This quality was measured through price by location, with Italian wine was seen as superior quality during this time, and thus commanded a better price around the empire.

After the fall of the Roman empire, wine quality was once again not generally considered important. Instead, a new grape subspecies was developed and used across Europe: *Vinis vinifera subsp.* occidentalis. During this Medieval period the main European grape growing regions were France, Italy, Spain, Germany, and Portugal. In each of these countries the mantle of growing vines was taken up by the monasteries, and this new subspecies, with its small bunches of small grapes, was cultivated extensively. For example, in Germany, the imperial and royal monastery Lorsch in Hessische Bergstrasse was said to have possessed 900 vineyards in around the year 850AD, and it is said to be then that the vineyards now famous for Resiling along the side of the river Rhine were started by the emperor Charlemagne[36]. Instead of a quality beverage, the monastic use of the wine was threefold. Firstly, as communion wine, secondly for drinking by pilgrims, and thirdly for soaking bandages to make them sterile. More than 100 modern appellations still refer to their monastic origins, most famously Chateau Neuf de Pape and Abbaye de Fontfroid in France[36,37].

The focus on wine quality started to improve again post-Charlemagne, especially once the Plantagenet Queen Eleanor of Aquitaine commenced free trade between Bordeaux and England in 1152. This trade was notable for the upper echelons of British society.

Bordeaux wine became a mark of quality, gaining the name claret. Claret comes from the Latin for clear and meant a pale or light-coloured wine. This linguistic change shows a distinction in quality of Bordeaux wines, especially noticed in the London markets. Bordeaux wines started to gain a reputation for quality, and the Bordeaux wine Haut-Brion was the first wine to internationally market itself with its own vineyard name in 1521, rather than its parish (or "appellation" in French) name. By starting the first wine brand, Haut-Brion was demonstrating their quality as an individual location, showing their prowess and distinctive wines from their single vineyard[38]. Quality here still dictated the price of the wine, as well as the status of it.

It was during this period that the conquistadors and colonial settlers took wine around the world with them. This was partly for the maintenance of quality wines as they travelled, but probably mainly for security of consumption reasons. As the settlers travelled, they took with them the first vines that produced the wines of Chile, Argentina, United States, Australia, New Zealand, and South Africa[39]. The first Chilean vines were planted in the 15th century[39], but it was not until the 19th century that the first Australian wineries were planted. As technologies advanced, so too did the colonial wines, and the so-called "noble" grape varieties which now make up the international wines were established globally in the 19th century. The number of noble grapes is said to vary depending on whom you ask[40,41], with any list being controversial but most lists including Cabernet Sauvignon, Merlot, Pinot Noir, Chardonnay, Grenache, Sauvignon Blanc, Riesling, Chenin Blanc, Gewürztraminer, Semillon, and Syrah/Shiraz[40]. The Noble grapes are known to retain their quality wherever they are planted, and the first six of them mentioned make up approximately an eighth of global vine area[42].

As time progressed the new vineyard brand of Haut-Brion was joined by more other wine brands seeking to demonstrate their quality. This increased the complexity of the Bordeaux wine market so much that in 1855, Emperor Napoléon III asked the merchants of Bordeaux to draw up a classification of the best wines of Bordeaux based upon reputation and price. This was the Grand Cru Classé classification system and is the most famous quality rating system for wine globally. Haut-Brion was joined by just three other chateaus in the Premier Cru (1st growth) classification[91]. Haut-Brion is also the only chateau from its locality (Graves) in the Grand Cru Classé system, the rest of the 58 chateaus are from the Médoc area of Bordeaux[91]. Only two changes have been made to this classification. In 1856 Cantemerle was added to the Fifth Growth, and in 1973 Mouton-Rothschild was added to the Premier Grand Cru Classé classification[43]. This Grand Cru Classé system was subsequently rolled out across France across all major growing regions to rank wines based on reputational quality.

In the current world the global wine market has grown rapidly. Global sampling suggested that wine has been consumed by 75% of people[44], and is regularly consumed by 24-44% of people[44,45]. Grapes are the largest global perennial crop by gross production value, and the 80 million tonnes of grapes grown in 2018 generated $74bn of value[28,29]. In 2018, 57% of these grapes were pressed and fermented into 292 million hectolitres of wine[46,47], a figure which has since remained stable[48].

On a more local scale, the parish system as a mark of quality is still present across much of the world, with, to use the English version of the EU and USA designations: Protected Designations of Origin (PDO) being found across most wine growing regions[49]. PDOs are called appellation d'origine protégée (AOP) in France, denominación de origen protegida (D.O.P.) in Spain, and denominazione di origine

controllata e garantita (DOCG) in Italy, and geographical indication (GI) in Australia and New Zealand. They are the highest level of legal protection a product can receive, and each legal specification dictates exactly what must be done to produce the product. Accordingly, geographical indications protect both the name of the product as mark of quality and indicate that certain characteristics of the wine are present. Thus, quality is supposedly retained through this marking.

Ranking systems like the Grand Cru Classé systems are still present as a method of determining relative quality of wine. These systems still agree with the original classification systems in the main[50], but they instead determine quality globally.

In 1978 the wine critic Robert Parker started the 50 to 100-point rating system in his publication *Wine Advocate* and is credited for driving the rise in the quantification of wine quality metrics during the 1980s. In the modern world critics scores abound, from numerous wine magazines to sommeliers, and wine merchants to consumer apps rating wines (e.g. Vivino). It has been controversially[7] argued that critics, most notably Robert Parker, have driven an increase in the production of stronger, bolder wines over the past 40 years[51] by driving their commercial interest and value.

Critics scores have been regularly used as measures of quality in publications, for example for both Bordeaux[52,53], and Burgundy[54] grapes. Another popular method includes examining the price paid for grapes[55], or by rating wines through scoring wine attributes using sensory analysis[56,57]. The latter has several limitations[56], including that expert opinions can vary regionally[58], and that the expectations and environment influence tasting[56]. Vintages also develop and vary with time, further impacting the perceived quality of the wine.

These wine rating systems only rate the final wines, post-fermentation, they do not rate the grapes themselves. In the modern understanding, wine grape quality has been attributed to the dimensionless term of "optimal ripeness"[8], and it has been acknowledged that it lacks a single measure[59,60].

Despite numerous compounds being both important and highly variable in the harvested grapes (e.g. tannins, flavanols, and phenols), multivariate molecular measurement is not widespread in viticulture[59,60]. Instead, the total soluble sugar (TSS) content of the pressed grape juice is the most widely used metric to assess ripening[8]. Maximum TSS varies depending on cultivar and the wine being produced: for example, Shiraz is 20° Brix[61], Merlot and Chardonnay are 24-25°Brix[62,63], and muscat is 27° Brix[8,61, 92].

This single sugar measurement of viticultural quality is frequently extended to a metric comparing the ratio of sugars and acids in the grapes[64], often called technical maturity. This may be because thresholds of sugar and acid contents are detailed in statute globally [65–67]. These ranges define what it means to be a still or sparkling wine, and accordingly, viticulturalists must grow grapes to surpass these thresholds set out in statute or risk being unable to produce wine[64]. The measurement is regularly expressed as a ratio of total soluble solids (measured in degrees Brix) to total acids (measured in grams per litre)[68–75]. Potential alternatives to such ratios have been proposed to better measure quality. For example, Jordan et al (2001) proposed BrimA (Brix - k·TA) where k is a coefficient between two and ten and varies depending on the variety of grape[76]. The relative merits of BrimA versus Brix:TA ratio are controversial and benefits appear to vary depending on grape cultivar and the consumer testing carried out[69,77].

More recently, the concept of grape quality has been extended to include the concepts of phenolic or physiological maturity (measures of tannins and pigments) and aromatic ripeness (olfactory features)[8]. This reflects a drive to expand the aspects considered when assessing quality, although ideal aromatic ripeness remains undefined[5,6]. Whilst studies normally directly measure aromatic ripeness[8], these measures have also been derived from sugar and acid concentrations[78]. However there does also exist a difference between ripeness and quality. Ripeness is a point in phenology representing a local maximum of quality for the year. Quality itself is a global property and represent the absolute relative goodness of the grapes compared to all grapes ever recorded.

Agricultural practises for grapevines are designed to optimise growth, yield, and quality. Grapes are grown as a simplified ecosystem, with vineyards often having tilled soil between vine rows, or at most some inter-row planting of species like vetch (*Vicia lutea*), or brown mustard (*Brassica juncea*). Choosing the best sites for vineyards includes considering aspect of slope and soil composition[84,87], and planting decisions include variety choice, spacing of vines, and pruning style. Vineyard management includes annual pruning, trellising, spraying with pesticides for diseases, and defoliation before harvest. Each of these factors represents options that vineyard managers can take, and all of them have impacts on the quality of the grapes and hence wines that are made.

The factors that impact ripeness and quality are combined into the term "terroir"[84-87]. Terroir roughly translates from the French as "landscape", and examines the multi-factorial combinations of soil composition, biodiversity (both micro and macro), management practises, grape varieties, topography, and climate which all combine to

form the wine[84-87]. Where PDOs are present these terroirs are codified into the specifications for producing the designated product. For example, in the French region of Champagne, AOP regulations from 1938 dictate that pruning must occur in the Chablis (most often for chardonnay) or Cordon de Royat (mainly for Pinot noir) styles for Grand and Premier cru grapes. The Guyot style is also permitted, and the Valée de la Marne style is used primarily for Pinot Meunier grapes[79,80]. As part of the AOP, harvest yields are also specified annually by the regulatory body, which in 2023 have been set at 11400kg/ha[81]. Harvest dates in these regions are also specified by the CIVC and have been every year since its inception in 1941. Since 1989 a new regime was introduced with the certification of press houses and methods, and the dates were set individually per village and variety to pick at optimal maturity, and hence maximise quality[82].

My thesis seeks to explore the impacts of weather and climate on the quality of wine. It does this through exploring the impact of weather on various measures of quality. In each chapter I will seek to explore how variation in weather or climate impacts the quality of grapes or wines in different major wine producing locations around the world. I do this through utilising large datasets, across multiple years, and utilising high-resolution weather data. As such, I attempt to holistically address the question of the impact of weather on wine grapes. Each chapter explores a different aspect of quality in a different location, firstly critics scores in Bordeaux, followed by grape composition in Chile, followed by an exploration of harvest dates in Champagne vineyards and finally exploring future climatic niches for quality bands of different varieties of grape. In doing so I seek to understand the historic impact of weather on wine, such that we can develop our understanding of how climate change will impact the quality of the largest perennial crop in the world.

The first chapter of this thesis` is an exploration of Bordeaux quality scores of *en primeur* wines. It matches high-resolution weather data to a range of standardised critics scores to determine the relative importance of precipitation and temperature on the quality of the wine. It uses two methods to do this. The first method uses a monthly approach related to Ashenfelter's Bordeaux equation[53,83], and the second method uses a novel technique based on changes in seasonality. This chapter focuses on linking the personal scores of critics to the weather data to examine the impact of weather on the wine quality itself.

The second chapter is a statistical model of grape composition. These models focus on Cabernet Sauvignon grape characteristics which are important for wine making and track them during the period of ripening for grapes in Chile. It uses path models – linked linear regressions, to predict the composition of the grape at harvest. The statistical models are based upon grape maturity and harvest data from across six degrees of latitude and account for the soil composition, altitude, clone, rootstock, management style, as well as the weather (temperature, light, and rainfall).

The third chapter is an exploration of the predictability of harvest dates, and the timing of optimal quality. As harvest can be seen to occur at the peak of quality for grapes, this chapter seeks to explore the impact that changes in climate have on the timing of the harvest, and its predictability around the world. By using machine learning models, this chapter endeavours to explore how variation in weather lead to changes in the timing of high-quality grapes. It also suggests that how variation in quality metrics lead to issues with the predictability and timing of the harvest across different grape varieties. This chapter uses two datasets, one is a record of harvest in every champagne

village since 1989, the second is from the German phenological network. Thus 4 different grape varieties (Chardonnay, Pinot Noir, Riesling, and Müller-Thurgau) are all examined and compared.

The fourth chapter is a global exploration of the future of viticulture at different price points. It uses a Maximum entropy species distribution modelling approach to determine the current regions which are suitable for growing wines of 7 different international grape varieties (Cabernet Sauvignon, Chardonnay, Muscat, Pinot Noir, Riesling, Sauvignon Blanc, and Shiraz), and then forecasts their distributions into the future up to 2100. In doing so it explores the changes in the grapes across space and time with changes in global climate.

The thesis concludes by exploring the factors which unite these chapters. It then explores more philosophically how we choose to build models. It examines why I have built each chapter in the way that I have. This thesis utilises a range of types of models, and hence the selection of the appropriate model was crucial at each stage.

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2

Seasonal weather impacts wine quality in Bordeaux (Wood et al., 2023, iScience)

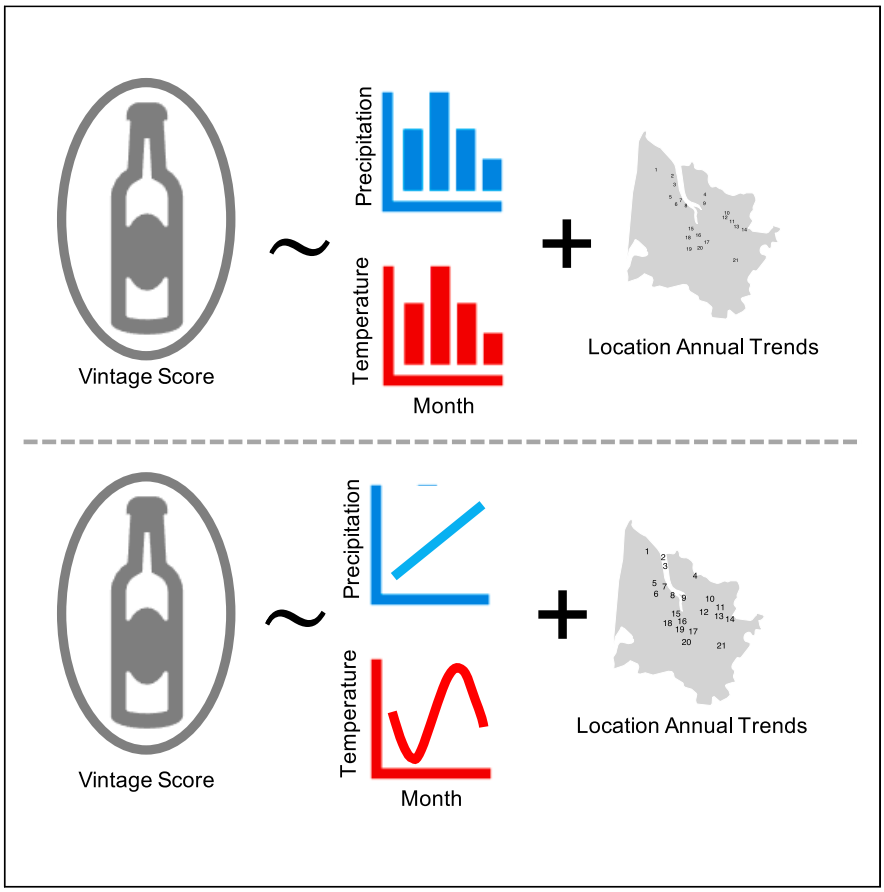
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Seasonal weather impacts wine quality in Bordeaux



Andrew Wood, Samuel J.L. Gascoigne, Gregory A. Gambetta, Elizabeth S. Jeffers, Tim Coulson

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Highlights

Wine quality measured through critics scores varies across space and time

Weather at multiple points during the year impacts wine quality in Bordeaux

Climate shifts suggest wine quality may improve with future predicted climate

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Seasonal weather impacts wine quality in Bordeaux

Andrew Wood,[1,3,*] Samuel J.L. Gascoigne,[1] Gregory A. Gambetta,[2] Elizabeth S. Jeffers,[1] and Tim Coulson[1]

SUMMARY

Critics judge quality based upon subjective characteristics of wine. These judgments are converted by critics into quantitative scores, which allow for comparison of vintages. This paper uses high resolution discrete and continuous time-based weather estimates at both a local and regional level to determine the role of weather conditions on producing high quality Bordeaux vintages, as determined by critics scores. By using discrete-time weather variables across local AOCs, this study reveals climate-quality relationships across the whole year, including previously ignored season effects. By using continuous time weather variables, we reinforce the evidence for these local effects by finding higher quality wine is made in years with higher rainfall, warmer temperatures; and earlier, shorter seasons. We propose management impacts of our results and suggest that as the climate continues to change, the quality of Bordeaux wines may continue to improve.

INTRODUCTION

Climate change is globally impacting agricultural produce, both in terms of yield and quality.[1,2] Despite these expected effects, the link between climate change and agricultural produce quality has not been widely explored. Wine (*Vitis vinifera*) presents the ideal system to study this relationship as wine price is governed primarily by quality,[3] which is dependent on weather during the vine's growing season.[4] Additionally, wine quality in Bordeaux (France) has been measured by many independent experts over time, meaning that there exists a multi-critic regional and local longitudinal dataset for quality.[5–11] With the availability of high-resolution weather data we can now use this information to examine how weather influences quality on both a regional and local scale.

Local variation in the quality of wine was first acknowledged with the introduction of wine rating systems. The Bordeaux Grand Cru system was created in 1855 to classify individual vineyards into one of five categories based on price and perceptions of quality. This Grand Cru classification system has been expanded such that there now exists 14 defined categories of wines in Bordeaux, with other wines simply being categorized as unclassified via this method.[11] A series of geographical protections were introduced in 1936, referred to as *appellations d'origine contrôlée*, or AOCs. Acting on the local scale, they create individualities for wines, with each AOC having distinct viticultural characteristics and vinicultural identities.[12] Such identities can link an AOC to perceived quality, with some becoming more famous than others. Regional and local disparities can be explored by comparing scores for the whole of Bordeaux to individual wine scores linked to an AOC. Consequently, each individual wine is wrapped in its own historic quality ratings which have the potential to shift perceptions of the current and future wines. Such perceptions must be considered in any attempt to understand quality.

Some studies have directly examined quality using tasting scores.[13–15] In Bordeaux these tasting scores traditionally take the form of a *primeur* score. These scores are bestowed by wine critics at tastings approximately 10 months after harvest and just after blending. While these wines are not mature and often highly tannic,[11] this scoring system provides a direct standardized measurement of quality and allows for an ascertainment of the quality of the wine before it fully ages. Other critics, mainly wine merchants, rate Bordeaux as a whole region, giving an overall classification as to whether or not a year is good or not. Due to this two-scale rating system, there exists the potential to compare regional tasting scores to local tasting scores.

Weather conditions have also been demonstrated to have an impact on the wine quality. Most famously, Ashenfelter's (1995) Bordeaux equation[6–8] suggested that the average price of wine in Bordeaux is a linear function of winter precipitation and summer temperature. Other models have used monthly weather, demonstrating that finer resolution weather data and local chateau characteristics[6,16] can contribute to explaining price variation in Bordeaux wines. These local effects have been examined using this same price-based approach by Lecocq and Visser (2006) using local weather stations.[17] The models in Lecoq and Visser (2006) found similar results at both regional and local scales and thus suggested that in most cases regional and local weather records are interchangeable.

Tasting scores have been correlated with single-year metrics of weather such as annual mean temperature and precipitation[7,9,18] in wine-growing regions from Australia[14] to California.[13] Consensus from the Bordeaux equation, price modeling and current quality scores suggest that higher temperature and lower precipitation leads to higher quality grapes.[5,7,11] Ashenfelter and Jones (2013) suggest that: critics scores "reflect qualitatively the same weather factors that have been documented to be determinants of wine quality."[6] Multiple studies have shown

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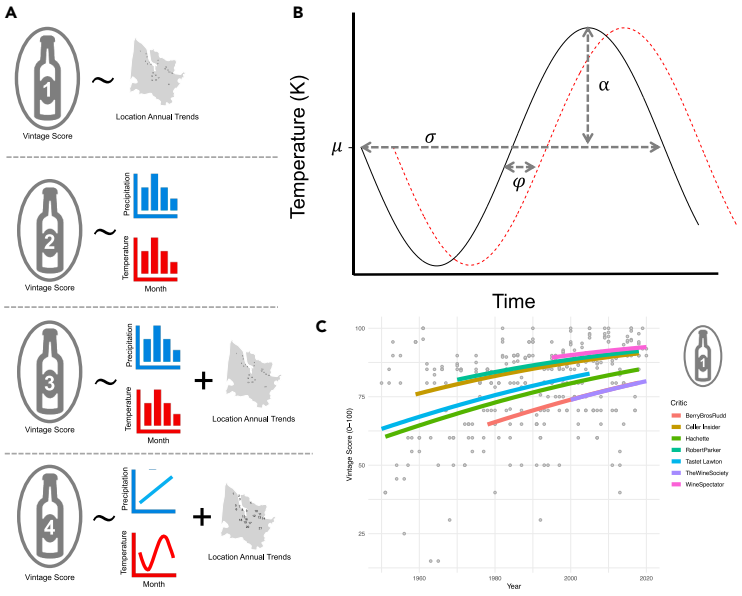


Figure 1. Methods panel plot

(A) Summary of the generalized linear models run to analyze the relationship between wine critics scores and the weather, controlling for location annual trends (location and year interactions). In each row the number on the bottle refer to the model number, and tilde means "is a function of".

(B) Depiction of sine wave with depiction of parameters fitted. μm is the mean temperature, α the amplitude, σ the wavelength, and φ the phase shift.

(C) Mean critics scores (scaled from 0 to 100) over time for Bordeaux as a whole with colored lines showing the GLM fitted.

that a higher number of warm days during flowering and at the onset of berry ripening (spring and summer) and lower precipitation during berry maturation (autumn) leads to higher quality.[5,19,20] But other conflicting studies have shown impacts outside of this time frame, with weather affecting quality across the year. Notably, the Bordeaux equation suggests that primarily winter precipitation and summer temperature is important. But Vittorio and Ginsburgh (1996) use the number of days of hail in April as well as temperature and precipitation during June to September.[16] Jones and Storchman (2001) look at phenological stages and find that four different weather aspects (evapotranspiration; total rainfall; and the number of days with temperatures more than 25°C and 30°C) all have an effect on the price of the final wine.[11] Baciocco et al. (2014) suggest that low rainfall and high heat accumulation over the year lead to higher ranked wines.[10] Bonada et al. (2020) claim that rainfall during winter dormancy impacts quality.[21] Alongside such varying insights in the literature comes a finding of a reduction in quality with high temperatures.[18,20] Other evidence also links spring frosts to changes in quality.[22] Overall, these findings suggests the potential for regional differences in climate change to potentially impact wine quality.[23] Thus, it is important to understand which features of the weather are affecting wine quality and when, in order to determine the precise impacts of climate change on a viticulturally relevant spatial resolution.

In this study, we explore the link between weather and critic quality scores, using weather and quality scores for Bordeaux wines, at both regional and local levels. We use discrete time models with time steps such that the impact of temperature and precipitation on wine quality scores across the year can be ascertained. We then use continuous time models which explore the weather across the whole year as single functions for rainfall and temperature. In turn, we aim to give greater understanding as to when wine quality is most susceptible to changes in temperature and precipitation, and how we can examine such changes.

RESULTS

Between 1950 and 2020 there was a general increase in quality scores for wine quality in the Bordeaux region. The maximal annual mean score was 98.67 points (1961), and the minimum was 32.5 (recorded in 1965). A generalized linear model was fitted to determine the location annual trends, as per model 1 in the model summary figure (Figure 1A). In this GLM, the overall critic score for Bordeaux is predicted by the year, controlling for critic. Year fitted as a continuous variable in the model was found to be statistically significant (coef = 0.0195, χ (1) = 4.4528, $p < 0.05$, $R^2 = 0.27$), meaning there is a general increase in critics' quality score over time (Table S3).

Quality scores were also examined on a local scale. The maximal mean critics score was 99 points (recorded once in 2019) and the minimum was 28 (recorded once in 2006). Critics showed high correlation between ratings (Figure S2). A binomial GLM was fitted, again as per model 1

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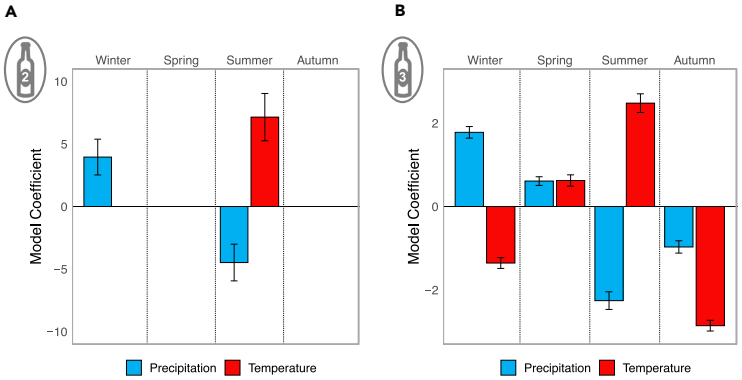


Figure 2. Weather variable model coefficients

(A and B) Weather variable model coefficients for generalized linear models (GLMs) fitted to explain (A) mean critic score for the whole of Bordeaux and (B) mean critic score controlling for AOC, Grand Cru status, and year. Bar presence signifies coefficient had a p value of less than 0.05 with standard error bars.

on the model summary figure (Figure 1A). It reported no significant coefficients for Year nor Year:AOC interactions. This suggests that, for the time period, there is no local increase in quality over time (for test statistics see Table S4).

Discrete time model

Generalized linear models were also built to explore the relationship between grouped monthly weather variables and the mean overall Bordeaux general score, controlling for the yearly trend of improvements (R^2 = 0.61; Table S5), as per model 2 in the model summary figure (Figure 1A). As weather has been normalized, only the sign (positive or negative) and the relative size of the coefficients are important. The largest significant ($p < 0.05$) coefficient in the model is the positive coefficient for summer temperatures (coef = −4.48, F (1,59) = 122.1716, p = 0.0004), followed by the negative coefficient for summer precipitation (coef = 7.14, F (1,59) = 114.0373, $p < 0.05$), and then the positive coefficient for winter precipitation (coef = 3.95, F (1,59) = 164.4203, df = 3, $p < 0.05$), as shown in Figure 2A. Models were found to fit well from visual inspection of residual plots (see Figure S3). According to this model, changes in temperature and precipitation at other times of year would not change the overall Bordeaux scores, excluding stochastic extreme weather events.

A generalized linear model was also run on the local (AOC) scale, as per model 3 on the wine model summary figure (Figure 1A). Model 3 examines the relationship between grouped monthly weather variables and individual wine scores, controlling for year increases, AOC, and Grand Cru status (n = 4521, R^2 = 0.35; for full details see Table S6). All weather terms were found to be significant, with coefficients shown graphically in Figure 3. Again, temperature and rainfall have been normalized for comparison purposes, and so exact coefficients are without real-world meaning. The largest coefficient is the negative term for temperature in autumn, followed by the positive coefficient for summer temperature, the positive term and the third largest impact is the negative coefficient for precipitation in summer. Models fitted well from visual inspection of plots (Figure S4). The variation in the coefficients shows the heterozygosity of the impacts, with positive and negative impacts occurring across the year. The coefficients appear to be in a wave formation, with both temperature and precipitation increasing and decreasing in a cyclical manner.

Results for models using parameters from continuous time weather models

Cumulative precipitation increases linearly with increasing month (Figure S5). Over time there exists a generalized trend of increasing precipitation with increasing year (year coef = 0.0000318, F(1,6185) = 1676.8, $p < 0.05$, for full results see Table S7). When mean critic scores are modeled against cumulative precipitation controlling for AOC and year, as per model option 4 in Figure 1A, a positive correlation is found (coef = 1779.8, F(1,6171) = 28.1, n = 4521, $p < 0.05$, R^2 = 0.29, Table S8). This suggests that higher whole year cumulative rainfall is beneficial for the production of higher quality wines.

Mean monthly temperatures have minima at around 3 to 4 months after September, in December and January. Peaks occur between 9- and 10-month past September—in June and July (Figure S6), increasing and decreasing in a wave pattern. Sine curves were fitted across each of the mean monthly temperatures and fitted the data well (mean R^2 is 0.95 and standard deviation of R^2 is 0.02, Table S9). μm and α were found to be the most variable terms, with means of 8.01 and 286.72 and standard errors of 0.79 and 0.65 (Table S9). σ and φ were found to have means of 0.52 and 3.07 and standard errors of 0.02 and 0.23 (Table S9). This suggests that mean temperature and temperature extremes can vary more than the timings of when seasons change.

Mean precipitation and the sine parameters of quality were used together as explanatory variables in a GLM, as per model 4 in Figure 1A. All factors, namely: mean precipitation (MeanPrecip), mean temperature (μ; C), amplitude (α; A), periodicity (σ, omega), and curve shift (φ; phi) were found to have significant ($p < 0.05$) positive coefficients (see Table S10 for test statistics). The marginal effects from this model can be

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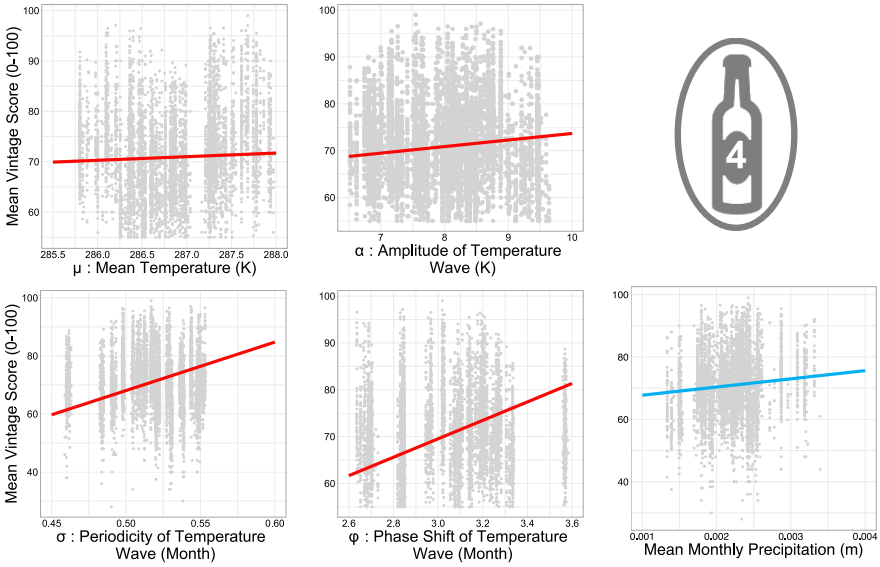


Figure 3. Model effects plots

Model effects plot showing the vintage score against the sine wave parameters and mean monthly precipitation, with the slope of the line being the coefficients of each parameter.

seen plotted in Figure 3. These results suggest that the greater the extremes in temperature (higher amplitude), the shorter and earlier the season (decrease in wavelength and positive temperature phase shift), and the larger the mean temperature and mean monthly precipitation, the higher the mean critic score of the wine.

DISCUSSION

All of the models suggest that weather is an important factor in the determination of wine quality. Taken as a whole, the models suggest that weather impacts the quality of wine over the course of the year, with importance varying between seasons and aspects of seasonal weather. This paper includes a new method of examining the weather-wine linkage, using continuous time rather than discrete time periods. It concludes that different aspects of temperature and precipitation are important to quality throughout the year, with high quality requiring periods of both high and low temperature and precipitation. Exploring weather as a continuous series, we find that higher quality wine is made in years with greater temperature extremes; earlier, shorter seasons; and potentially a higher mean temperature.

At a regional scale, quality can be seen to have increased over the last several decades (Figure 1C). The cause of such a trend cannot be distinguished statistically on such a scale. Multiple factors all act in concert to improve wine critics scores, namely: climate change, increasing technology, increased positivity in critics reviews, and increased matching of wines consumer pref. [4,28,29]. This increase in technology and consequential changes in wine characteristics since the 1960s have been described as the "Peynaudization" of Bordeaux wines.[30] Controlling for such trends therefore allows for greater exploration of the impact of individual aspects of wine quality scores. At a local scale, no increase in trend can be seen to exist, and thus no universal increase in quality can be detected (Table S4). This may be due to the shorter time duration, variation in wine making techniques, or potentially even that the regional trends reflect critic regional sentiment rather than specific wines and thus no actualized trend exists.

The overall Bordeaux generalized linear model (model 2 in Figure 1A) suggests the traditional view of high winter precipitation, high summer temperatures and low precipitation in the summer and autumn lead to high quality grapes (Figure 2A). This combination of precipitation and sunshine has previously been termed the "Bordeaux Equation,"[7,8] and has shaped the global understanding of grapevines.[29,31] However, the weather location we used to examine these regional scores is in the city center of Bordeaux. This is an urban area not related to viticulture. This suggests that general regional weather has some effect, but that this is not the whole story.

Like the Bordeaux equation, our overall models also advocate for the impact of out of growing season effects too, corroborating statistically with findings from Bonada et al. (2020) that an increase water availability during the dormancy phase (in our case from precipitation and in their case due to irrigation) leads to an increase in quality.[21] During winter the grapevines are experiencing dormancy, and a negative temperature coefficient here suggests a cooling period is required for high quality wine. The models also concur with previous findings that rainfall during the winter leads to higher quality,[17,21] with agricultural suggestions that this may be due to lower soil salinity.[32] It has been suggested that more rain in the winter could lead to a better water balance during the growing season, however, it has previously

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been shown that in Bordeaux only 3 of the last 70 years have started the growing season not at full water soil capacity.[2] Flowering, fruit set, and potentially the onset of berry ripening (depending on the year) all occur in summer, with hotter and drier weather again being suggested to make high quality wine in this time period, potentially due to lower promotion of major grape diseases.[7,19]

The individual AOC model (model 3 in Figure 1A) suggests a more complex view of the relationship and quality. While the same relationships between weather and quality are there during the summer and autumn for temperature and precipitation, additional effects are also present (Figure 2B). These are the negative effects of temperature in winter and autumn and precipitation in autumn, as well as the positive effect in temperature and precipitation in spring. The higher number of significant time periods suggests that weather impacts occur right across the year, with impacts of weather on quality score potentially varying due to the phenological stage of the grapevine.[5] As well as the dormancy effects, higher precipitation and higher temperatures in spring advocate for wetter and warmer weather for bud and leaf burst. Finally, cooler and drier weather is best for ripening in autumn and the optimal harvest to make a high-quality vintage. There is also an element of susceptibility suggested, with the impacts of water deficit on wine quality having greater impact on wine quality during the winter and summer months, and wine quality being more susceptible to temperatures in summer and autumn.

Combined, the two normalized weather models (models 2 and 3) suggest a difference between the regional and local levels. They suggest that heterogeneity at the local (AOC) level is being masked when only examining the regional level. They therefore suggest that, in order to improve the viticultural understanding and hence relevance of such modeling approaches, more local scale weather effects should be considered.

While these discrete-time suggestions are useful independently, they do not inform about time sequences of weather, which is exactly how it occurs. To explore this more fully, weather was treated as a continuous time variable. When examined in continuous time, monthly precipitation was found to be erratic and thus suited a cumulative approach, with increases being added and forming a linear accumulation. The fact that such an accumulation is well approximated by a linear model suggests an almost constant aseasonal pattern of precipitation, with the slope of this linear accumulation being the mean monthly precipitation. Conceptually, examining this mean monthly precipitation allows us to consider whether a whole year is wet or dry, rather than just the segments set out in the discrete GLMs. The significant precipitation term suggests that, even controlling for temperature, year, location, and class, a positive relationship exists between mean monthly precipitation and wine quality (Table S10). Wetter years appear to lead to higher quality wines. Coupled with the discrete time models (Figure 2), this model therefore suggests that this high rainfall should optimally occur post-harvest and pre-growth, during the dormancy period.

Temperature is not linear, rather it fluctuates according to seasonality and thus can be well approximated with a sine curve. Each of the parameters of the sine curve informs aspects of a temperature regime over the course of a year. In the GLM exploring the impact of temperature and precipitation parameters on mean quality score (again controlling for year, class, and AOC), the coefficients of each of the terms are found to be positive (Table S10). This suggests that, aside from being wetter, years that make higher quality wine are characterized by greater temperature extremes, with a higher mean temperature, and earlier, shorter seasons. While the increase in mean temperature concurs with previous research,[7,20] more extreme weather suggests colder winters and hotter summers give higher quality. Earlier seasons suggests that consistently warmer weather during early phenological stages is also beneficial. Warmer weather means lower risk of frost, suggesting that damage to crops extends beyond losses and into quality.[22,33] Warmer weather also potentially suggests that higher metabolic rates and higher photosynthetic rates lead to higher quality grapes. Shorter seasons suggest that the cooling of temperatures toward the end of the growing season may positively impact the ripening of grapes. With increases in both mean and extreme temperatures predicted across France,[34] and changes in timing and length of growing season also predicted across growing regions,[35] this leads to the potential suggestion that wine in Bordeaux may continue to improve over time.

Among these trends there still exists the question of the local versus regional disparities. The differences between the local and regional models in both their model coefficients and statistical significances suggest the impacts from the local scale are being masked when examined at the regional scale. This may be because of the individual differences in weather, or due to disparities in the wine making in each of the AOCs. For each of the models that are built, the Grand Cru classification system suggests significant differences between the classification levels, and similarly AOC level differences appear to exist (see Tables S6–S10). However, one potential source of variation in these data may be bias in expert opinion.[36–40] Statistically, it is impossible with these data to fully disentangle wine bias from perceived quality. Future studies where the data for wine quality is both linked to local weather and also rated in a double-blind fashion, will be necessary to capture the degree to which expert bias informs or weakens our predictions.

We suggest that such variation in quality classification between regions has masked local variation in impacts of weather on quality across the year. While we accept that biases exist within wine, both for a specific locale or classification, we have also demonstrated a significant shared understanding of quality.

There are clear management implications of these findings, which result from trying to optimize the environment for vine growth and fruit composition. Our models suggest that water regime is critical in determining higher quality wines. Specifically, to increase wine quality, ideal conditions include high water abundance during the winter months and low water abundance in the summer, coupled with high temperatures. Climate change in Bordeaux will likely lead to more extreme weather, with variation depending on the location.[41] While some places will be in drought, others will encounter less total rainfall punctuated with short heavy rain events.[41] For red wine production we suggest that if irrigation were to be considered, it would be best to target the water regimes highlighted in this work: a well-replenished soil water profile over the winter months followed by moderate to severe water deficits during the summer months (depending on yield and wine style considerations). In cases where heavy rainfall could be an issue in summer, increased drainage, erosion control, or, at an extreme, rainfall covers could be necessary. With regard to temperature management, summer management strategies which promote localized higher

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temperatures are suggested (especially during the ripening period). This can be achieved by increasing defoliation around the berries to reduce shading, but caution is warranted to guard against exposing fruit to temperature extremes. Finally, we agree with common practices of avoiding frost damage by raising temperatures around the vines during the spring months. With predicted phenological and weather changes leading to hotter and earlier summers, our results suggest that average Bordeaux quality scores may continue to increase.

This paper has explored the impact of weather on wine, seeking to determine the optimal growing conditions for high quality Bordeaux vintages. It explores the infamous Bordeaux equation, finding that the equation works well for explaining regional patterns, but that for individual AOCs the weather impacts occur over the course of the year. Exploring this weather sequentially, this paper finds that higher quality wine is made in years with greater temperature extremes; earlier, shorter seasons; and a higher mean temperature. This all suggests that as climate change increases, the wine quality may continue to get better.

Limitations of the study

We appreciate that the study was only conducted using ratings for Bordeaux chateaus, and that the corresponding limitations are therefore that we can only control for the winery at the winery level. We cannot control for the winemaker changing, or any potential changes in the exact plots used to make the wines. Finally, it is statistically impossible to tell the difference over time between improvements in wine due to climate and winemaker (and hence this trend has been removed from dataset). Despite these limitations, we have shown a robust trend within the dataset concerning the impact of seasonal weather on the quality of wines.

STAR★METHODS

Detailed methods are provided in the online version of this paper and include the following:

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SUPPLEMENTAL INFORMATION

Supplemental information can be found online at https://doi.org/10.1016/j.isci.2023.107954.

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AUTHOR CONTRIBUTIONS

A.W. and S.G. conceived the main ideas and initial methodology; all authors contributed improvements to ideas and the methodology; A.W. collected the data and A.W. and S.G. analyzed the data; A.W. led the writing of the manuscript, with edits from all authors. All authors contributed critically to the drafts and gave final approval for publication.

DECLARATION OF INTERESTS

We declare no conflicts of interest.

INCLUSION AND DIVERSITY

We support inclusive, diverse, and equitable conduct of research.

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STAR★METHODS

KEY RESOURCES TABLE

REAGENT or RESOURCE	SOURCE	IDENTIFIER
Deposited data		
ERA-5 Land Hourly Weather Data	https://doi.org/10.24381/cds.e2161bac	
BordOverview Wine Database	https://www.bordoverview.com/	
Software and algorithms		
RStudio		
tidyverse packages		
Krigr package		

RESOURCE AVAILABILITY

Lead contact

Further information and requests for resources and reagents should be directed to and will be fulfilled by the lead contact, Andrew Wood (wood_and@hotmail.com).

Materials availability

This study did not generate new unique reagents.

Data and code availability

This paper analyses existing, publicly available data. All data is publicly available at locations referenced within the text. Wine data is available here: https://www.bordoverview.com/ and climate data from: https://cds.climate.copernicus.eu/cdsapp#!/dataset/10.24381/cds.68d2bb30?tab=overview as documented in the reference list and the key resources table. Any additional information required to reanalyse the data reported in this paper is available from the lead contact upon request.

METHOD DETAILS

This study is an analysis of the linkage between two key weather variables: temperature and precipitation, and the critic scores at a regional and local (AOC) level for the Bordeaux region. As in previous approaches,[7,23] analysis of the relationship between weather variables and wine quality scores are based upon the assumption that beneficial weather influences will lead to higher wine quality. The quality-weather interaction methodology can be split into two approaches. Both approaches fit critics scores against weather using a generalized linear model (GLM), but each uses different quantifications of weather as variables. The first approach uses the mean temperature and precipitation during discrete time-steps as the variables; the second approach uses the parameters of functions fitted to the temperature and precipitation data as the variables in statistical models of quality. All data extraction and analysis were undertaken in R version 4.2, using the *tidyverse*[24] and *baseR* packages.

Weather data

Historical weather data were extracted from the ERA-5 land reanalysis weather dataset[25] for each Bordeaux AOC region and central Bordeaux on a monthly time-step using the *Krigr* package[26] (see Table S1 for AOCs and their locations). ERA-5 land is a high temporal and spatial resolution interpolated dataset which is available on a 0.1° grid at time scales varying from hourly to monthly since January 1950.[25] Temperature and precipitation data were extracted on a monthly time-step for a 1km radius from the latitude and longitude point given per AOC for a period of January 1950 to December 2020. Temperature was measured in Kelvin (K), and precipitation in meters (m), both SI units for their respective measures. A growing season was defined as running from 1st November to 31st October, with harvest occurring at the end of the year. This aligns with standard growing season measurements (May-October) but extends them to include the overwintering effects (November-May).

Monthly weather variables were expectedly found to be strongly autocorrelated (Appendix 6), and thus unable to be used individually for building GLMs. Accordingly, months were grouped into autocorrelated groups, which could be roughly thought of as seasons. These groups were determined by those consecutive months by which the inter-month temperature or precipitation Pearson correlation coefficient was above 0.4. Winter was defined as being November and December, Spring as January to May, Summer as June to August, and Autumn as September and October.

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A second way of dealing with this temporal autocorrelation is to describe temporal variation in the weather data to a continuous function. Precipitation is erratic, and hence to examine it in a continuous fashion, cumulative precipitation was used. The cumulative monthly precipitation was modeled linearly using a GLM, meaning that the cumulative precipitation can be approximated using the mean monthly precipitation.

Monthly mean temperature across the year were also described using a sine curve, as in Figure 1B. Non-linear least squares used to fit the data to the following equation:

$$\alpha \sin(\sigma M + \varphi) + \mu$$

Where M is the number of months since October, and $\alpha, \sigma, \varphi,$ and μ are parameters to be fitted. Figure 1B shows how each parameter relates to a part of the sine curve. Starting values for parameters were chosen based upon a fixed periodicity for σ and φ ($\sigma = \frac{2\pi}{12}, \varphi = 3$). σ was chosen because of the annual cycle, hence division by twelve, and φ was chosen as October is 3 months after the approximate peak annual temperature. α and μ were fitted using the maximum, minimum and mean values of the temperature data per site and year using the equations: $\alpha = (\max(t) - \min(t))/2$; $\mu = \text{mean}(t)$.

Quality data

Annual quality scores were collected on two scales, regional and local. Regional critic scores are based on the opinions of how Bordeaux performed as a whole, with individual variation largely ignored and general trends suggested.[20] Local scores are based on individual wines, which are tasted *en primeur* and then rated based upon this premature wine.[27] For each, publicly available wine critic, scores were transformed into a standardized 0–100 scale. Whole region scores were available for the period of 1950–2020 and were drawn from several sources,[9,20] with additional data drawn from online vintage charts (see Table S2). Regional primeur critics scores for the period 2014–2020 were compiled by Bolomey Wijnimport[27] and consist of published ratings from major wine experts from France, UK, US, the Netherlands and Germany. All publications were tested for correlation between their scores, and 14 wine publications were chosen based on having a Pearson Correlation Coefficient of more than 0.4 with at least 3 other selected publications. This cut-off was chosen as a liberal threshold for the inclusion of publications in our analysis. The chosen cut-off means that at least 16% of the variance in critics scores can be attributed to a shared understanding of quality across 3 other publications. These scores were standardized within publications such that each was on a 0 to 100 scale. If wines were rated by more than one publication (78% wines) mean standardized scores were taken.

QUANTIFICATION AND STATISTICAL ANALYSIS

Generalized linear models

Generalised linear models (GLMs) were used to explore the relationship between weather and quality. A summary diagram of the models fitted can be found in Figure 1A. In the diagram, the number in the bottle refers to the model number, and tildes mean "is a function of". GLMs were chosen because they are a flexible modeling approach which does not require any particular error structure or variance.

As per model 1 in the summary diagram (Figure 1A), mean quality scores over time were investigated using a GLM with a binomial distribution and logit link, controlling for the critic. This was due to the bounded nature of the scoring system (0–100) and decreasing variation in quality scores over time. This allows for a comparison of longer-term regional versus local trends over time. At a regional scale, the yearly trend interacted with region to determine the differential baseline trend over time.

For both the regional (model 2, Figure 1A) and local (model 3, Figure 1A) level scores, a GLM with a Gaussian distribution was fitted between the mean of the annual critic scores and the normalized temperature and precipitation during each weather grouping, controlling for year and, in model 3, the AOC and Grand Cru status of the vineyard. Normality of residuals was checked visually using a qqplot and residuals vs. fitted plot. The seasonal means of temperature and precipitation were normalized by subtracting the mean of the weather group and dividing by the standard deviation (Standard Score normalisation). This means that the GLM examined the proportional positive or negative impact of each of the variables on quality, rather than the absolute value. In normalizing such environmental data, comparisons could be made between the variables and therefore the relative contributions of each can be ascertained. The year was controlled for by adding it as a continuous variable, and, in the AOC model, the locality was also controlled for by adding it as a factor.

GLMs were also built to compare the mean vintage score with weather treated as a continuous function (model 4, Figure 1A). This model utilized an additive Gaussian GLM to examine how each of these variables explained the variance within the mean critic scores, controlling for AOC, year, and class. These models were run for both temperature and precipitation separately and then together. We also ran a GLM without year as an explanatory variable due to covariance.

Additional Discussions Resulting from Viva

During the discussion of this chapter during my viva, several points were made and discussed. The first was concerning the difference between using calendar data and phenophase data. The latter would be examining quality against periods during the annual lifecycle of a grapevine (harvest-budbreak; budbreak-flowering; flowering-veraison; veraison-harvest), which could be calculated based-upon accumulated temperature. However, it raises lots of additional complexities with varietal differences in phenological thresholds varying and unknown spatial variation in varietals across Bordeaux as a whole. Further, it would shift the intention of this piece towards a modelled phenology paper, rather than examining the changing quality due to variation in weather patterns. The two questions – modelling climate impacts on phenology verses weather variation on quality are subtly different. One question concerns the timing for weather-related interventions during the year for humans, the other a specific phenological vulnerability at the vine-level examined from a different perspective. As a next stage though, the addition of phenophase data and the perspective would certainly be an interesting extension to this work. The other discussion centred around the temporal resolution of the work. As is already mentioned in the manuscript, there is high autocorrelation between the monthly temperatures, as well as for monthly rainfall. Greater temporal resolution, whilst it would increase the amount of information in the model, would not help the model building. This is because the autocorrelation would mean that the model could not use the information provided and spurious correlations would abound. Thus greater resolution of data may lead to incorrect statistical patterns being identified, but may be useful for making better predictions – although chapter 4 of this thesis suggests otherwise.

Additional clarifications:

- Pg 28: The full name is the Grand Cru Classé system
- Pg 30: graphical depiction of coefficients is shown in figure 2 not 3
- Pg 31: Dormancy is a complex phenomenon. Paradormancy is the inhibition of bud growth and is an internal process which occurs within the plant. Endo- and eco-dormancy are two alternative forms which are temperature dependent and occur whenever the plant is subjected to cold weather during the winter. This temperature-dependent winter dormancy, sometimes called winter rest, is the primary meaning for the term dormancy in this chapter.
- Pg 31: Excess salinity is unlikely in Bordeaux due to high winter rainfall, but small changes in soil composition are possible due to variation in such winter rainfall.

Appendix For Chapter 2

Appendix For "Seasonal Climate Impacts Wine Quality in Bordeaux"

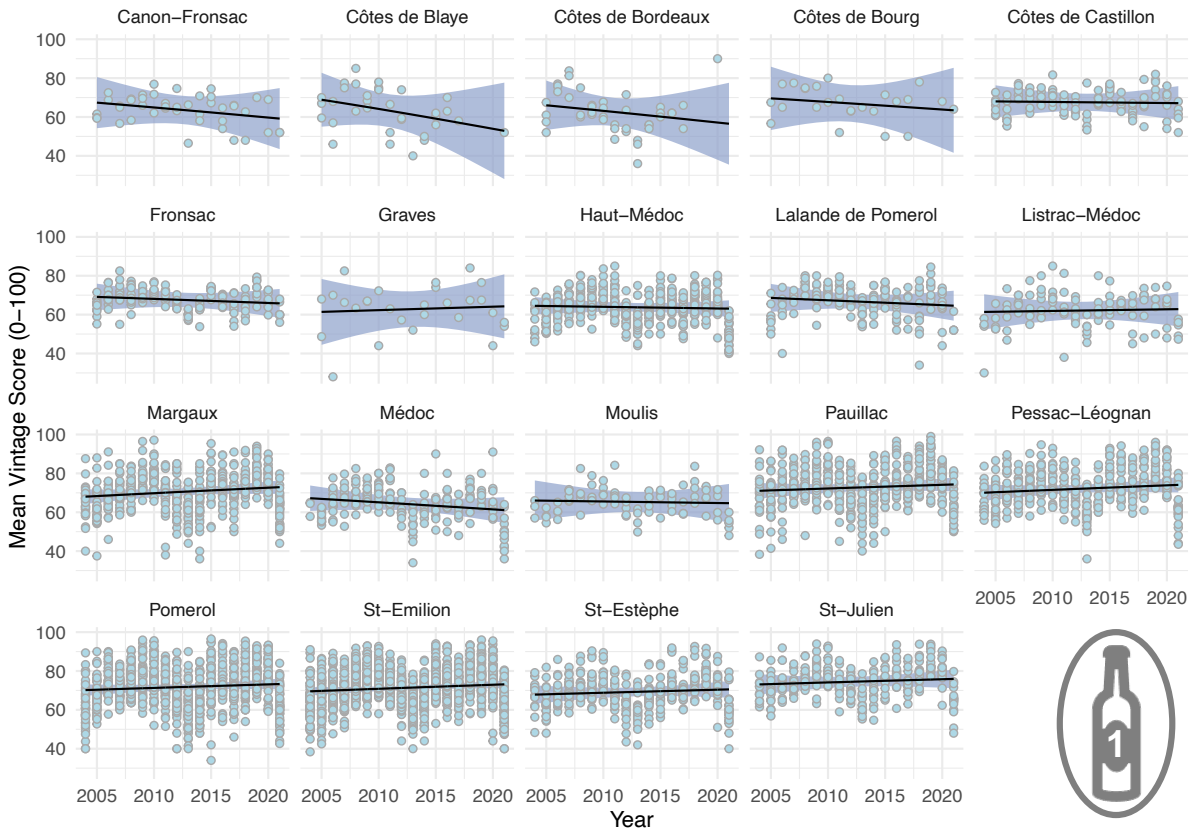
Supplementary Table 1: AOC locations used for weather data extraction

Region	Latitude	Longditude
Bordeaux (City Centre)	44.841225	-0.5800364
Haut-Médoc	45.3745047	-0.8788471
Pomerol	44.9311234	-0.1999904
Moulis	45.0564852	-0.7736381
Listrac-Médoc	45.0736769	-0.7905774
Côtes de Bourg	45.0343476	-0.4954363
Côtes de Castillon	44.8706805	-0.0754746
Pauillac	45.1995626	-0.7484994
St-Estèphe	45.5925	0.6633333
Côtes de Bordeaux	44.7311086	-0.3187064
Graves	45.6500048	-0.1060768
Margaux	45.046232	-0.6728851
Pessac-Léognan	44.7294474	-0.5997267
Côtes de Blaye	45.127548	-0.4368037
Premières Côtes de Bordeaux	44.7790343	-0.461452
Médoc	44.5563705	-0.0385057
St-Emilion	44.8931452	-0.1560662
Canon-Fronsac	44.7007217	-0.5288963
St-Julien	44.817706	1.1745895
Lalande de Pomerol	44.9560756	-0.2104434
Fronsac	44.9229141	-0.2740925

Supplementary Table 2: Quality Critics

Bordeaux Overall Quality Ratings	Bordeaux Individual Wine Quality Ratings
Berry Bros & Rudd	Wine Advocate (Robert Parker & Lisa Perotti Brown)
Hachette	Neal Martin
Tastet Lawton	Jancis Robinson
Wine Spectator	Tim Aitkin
Wine Society	TASTE (Michael Betanne & Thierry Desseauve)
	James Suckling
	Wine Cellar Insider (Jeff Leve)
	Decanter
	Revue de France
	Bordeaux Insider (Jane Anson)
	Le Point
	Perswijn
	Wien Wisser (Rene Gabriel)
	Wine Doctor (Chris Kissack)

Supplementary Figure 1: AOC scores over time



Supplementary Table 3: ANOVA table of GLM comparing quality increases over time across the whole region

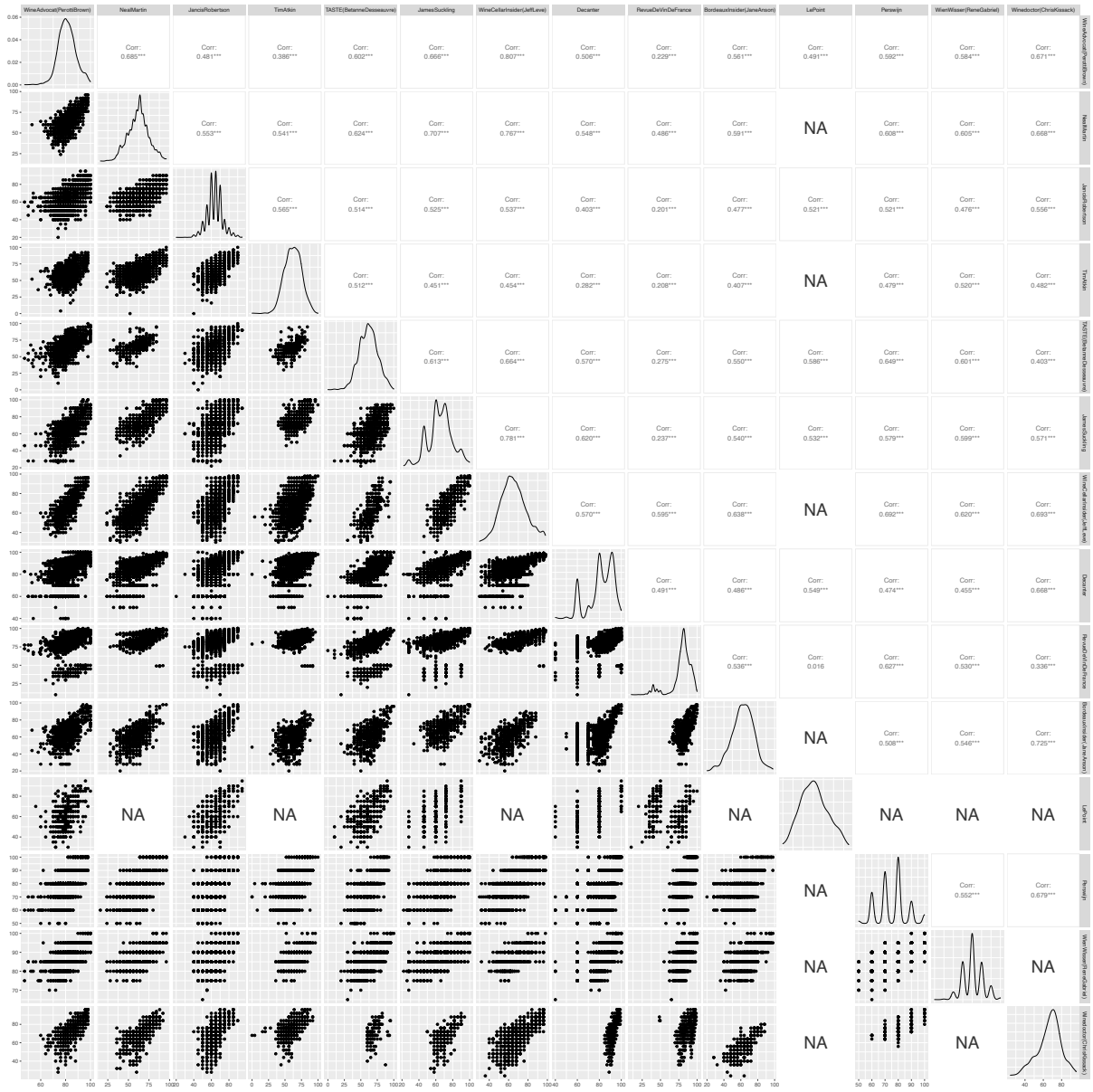
glm(formula = MeanScore/100 ~ Year+Critic, family = binomial(link = "logit"))

Null deviance: 47.397 on 313 degrees of freedom
Residual deviance: 34.221 on 306 degrees of freedom
AIC: 204.98
R^2 = 0.2779923

ANOVA table:

term	df	χ-statistic	p.value	p-§
Year	1	4.4528	0.03484	Y
Critic	6	6.6488	0.35455	N

Supplementary Figure 2: Plot of individual critics scores plotted against each other and Pearsons correlations between them



Supplementary Table 4: ANOVA Table of GLM comparing quality increases over time in different AOC regions

glm(formula = MeanVintageScore/100 ~ Year * AOC, family = binomial(link = "logit"))

Null deviance: 307.30 on 6566 degrees of freedom
Residual deviance: 273.44 on 6529 degrees of freedom
AIC: 5051
$R^2 = 0.1101906$

ANOVA table:

term	df	χ-statistic	p.value	p-value < 0.05
Year	1	1.3046	0.25337	N
AOC	18	30.2727	0.03488	Y
Year:AOC	18	2.5457	0.99999	N

Supplementary Table 5: ANOVA Table for Whole Bordeaux (Regional) Generalised Linear Model of Weather on Quality

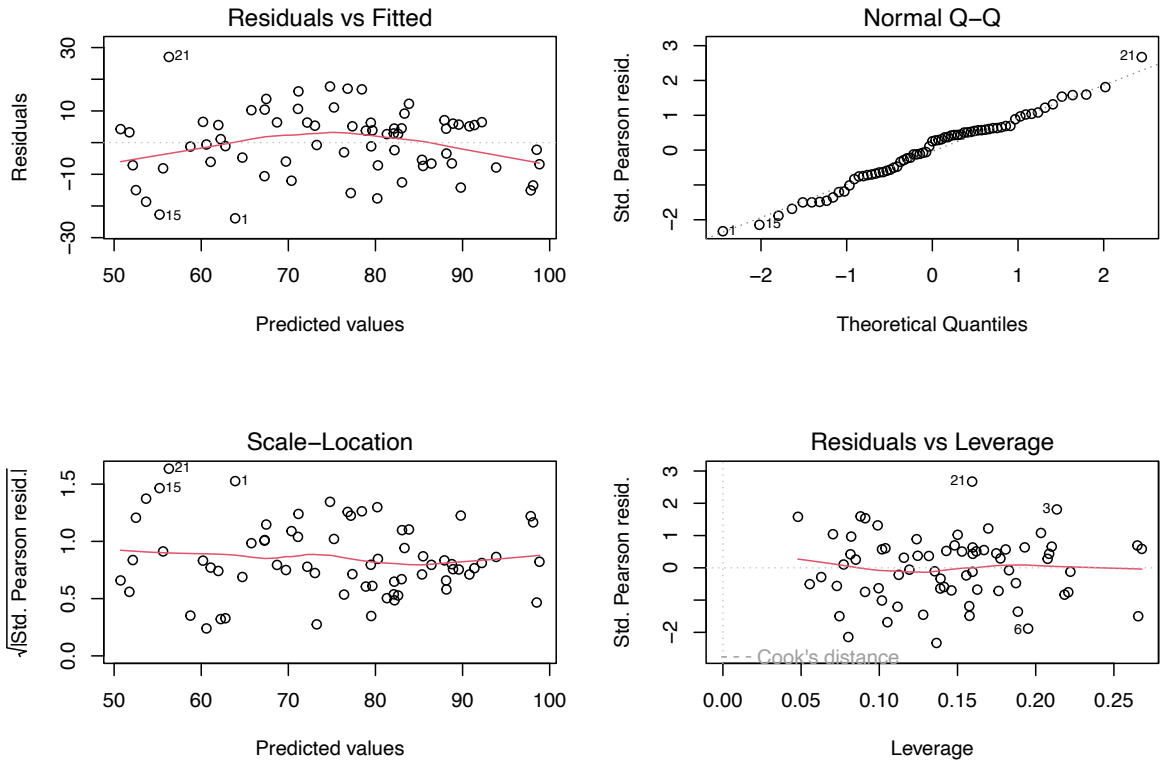
glm(formula = MeanScore ~ Year + NormalisedWinPrecip + NormalisedSprPrecip + NormalisedSumPrecip + NormalisedAutPrecip + NormalisedWinTemp + NormalisedSprTemp + NormalisedSumTemp + NormalisedAutTemp, family = gaussian(), data = OverallGLMData, na.action = "na.omit")

Null deviance: 18587.0 on 68 degrees of freedom
Residual deviance: 7190.9 on 59 degrees of freedom
AIC: 538.42
$R^2 = 0.6131224$

ANOVA table:

term	sumsq	df	F-statistic	p.value	p-value < 0.05
Year	14.2161105	1	0.11664064	0.73392035	N
NormalisedWinPrecip	926.652503	1	7.60301804	0.00774375	Y
NormalisedSprPrecip	56.7666213	1	0.46575997	0.49761512	N
NormalisedSumPrecip	1133.65482	1	9.30143505	0.00342646	Y
NormalisedAutPrecip	214.658287	1	1.76123285	0.18958385	N
NormalisedWinTemp	3.74231222	1	0.030705	0.86150013	N
NormalisedSprTemp	286.087625	1	2.34729779	0.13084528	N
NormalisedSumTemp	1738.03832	1	14.2602936	0.00037225	Y
NormalisedAutTemp	259.55029	1	2.12956371	0.14978582	N
Residuals	7190.89411	59			

Supplementary Figure 3: Goodness of fit plots for overall generalised linear model for weather against quality score controlling for year



Supplementary Table 6: ANOVA Table for AOC (Local) Scores Generalised Linear Model of Weather on Quality

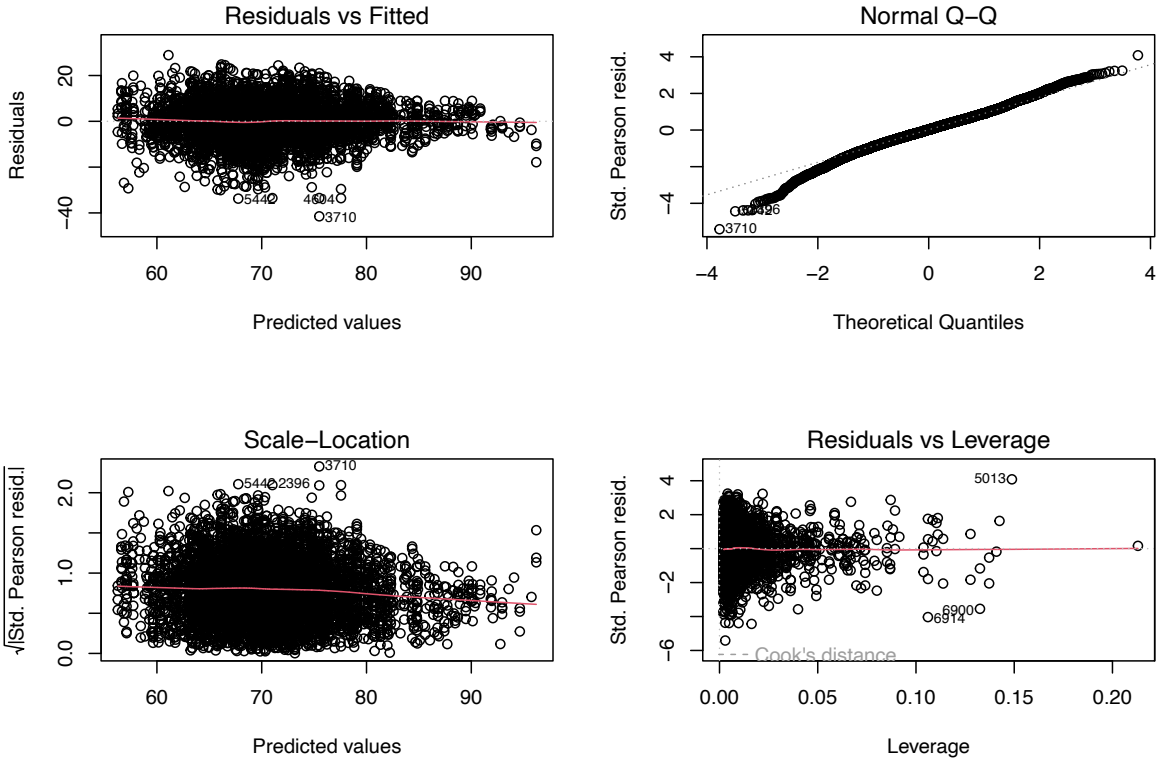
glm(formula = MeanVintageScore ~ AOC * Year + Class + NormalisedWinPrecip +
NormalisedSprPrecip + NormalisedSumPrecip + NormalisedAutPrecip +
NormalisedWinTemp + NormalisedSprTemp + NormalisedSumTemp +
NormalisedAutTemp, family = gaussian(),
na.action = "na.omit")

Null deviance: 560005 on 6222 degrees of freedom
Residual deviance: 362802 on 6163 degrees of freedom
AIC: 43082
$R^2 = 0.3521448$

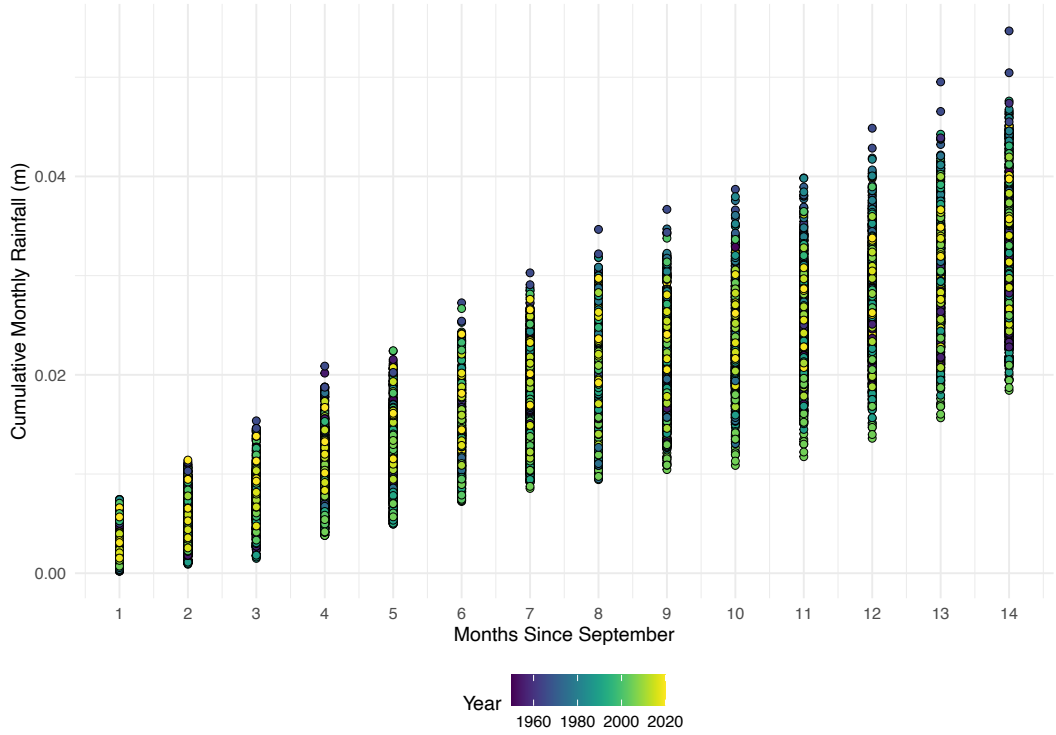
ANOVA Table:

term	sumsq	df	F-statistic	p.value	p-value < 0.05
AOC	22855.9498	18	21.5699504	5.62E-69	Y
Year	2050.56773	1	34.8334506	3.78E-09	Y
Class	74847.8129	14	90.8183186	2.96E-238	Y
NormalisedWinPrecip	9679.06002	1	164.420347	3.64E-37	Y
NormalisedSprPrecip	2019.30686	1	34.3024151	4.96E-09	Y
NormalisedSumPrecip	6713.12406	1	114.037333	2.17E-26	Y
NormalisedAutPrecip	2523.45657	1	42.8665185	6.33E-11	Y
NormalisedWinTemp	6515.22182	1	110.675523	1.15E-25	Y
NormalisedSprTemp	1248.50272	1	21.2085936	4.20E-06	Y
NormalisedSumTemp	7191.97238	1	122.171636	3.89E-28	Y
NormalisedAutTemp	29009.5685	1	492.791998	4.23E-105	Y
AOC:Year	6149.22928	18	5.80324037	4.59E-14	Y
Residuals	362802.098	6163			

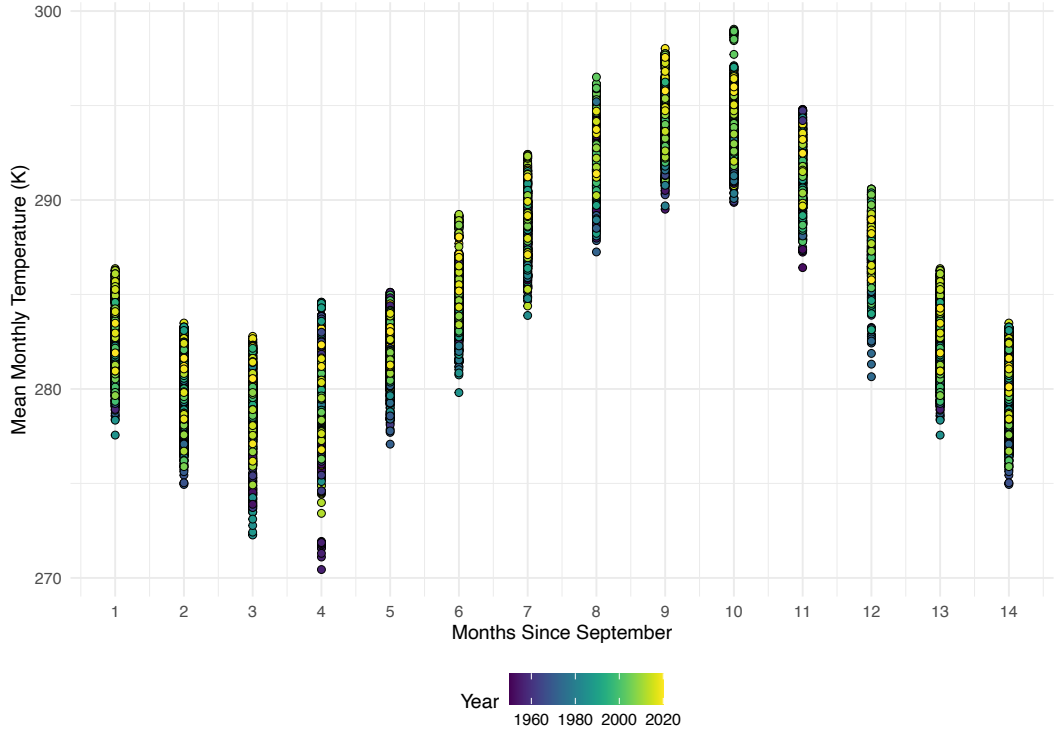
Supplementary Figure 4: Goodness of fit plots for local generalised linear model for weather against quality score controlling for year, AOC, and class



Supplementary Figure 5: Cumulative Monthly Precipitation Across all AOC of Bordeaux (1950-2020)



Supplementary Figure 6: Mean Monthly temperature across all AOCs in Bordeaux (1950-2020)



Supplementary Table 7: ANOVA Table For Precipitation-Year GLM

glm(formula = MeanPrecip ~ AOC * Year)

Null deviance: 0.00063460 on 4819 degrees of freedom
Residual deviance: 0.00048849 on 4784 degrees of freedom
AIC: -63872
R^2 = 0.2302302

ANOVA table:

term	sumsq	df	f-statistic	p.value	p-value < 0.05
AOC	5.93E-06	18	3.39182943	1.50E-06	Y
Year	0.00016285	1	1676.79052	0	Y
AOC:Year	3.97E-06	18	2.26854534	0.00164684	Y
Residuals	0.00060068	6185			

Supplementary Table 8: ANOVA Table for Generalised Linear Model of Vintage Score and Precipitation

glm(formula = MeanVintageScore ~ MeanPrecip + AOC * Year)

Null deviance: 421986 on 4520 degrees of freedom
Residual deviance: 347495 on 4484 degrees of freedom
AIC: 32536
R^2 = 0.1765253

ANOVA table:

term	sumsq	df	f-statistic	p.value	p-value <0.05
MeanPrecip	1813.6452	1	28.0821828	1.20E-07	Y
Class	74404.4808	14	82.290478	7.97E-217	Y
AOC	24729.4977	18	21.2726366	6.25E-68	Y
Year	8669.74509	1	134.240901	1.00E-30	Y
AOC:Year	6801.80703	18	5.85100314	3.21E-14	Y
Residuals	398480.097	6170	NA	NA	

Supplementary Table 9: Mean and standard deviation of sine curves fitted to monthly temperature data (1950-2020)

$$\alpha \sin(\sigma M + \varphi) + \mu$$

α (A)		σ (omega)		φ (phi)		μ (C)		R^2	
Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD
8.01	0.79	0.52	0.024	3.07	0.23	286.7156	0.65	0.954	0.017

α >> amplitude
σ >> periodicity, length of waves
φ >> phase shift (positive = earlier)
μ >> mean temperature

Supplementary Table 10: Model ANOVA Table for GLM of mean vintage score described by mean precipitation and sine parameters of temperatures

glm(formula = MeanVintageScore ~ A + AOC + C + Class + MeanPrecip +
omega + phi + Year + AOC:Year + 1, family = gaussian())

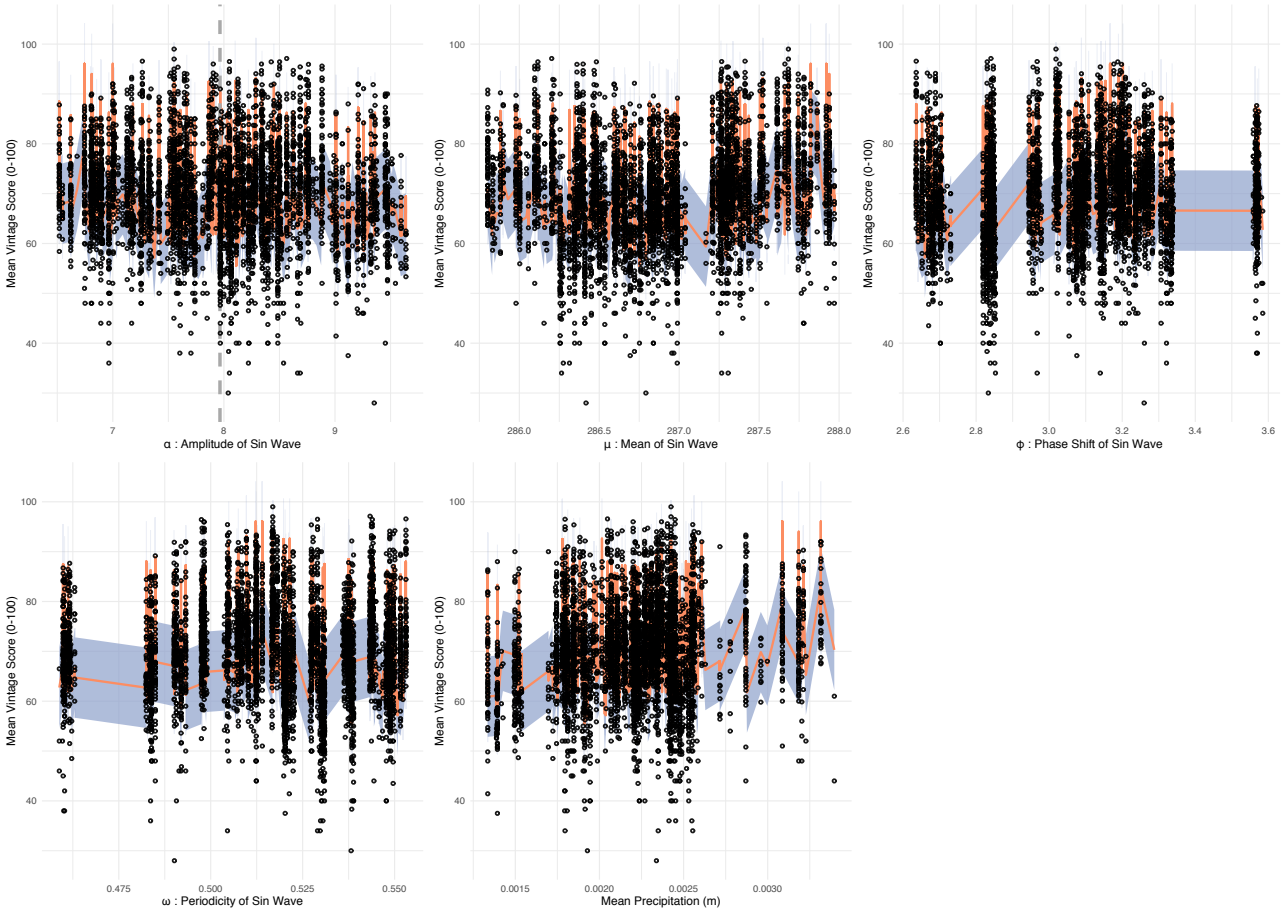
Null deviance: 425248 on 4520 degrees of freedom
Residual deviance: 291112 on 4469 degrees of freedom
AIC: 31766
R^2 = 0.3154307

ANOVA table:

term	sumsq	df	F-statistic	p.value	p-value < 0.05
A	4149.6994	1	66.4808914	4.24E-16	Y
AOC	24050.1539	18	21.4055086	2.13E-68	Y
C	256.8952	1	4.11562868	0.04253162	Y
Class	75250.522	14	86.1116037	1.82E-226	Y
MeanPrecip	3328.49824	1	53.3247131	3.18E-13	Y
omega	9461.38421	1	151.577547	1.98E-34	Y
phi	12153.4513	1	194.706219	1.37E-43	Y
Year	3536.46822	1	56.6565279	5.93E-14	Y
AOC:Year	6253.52076	18	5.56586011	2.72E-13	Y
Residuals	384878.21	6166	NA	NA	

Supplementary Figure 7: Goodness of Fit For Model

GLM predictions plotted (orange, with error in purple) against data points (black). Vertical dotted lines indicate the mean predicted values. Plotted to test goodness of fit



3

Modelling the Climate Changing Concentrations of Key Red-Grape Quality Molecules Using a Flexible Modelling Approach

Words in Abstract: 150

Words in Chapter: 7289

Abstract

Grape (*Vitis vinifera*) composition is weather-dependent, and an important determiner of wine quality. As the climate changes, so too will the grape composition. To understand the extent of this, path models were built to create a generalised Cabernet Sauvignon grape quality model focusing on the total concentrations of 6 important molecular groups (sugar, pH, phenols, tannins, flavanols, anthocyanins). The impact of changes in composition under several climate change scenarios (light, temperature, and rainfall) for a Chilean region were then explored. This paper predicts, under the projected climatic changes, higher concentrations of sugars; lower acidity (a more neutral pH); and higher total concentrations of aromatic compounds (tannins, phenols, flavanols, and anthocyanins). Changes in phenology changed the rates of accumulation and total concentrations. These two results combined suggest the potential for stronger red wines in future for this region, with more flavour-related compounds and in particular tannins which may give greater aging potential.

Introduction

Changing climate conditions are impacting the quality of agricultural produce[1,2], most notably perennial crops such as wine grapes (*Vitis vinifera*)[3–5]. In these systems, crop value is more dependent upon quality than quantity. A major part of wine quality is determined by grape must composition: a more optimal composition of grapes at harvest generally gives better quality wines[6]. Naturally varying wine quality occurs due to variation in weather leads to an increased desire to understand the impacts of climate change on composition of the grape. The precise optimal make-up of grape composition compounds is determined by the opinions of individual winemakers, with different wine makers preferring different must compositions depending on preference. Hence prediction tools must allow flexibility in output to allow for variation in individual preference. This paper seeks to understand and quantify the impact of changes in weather during the ripening period (from veraison to harvest) on the composition of the grapes at harvest. In doing so it provides and demonstrates a flexible framework for the exploration of the accumulation of important compounds in perennial crops, thus demonstrating a technique by which important compounds can be modelled in any perennial crop globally.

This desire to understand climatic impacts on the composition of the grape is set in the context of changing climate suitability for winegrowing in current winegrowing regions. Winegrowing suitability in these areas is predicted to decrease by between 8 and 65% under "conservative" climate change predictions (RCP 4.5)[7,8]. This large range suggests a range of potential outcomes depending on realised climate effects, and non-linearities in the outcomes[8]. These models suggest a 1-2°C increase in temperature in wine growing regions globally and a large increase in variability of rainfall between regions, with some years and regions experiencing drought, and others experiencing an increase in strong rainfall events[7–10]. However, little is known about the change in grape quality in such situations, with quantified changes in grape and wine composition not yet predicted. Qualitatively the general global impact of the predicted climate changes has been posited to lead to better and stronger wines, with higher concentrations of many aroma-causing compounds[11–13].

A grape anatomically consists of three parts: pulp, skin, and seed, each of which contains important compounds for quality (as seen in Table 1). These compound groups: sugars, acids, phenols, tannins, flavanols, and anthocyanins have previously been quantified chemically using laboratory and spectroscopic techniques. Spectroscopy has also subsequently been used to monitor the composition based on observed characteristics[14–17].

Air temperature is frequently cited as having the greatest impact on ripening and maturity, with impacts on vigour, ripening rate and consequential harvest date[18,19]. Accordingly, some models of grape maturity rely on temperature thresholds in growing degree days to help ascertain the maturity levels of the grapes and assist in the harvest of the grapes[20–24]. These models evaluate the entirety of the grape as an ensemble, and thus incorrectly suppose that ratios between the compounds within the grapes change in concert[25].

Temperature is not the only factor that affects the quality of the grape. Wine grapes require hot, dry summers and cool, wet winters, with plenty of sunshine[13,26–30]. Berry development during ripening is thought to require moderate temperatures (15-40°C) coupled with high light and low humidity[11,26,29–35]. Each of these factors impacts different aspects of the grape differently[32,36], as each set of compounds has a different biological purpose and property. Climate change is also leading to a decoupling of the impacts of drought and temperature[36], with changes in extreme heat and water availability occurring differently. This has strong phenological effects, and consequently changes in the grape maturity and composition[37].

Chile is the 6th largest wine producer and the 8th largest country under vines[38]. The wine growing area covers 8 of the 15 regions, with 87% found in the 4 central regions of Maule, Valparaiso, Bio Bio, and O'Higgins[39]. Most of the grapes grown are for producing still red wine, with Cabernet Sauvignon (39.3%) making up the largest share of vineyard area[39,40]. Accordingly, the same grape varieties are planted over a large geographic area, meaning that space for time comparisons can be used for determining the best climate and growing conditions. Whilst there exists a latitudinal gradient along these regions of Chile, there also exists an altitudinal gradient too, with longitudinal variation existing as the coastal regions give way to the Andes mountains. As such there exists historic wine growing over a large longitude and altitudinal radius, with enough scope to explore the impact of weather on the grape composition over the ripening period.

Whilst Cabernet Sauvignon is thought to have originated from Bordeaux (France) in the 17th century, it is now an "international variety" and makes up 5% total world area under vines, the largest of any wine grape[41]. These vines are thought to cover an area of approximately 341,000 hectares in countries from Chile and South Africa, to China, Italy, and France[41]. It is generally made into a still red wine, famed for its strong taste, full-body, and ageing potential.

The key compounds of sugars, acids, phenols, tannins, flavanols, and anthocyanins together comprise much of the maturity of wine (technical, phenolic, and partially aromatic maturities). They are key compounds in the determination of when to harvest and contribute in a major way to the organoleptic quality of the grapes. Accordingly, these compounds groups were chosen to be modelled for their impact on quality. General reviews have predicted changes in each of the individual compound groups[11], but little work has been done to quantitatively model them, especially to determine the impact of climate change on the composition of the grapes.

Path models statistically connect factors to each other to create a model of a multi-stage dependencies. In this way they are a series of linked models which describe flow through a network from input to output, via any latent variables. They are highly flexible and agnostic to mechanism, and hence can be used statistically to represent a series of undefined metabolic pathways. Other grape models seek to precisely mimic some aspects of grapevine behaviour. This can be either physiological through the flow of water[42–44] or biomass of plant[45–48] or grape[49] or chemically through their allocation of carbon[43,50–52]. But these other models fail to capture the metabolic complexity required for grapes to make compounds important for quality, taste, and flavour. In grapes these metabolic reactions start with sugar being imported into the grape from the parent plant's phloem, and then converted in the grape into myriad other forms. Different compounds and observed characteristics are important for different wines, and thus any modelling approach which seeks to address quality must be flexible enough to deal with this. By using a path model and simulation approach we can therefore explore the impact of changes in climate on any potential compound or property, no matter the detail known about its metabolic synthesis.

This paper seeks to examine the impact of interannual variation in weather on the concentrations of quality-related compounds within the wine grape. It does this through creating linear models based upon existing viticultural data which are subsequently used to estimate how projected climatic changes might affect the wine-grape composition in Chile by 2050. In doing so, this paper first demonstrates a generalised approach to determining the concentrations of important molecules within the grape. We use path models to create a generalised Cabernet Sauvignon grape model focusing on the total concentrations of 6 key molecular groups (sugars, pH, phenols, tannins, flavanols, anthocyanins). We then explore

the impact of changes in composition under several climate change aspects, namely changes in light, temperature, and rainfall.

Table 1: Table showing various components of grapes important for the making of wine

Compound Group	Molecules	Location in Grape	Wine Quality Aspect	Maturity Aspect
Sugar	Fructose, sucrose	Pulp	Alcohol and sweetness	Technical maturity
Acids (pH)	Malic acid, phenolic acids	Pulp	Acidity, balance with Sweetness, ageing potential[67]	
Polyphenols	Hydroxybenzoic acids (Gallic acid)	Pulp	Astringency and flavour [68]	Phenolic maturity
	Hydroxycinnamic acids	Pulp	Browning and aroma of wine[69]	
Flavanoids	Flavanols (myricetin and quercetin)	Skin	Stabilisation of the colour and flavour – primarily astringency and bitterness [67].	
	Anthocyanins (malvinidin and petunidin[70])	Skin	Colour of the wine, mild bitter taste, astringent mouthfeel[71]	
	Tannins (catechin, epicatechin, and proanthocyanidins)[69]	Pips and Skin	Structure (mouthfeel) and taste of wine[71] Ageing potential	

Methods

This study seeks to understand how weather influences the composition of the wine grape (*Vitis vinifera* subsp. 'Cabernet Sauvignon') between the onset of ripening and harvest. It builds a mathematical simulation model which describes the linkage between weather and key metabolite groups within grapes as they ripen and then simulates outcomes based on weather regimes. The weather for this simulation is then manipulated to represent predicted climatic changes and the predicted change in grape composition are simulated. To parameterise this simulation, a statistical description of the system was built via a path model. This path model phenomenologically links the weather to the key metabolite groups which make up technical and phenological maturity. As it is a series of simple linked models, it is a highly flexible approach that could be applied to multiple systems across all perennial crops.

Simulation: We wanted to investigate how predicted changes in the climate would impact the composition of the wine. In order to do this, we simulated current (2000-10s) and mid-century (circa 2040s) weather regimes for one location in El Boldo, Chile. Whilst we could have run the model for multiple different combinations of clones, rootstock, training systems, and quality productions, for the purposes of exploring the impact of climate change on quality we examined one singular grape-vine type in this location. This we selected as a vine of clone 170, with rootstock 110R, being grown in a cordon-libre training system, to produce premium wine. For this grapevine we iterated the path model through the full ripening period (weeks 7 to 15 of the year in Chile). Grape values from one time step (t) were used alongside simulated weather at time t to predict the next time step (t+1). A single simulation took a vine from the point of veraison until full-ripeness (and thus readiness for

harvest), creating outputs for all 9 steps in the pathway. To run the model for other combinations of weather, grape-vine, and production system please see the Shiny application: (https://andrewwood.shinyapps.io/Vitis_v1_PathModel/).

For each of the 500 simulations run, a weather regime was created by sampling from a distribution for each variable during the time period. The normal distribution was used for both mean temperature and cumulative light, and the gamma distribution was used for the precipitation. The gamma distribution was used due to the high number of very low values of rainfall. For the gamma distribution the shape parameter was calculated using the formula: $(\text{mean}/\text{standard deviation})^2$ and the rate parameter by: $\text{mean}/(\text{standard deviation})^2$.

For the middle century predictions, distributions of each component of weather were changed depending on literature predictions of weather. Mean temperature increases of 1.5 degrees were predicted by Cabre et al. (2016)[57], a 35% reduction in cumulative precipitation was predicted by Araya-Osses et al. (2020)[58] and increases of light by 15% were predicted by Zhang et al. (2021)[59]. Variability of all three was also predicted to increase, and we have therefore doubled the standard deviation in the climate change scenario to account for this. This was modelled both in concert, and independently, to explore the impact of coupled and decoupled climate effects.

A secondary impact of changes in climate is a change in phenology, most notably the beginning of the ripening period. To determine the impact of this change in ripening period, we simulated changes in the date of veraison (and thus the start of the latter ripening period). This was done by starting the simulation at the same sugar

concentration and pH at different weeks around the mean veraison date but keeping the weather the same.

The first step in building the simulation was the creation of the statistical path model. This required three sets of data: weather, site (vineyard) and grape data.

Weather Data: Historical weather data were extracted from the ERA-5 land reanalysis weather dataset[60] for each plot location using the Krigr package[61] (see Supplementary Data for locations). ERA-5 land provides gridded interpolated data on a 0.1° grid at hourly time scales since 1st January 1950[60]. The data is interpolated from both Earth-based datasets (weather stations, buoys, aircraft, weather balloons, ships, and radar), and various satellite data (around 50 satellite datasets). We extracted the temperature (K) as a daily mean value, and precipitation (m), soil moisture for 7 to 28cm beneath the soil (m^3 m^{-3}), and solar radiation (J m^{-2}) as daily cumulative totals, all in their standard untransformed units. From this, mean temperature was extracted for a rolling window of either 7 or 30 days before the measurement was taken, allowing for the mean weather over the previous week or month to be calculated. Cumulative precipitation, soil moisture, and light were extracted using the same rolling window of 7-, or 30-days previously.

Site Data: Altitude data were extracted on a 0.1-degree resolution from the AWS terrain tiles using the *elevatr* package in R[62]. Four aspects of soil composition (percentages of clay, sand, silt and gravel/cfvo content) were extracted from NCSS database on a 0.1-degree resolution using the *SoilDB* package[63], and values for composition extracted between the horizons 5-15 centimetres were used.

Grape Data: Two datasets were used for this work, both from commercial vineyards of Viña Concha y Toro (VCT) in Chile. Dataset 1 (harvest tracking) comprised of maturity measures of weekly samples of sugar concentration and pH for 749 parcels of vines ("plots") across 35 vineyards during the ripening period, (starting at the earliest date of 19/01 and finishing at the latest date of 03/05) between the years 2013 and 2021. The samples cover a 5.5-degree latitudinal range and a 1.7-degree longitudinal range and can be seen as purple triangles on the map (Supplementary Figure 1). Sugar and pH measurements were taken using the Dyostem Measuring system (via spectroscopic techniques) for 1600 plots for up to 10 years (see table 1 for vineyard locations and table 2 for years each region was sampled). This dataset consisted of 111,358 total samples.

Dataset 2 (HPLC) comprised of 300 grape samples taken at harvest across three years (2018-2020), for 300 plots across the same vineyards (one bunch per plot) for a similar 6-degree latitudinal range and a 1.8-degree longitudinal range. Six important aspects of grape compositions were measured using standard protocols as per Schober et al (2022) at the experimental winery of the VCT Centre for Research and Innovation (CII)[17]. The aspects of grape composition measured were total concentrations of: sugars (g/L), acidity (pH), phenols (mg/L), tannins (mg/L), flavanols (mg/L), anthocyanins (mg/L).

Statistical Analysis (Path Model): The data was then used to build a path model. A path model is a series of linked linear models, each assuming a gaussian distribution of the predictor variable and an identity link function (*Supplementary Formula 1*). Each step connected the inputs to an aspect of grape composition. Below are the nine

steps which formed the steps in the pathway, with the output (target, dependent, y) variable, in bold:

1) From climate and vineyard (C+V) to **soil moisture**
2) From climate, soil moisture and C+V to **sugar concentration.**
3) From climate, sugar concentration, soil moisture and C+V to **pH.**
4) From climate, sugar concentration, pH, soil moisture and C+V to **reflectance at 520nm wavelength.**
5) From climate, sugar concentration, pH, soil moisture and C+V to **reflectance at 280nm wavelength.**
6) From climate, sugar concentration, pH, soil moisture, reflectance at 280 and 520nm wavelengths, and C+V to concentration of **total anthocyanins.**
7) From climate, sugar concentration, pH, soil moisture, reflectance at 280 and 520nm wavelengths, and C+V to concentration of **total tannins.**
8) From climate, sugar concentration, pH, soil moisture, reflectance at 280 and 520nm wavelengths, and C+V to concentration of **total phenolics.**
9) From climate, sugar concentration, pH, soil moisture, reflectance at 280 and 520nm wavelengths, and C+V to concentration of **total flavanols.**

Each step mimics a transfer of energy, starting with an external process (the soil moisture) and then moving to the characteristics of the grape that define the technological maturity (sugar concentrations, pH). From this technological maturity, two spectroscopic measurements were analysed as intermediaries (the reflectance at 280nm and 520nm), and then from these the analysis considered the wider maturity characteristics (total concentrations of tannins, flavanols, anthocyanins, and phenols). The spectroscopic measurements were chosen to represent the growth of the pulp and the skin respectively.

For each step in the pathway, a fully connected model was created between the output variable and the named input parameters detailed in *Appendix Table 1,* with the linear models encoded as in *Supplementary Formula 1*. There are two issues with just running the model as per this fully connected model. The first is covariance. To remove this from the model, a correlation pairs plot was created, and variables which were co-linear above the 0.4 covariance threshold (Pearson's correlation coefficient) were removed from possible models, such that no two covarying variables were allowed in the same model.

The second is the high number of redundant non-significant terms in the model. To remove this, the statistically significant variables ($p<0.05$) were fixed in the model evaluation stage, and all other possible models were evaluated (using dredge function, *MuMln)*. The model chosen was that with the lowest AIC value. Model goodness of fit was also examined for each linear model using plots of predicted values against true values, coupled with R^2 values.

Results

The path model is a statistical understanding of the network of factors that impact the composition of the grape. The linear models built during the statistical analysis suggest a statistically robust and complex network of inputs from across terroir – from climate, human management, and soil. Figure 1 shows the statistically significant ($p<0.05$) connections in the most parsimonious (lowest AIC) models for each output or latent variable (interior node in the graph). There are 67 connections in the network, out of a possible 130 connections, making the graph 51.54% connected. No output variable has fewer than 4 predictors (the minimum is anthocyanin concentration), up to a maximum of 9 predictors (for both tannin and flavanol concentrations), as seen in Table 4 in the Appendix. The most connected input variables are altitude and the cumulative monthly precipitation, with 7 connections each. This suggests that grape composition is a complex phenomenon, with many influencing factors that each contribute additively to the final composition of the grapes.

The statistical analysis suggests that there exists a strong link between the environment of the grape vine and the concentrations of key molecular compounds within the grape. The model predictions all sit on the y=x line of the predicted against true value plots (Figure 2), suggesting a strong link and good fit of the models. The mean R^2 value of the models is 0.86 (Table 4 in Appendix), meaning that on average 86% of the variance within the data is captured by each model. The high R^2 value of the models (Table 4 in Appendix), coupled with the straight Predicted-Actual Plots (Figure 2), suggests that the linear models are a good fit for the data, and suitable over a breadth of variation in climate and soil space.

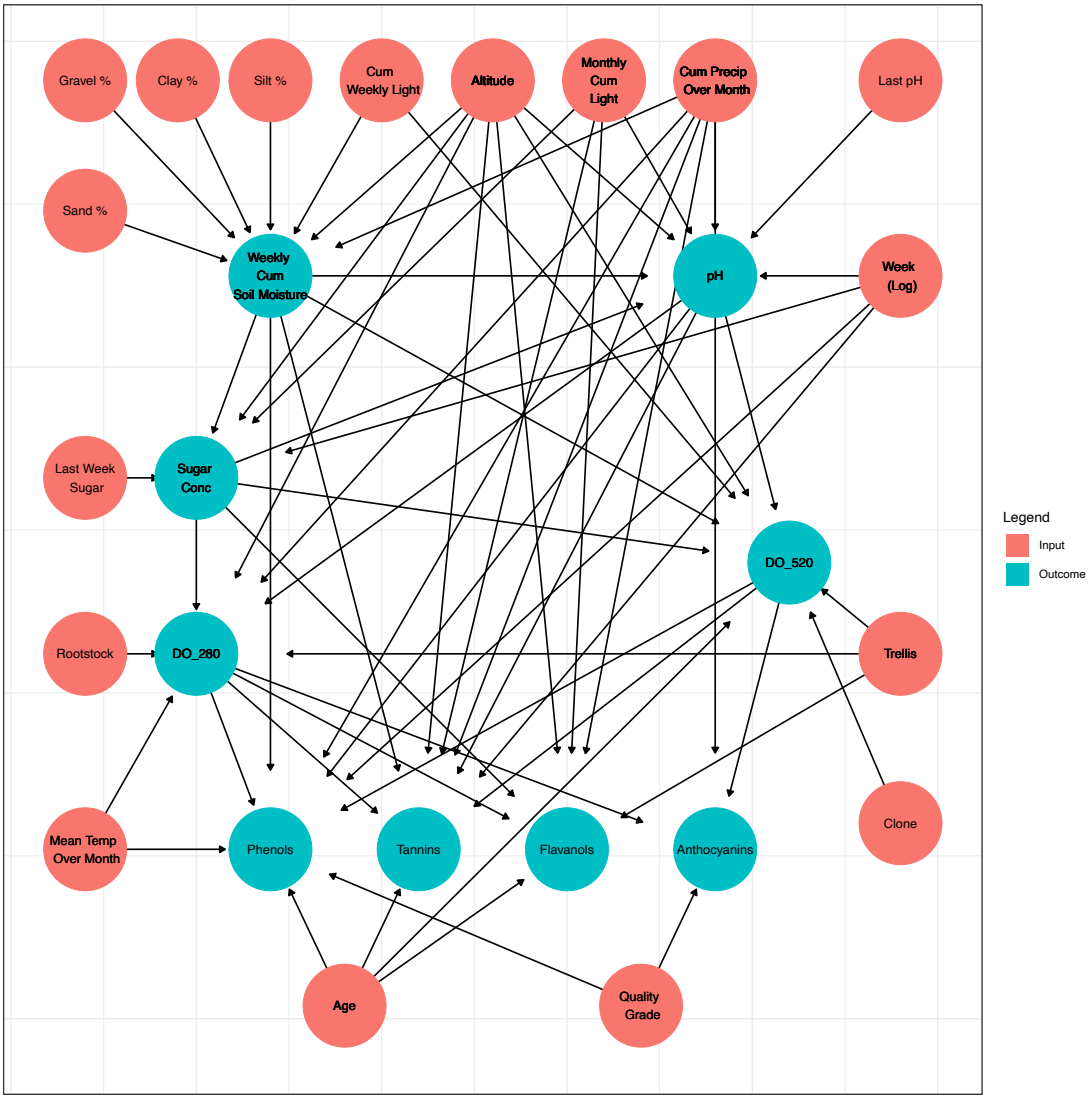


Figure 1: Path model showing the statistically significant relationships between input (red, outside) and output (blue, inside) variables. Each linkage is a statistically significant term.

To determine the change in composition caused by climate change we firstly simulate a baseline of the current weather patterns. The output from the simulation using the current weather regime suggests a general increase in concentrations of most molecules over the course of the ripening period (except for tannins, flavanols, and phenols). Weekly cumulative soil moisture remains constant for the first 10 weeks, before increasing in an almost exponential fashion (Figure 3, solid line). Sugar concentration, pH, and anthocyanins rise in a logarithmic growth curve over the

course of the season, never completely reaching the stationary phase but declining in rate of accumulation after week 10. Tannin, flavanol, and phenol concentrations rise slowly to begin with, but then decline, with tannins ending in week 15 at a concentration lower than they started, phenols ending slightly higher, and flavanols at about the same concentration. The variance for the baseline (depicted as a shaded areas in Figure 3 centred on each line), is quite small, suggesting a high degree of certainty around these trends, however it is worth noting that particularly for tannins, flavanols, and phenols, there is a larger variation than for sugar and pH. This leads to the potential for some variation within these concentrations. The evolution of grape composition over the course of ripening suggests that grapes change dramatically in quality and flavour over time, with wet weather having a negative effect on the final harvest concentration and warm weather having a positive effect on the final harvest concentration.

We then hold all other factors aside from the weather regime constant (soil, altitude, rootstock, and scion clone) and re-run the simulations with the literature-predicted weather changes. Under this climate change scenario there is lower soil moisture across the whole growing period (Figure 2, dotted lines). Concentration of all molecules is found to increase at a faster rate in this simulation. The increase in concentration also continues until it reaches a higher total concentration. This is particularly interesting in the case of the more variable compounds (tannins, flavanols, and phenols) which show a clear increase in the climate change scenario. The notable exception to this increase is acidity, which, as pH increases more, suggests a faster and greater decrease in acidity. This suggests that grapes are higher in sweetness, lower in acidity, and higher in compounds which give flavour and structure to wine. In short, the grapes are riper, which could lead to stronger wines.

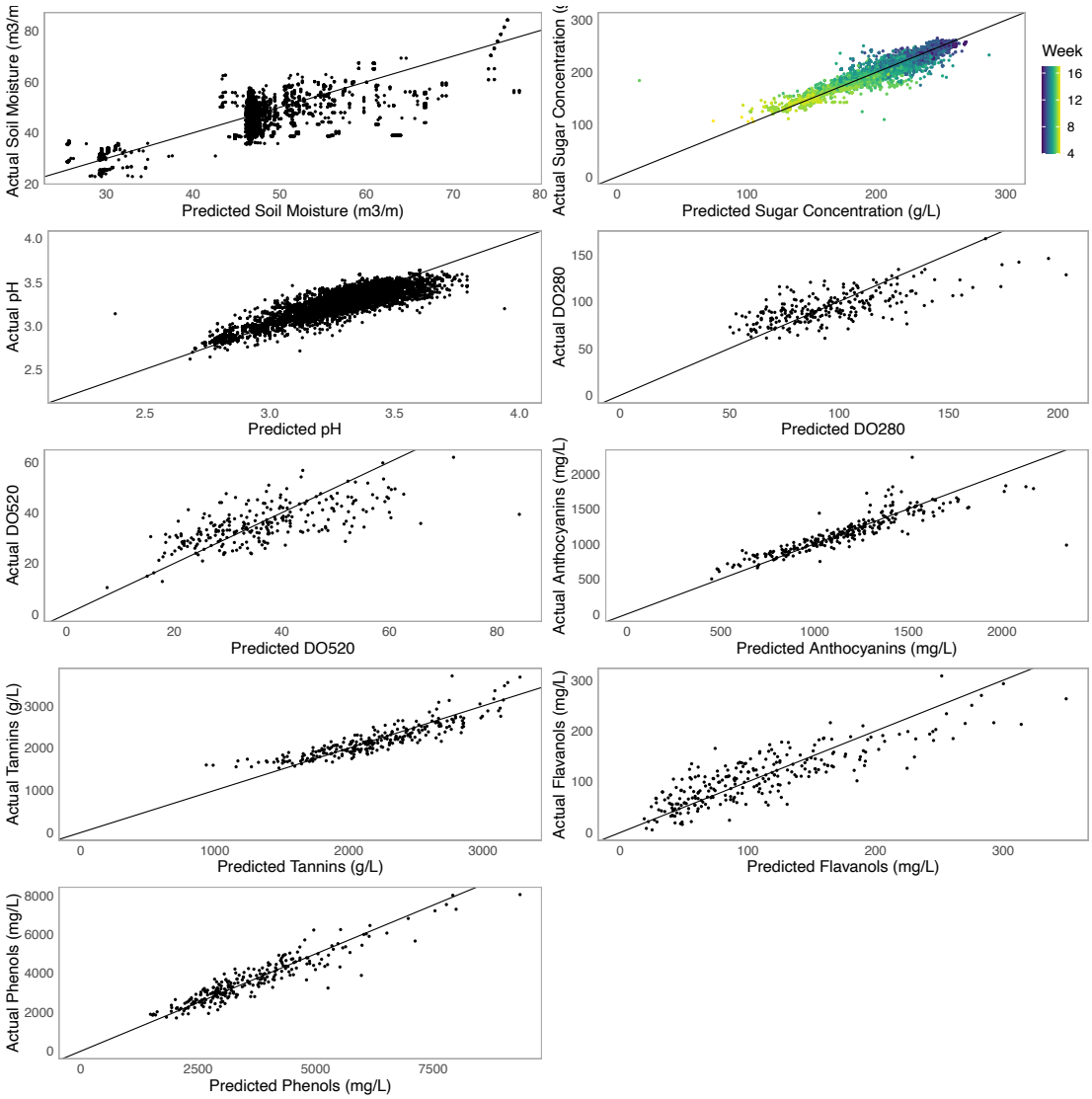


Figure 2: Plots showing the predicted output from the statistical model (x) against the actual (true) value of the model (y).

The independent changes to weather regime were conducted as a form of sensitivity analysis, and have a more varied effect, as seen in Supplementary Figure 3. For sugar, pH, and anthocyanins the largest single effect comes from changes in mean light, for tannins, flavanols, and phenols it comes from increases in mean temperature. This suggests that light and temperature are more important in the development of higher concentrations of key grape compounds, and hence for the potential of making stronger wine.

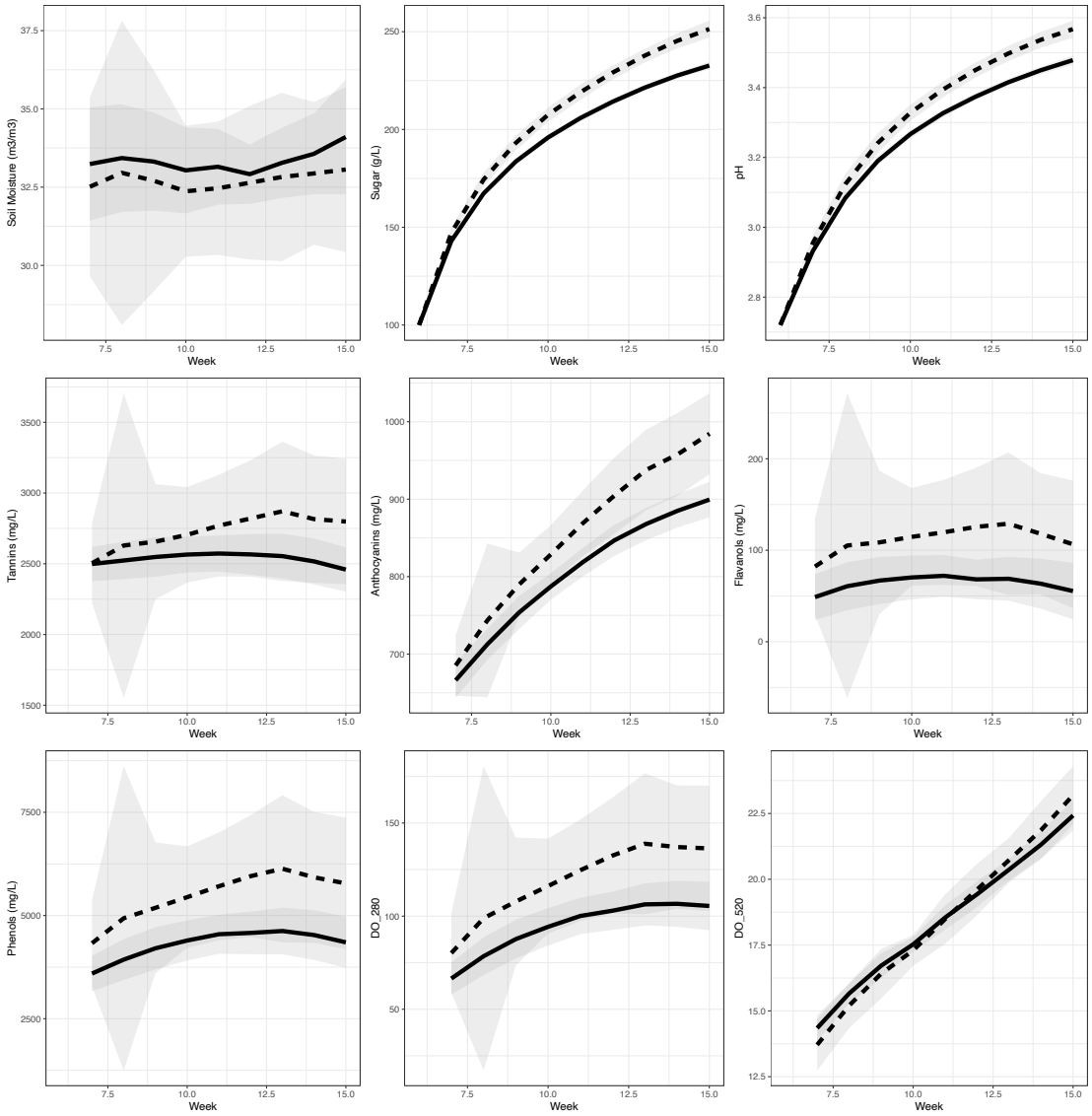


Figure 3: Output from the simulation models run, with the current climate scenario in the solid line and the future (2040) scenario in the dotted line

But climate changes are not confined to specific weeks of the year, and hence lead to changes in the phenology of the vine. Most importantly for this simulation, we changed the start date of the simulation to change the timing of the onset of ripening. We find that the soil moisture remains approximately the same in trend throughout the simulation, however there is a consistent trend of later starts leading to consistently lower concentrations of the grape molecules (Figure 4, with error Supplementary Figure 3). Each week that the delay occurs reduces the maximum reached by a

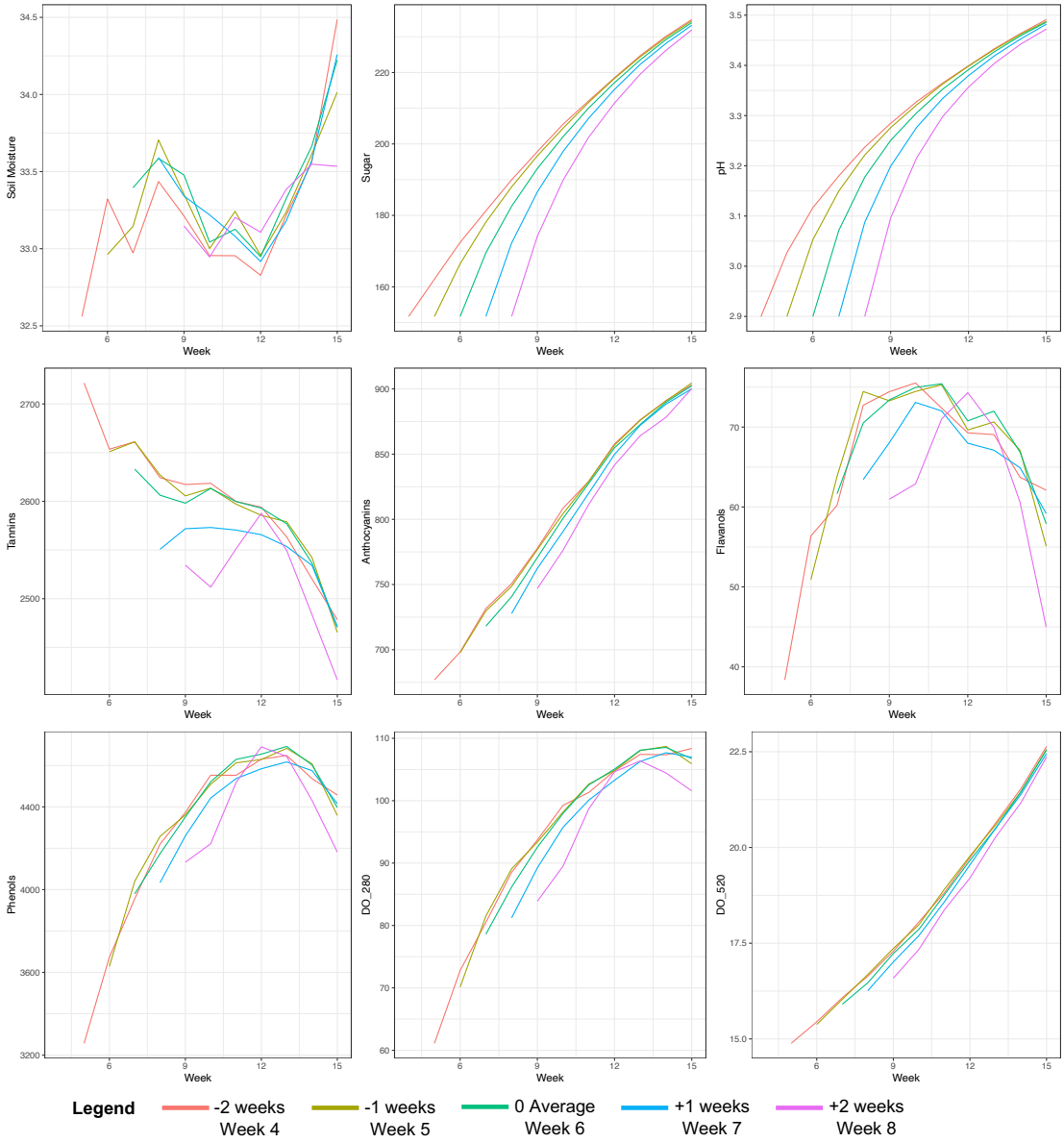


Figure 4: Output from changing the start date of the model simulation models run, starting in week 4 of the year and ending in

constant amount. Comparing the earliest with the latest starts to ripening it can be seen that there is comparable rate of accumulation of sugars and increase in pH (decrease in acidity). A similar trend is seen for anthocyanins and phenols, with sharp increases occurring post onset which do not catch up with the earlier ripening berries. Tannin concentration starts lower when ripening is delayed and as it declines at a similar rate (and all simulation outputs plateau between weeks 10 and 13 before declining again), parity is not reached until approximately week 15 (early April). This

is similar to the other molecules too, with parity not being reached by the extremes in ripening times until this time. The phenological changes suggest that earlier onset of ripening will also lead to stronger grape concentrations, and hence the potential for stronger wines.

Combining the two aspects of the scenario lead to the potential for much stronger concentrations of important flavour molecules in grapes under the predicted climate changes for Chile. This leads to the potential for stronger, higher-flavour wines, with greater structure, and potentially longer aging potential.

Discussion

This paper suggests a quantitative method of forecasting the composition of major components within a wine grape that contribute to quality. It utilises a path model method to determine how climate change will impact the composition of grapes at harvest. It finds that, under the projected climatic changes the reduced rainfall, and increased temperature and light will lead to higher concentrations of sugars; lower acidity (a more neutral pH), and higher total concentrations of phenolic and other chemically aromatic compounds (tannins, phenols, flavanols, and anthocyanins). It also suggests that phenological changes are important too, with an earlier start to ripening resulting in the same as the 2040s climate change scenario - higher total concentrations are reached (with a more neutral pH). These combined suggest the potential for stronger red wines in future, with higher concentrations of flavour-related compounds and in particular tannins which give longer aging potential.

The simulation findings are in accordance with previous qualitative and synthesis works. Van Leeuwen et al (2022) suggest in their recent synthesis that climate change in wine growing regions may lead to stronger wine flavours, with deeper colours and greater structure[12]. This is in line with their previous work, which shows “hotter” climates give stronger wines[64–66]. Experiments in Northern Portugal by Costa et al. (2020) showed that hotter weather leads larger pH and sugar values (the latter leading to potential alcohol)[32]. They found no heating trend in the phenolics and anthocyanins across temperature gradients between regions but found a difference between high and low maturity years. This is similar to what we find in our model (Figure 3), with higher sugar and pH in hotter climates, and higher variation in the phenolics, anthocyanins, tannins, and flavanols. Unlike Costa et al. (2020) we do find a general

climate change effect in the chemically aromatic compounds, however this may be due to the differing location, or specific changes in climate factors, such as changes in light intensity. This paper's predictions are also similar to the predicted changes suggested by Mura de Orduna (2010) in their review on the topic, with increased climate leading to increases in concentrations of sugars, acids, and chemically aromatic compounds, until such a point that it reaches a physiological limitation[11]. We therefore suggest that in this instance the environment that this model system is parameterised on has not reached its physiological limitation. The linear nature of the simulations means that the system cannot predict this threshold of decline, as the data from which it has drawn has not had that occur. The large sample size within this dataset means that many events have been captured in the data, but non-linearity means that at extreme values outside those currently seen, the model will not perform as well as for scenarios within which it has been parameterised.

The path model and simulation framework form a general model of Cabernet Sauvignon grapes. As such, it is also possible to use it to predict composition of the grapes several weeks into the future in any given year, and thus could be useful for the planning of harvesting of the grapes. Quality is a subjective measure which depends on the desired outcome of the viticultural management team, and the desires of the winemakers utilising the grapes. Hence by predicting the composition of the grape, rather than the date of harvest itself or the status of the vine, we can give choice to the vineyard managers and winemakers as to when they would like to pick their own grapes.

As well as understanding the potential impacts of unmitigated climate change on a single vineyard, the model is also useful for understanding the potential impacts of

climate change interventions. As we have demonstrated through our climate change forecasting, by understanding the impact of the intervention on the environment that the grape vines experience can understand the changes of the intervention to the composition of the grape. For example, a sun cover would reduce light and precipitation but may increase temperature around the vine, and thus the model could be parameterised to see what impact this intervention would have on the grapes. This tool could therefore be used to understand the impact of these interventions on the composition of the grape. It is worth noting that, due to the high co-linearity between temperature and light, there is no information gained by using both variables in a given statistical model and hence the path model built was constrained such that only one was included per statistical model built. Thus, any conclusion drawn for light can be applied to temperature also. Also, Chilean vineyards are often irrigated when water is in short supply, and no irrigation information was included in this model. Despite this, cumulative precipitation was found to be the most connect node, underlining how important water is in determining the concentration of key quality molecules within the grape. This paper has also demonstrated that it is possible to model the impact of changes in each weather factor separately, allowing for future changes in the covariance structure between the two climate variables to be accounted for[36].

But this paper is not just about the specific regional results for one specific variety of wine grape. The model parameters are both globally relevant and easily calculable for any grape variety, and the gridded input data used in the model are available for any point on the planet. Further, whilst we explore the impact of climate on one set of quality parameters – namely the total concentrations of many quality component compounds, this framework is flexible enough to accommodate any target variables. This flexibility means any combination of possible molecules could be modelled and

predicted, potentially in any crop. Staying with viticulture, white wines would require different characteristics to be tracked than red wines, with tannins and anthocyanins being less important and other aroma-causing compounds being more important. For example, naphthalene compounds give Riesling wines their characteristic petrol smells and thus are particularly important for quality in this specific wine grape variety[72]. Thus, when Riesling grapes are growing it is important to know their concentration to determine when to harvest. This modelling approach would be able to do just this by adding naphthalene compounds as an output predictor in the model.

As a flexible statistical modelling approach, our path model framework is able to be used for any crop, and in particular for any crop in which quality is more important than yield. The structure used in our path model is based upon the underlying metabolism[73]. which is conserved across many perennial crop species. Thus, the same structure, with sugar being fixed first and then other compounds and properties evolving from it, would be a highly possible new method for modelling the composition and hence quality of many perennial fruits.

To grow perennial crops under changing climate conditions requires new tools and new approaches. The use of models such as the ones we have developed suggest that there is a new future for perennial crop quality. With warming climates dramatically altering the composition of the grapes at harvest, the quality of the wines made from these grapes will also vary. This new modelling strategy allows important aspects of the grape to be estimated and serves as a potential platform for interventions to be planned. The metabolic-style statistical structure of the model also allows for great flexibility in the model applications, with potentials here to model target variables of interest, both within wine grapes and beyond into other perennial crops. In the case of

Cabernet Sauvignon in Chile, from our simulations it appears that the predicted climate changes will lead to stronger concentrations of grape metabolites in the future. This should give wine makers the opportunity to make wines with a relative increase in their complexity, structure, and concentration of chemically-aromatic compounds. These wines should have both great flavour and aging potential, and hence suggest an increase in desirability in wines in the future from this region.

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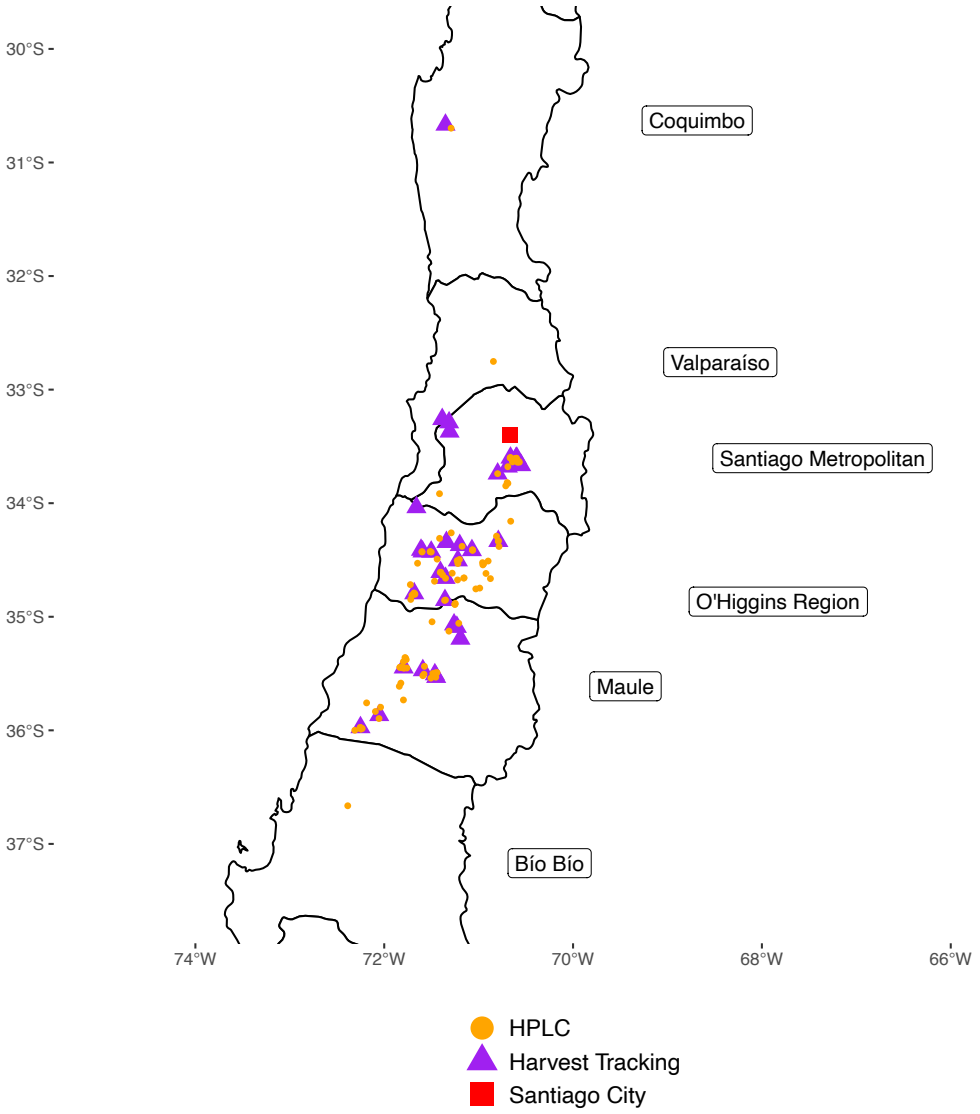
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Appendix For Chapter 3

Table 1: GPS Location for Vineyards

Vineyard Name	*Region*	*Latitude*	*Longitude*
El Boldo	Maule	-35.97224	-72.248466
Agua Santa	Libertador General Bernardo O'Higgins	-34.42692	-71.50539
RH	Maule	-35.472	-71.591167
Don Melchor	Región Metropolitana de Santiago	-33.607556	-70.604417
Lo Ovalle	Valparaíso	-33.266404	-71.389075
Ucuquer	Libertador General Bernardo O'Higgins	-34.036501	-71.658897
Chomedahue	Libertador General Bernardo O'Higgins	-34.659235	-71.350461
Rauco	Maule	-34.876104	-71.344644
Requinoa	Libertador General Bernardo O'Higgins	-34.331304	-70.793039
Santa Isabel	Región Metropolitana de Santiago	-33.660882	-70.542616
Lourdes	Maule	-35.444289	-71.805913
Mariposas	Maule	-35.535403	-71.452913
Quebrada de Agua	Maule	-35.512735	-71.459162
El Mariscal	Región Metropolitana de Santiago	-33.600979	-70.666869
El Triangulo	Región Metropolitana de Santiago	-33.371768	-71.302634
Yungay	Maule	-35.090554	-71.230752
Idahue	Libertador General Bernardo O'Higgins	-34.501245	-71.221709
Keule	Maule	-35.868566	-72.051819
La Protectora	Región Metropolitana de Santiago	-33.602894	-70.59467
Las Mercedes	Libertador General Bernardo O'Higgins	-34.793047	-71.691197
Las Pataguas	Libertador General Bernardo O'Higgins	-34.34308	-71.339631
Los Perales	Región Metropolitana de Santiago	-33.289834	-71.310799
Marchigue	Libertador General Bernardo O'Higgins	-34.411636	-71.610285
El Mirador	Maule	-35.19425	-71.19019
Palo Santo	Libertador General Bernardo O'Higgins	-34.420474	-71.59959
Pirque	Región Metropolitana de Santiago	-33.643245	-70.599737
Peumo	Libertador General Bernardo O'Higgins	-34.375542	-71.173559
La Puerta	Libertador General Bernardo O'Higgins	-34.610655	-71.404627
Quinta Maipo	Región Metropolitana de Santiago	-33.74886	-70.805433
El Recurso	Región Metropolitana de Santiago	-33.678778	-70.691111
Rucahue	Libertador General Bernardo O'Higgins	-34.409634	-71.066534
San Adolfo	Región Metropolitana de Santiago	-33.636718	-70.642031
San Ignacio	Maule	-35.072909	-71.260455
San Julian	Coquimbo	-30.667817	-71.350772
Tocornal	Región Metropolitana de Santiago	-33.604425	-70.597657



Supplementary Figure 1: Locations of the individual plots within the central regions of Chile. The data comes from three different datasets, orange circles is laboratory analytical data (generally High-performance liquid chromatography) to extract the concentrations of aromatic and volatile compounds at harvest (flavanols, tannins, phenols, as well as sugar and pH measures. The harvest tracking data (purple triangle) is a spectroscopic dataset from the Dyostem measuring system. The red square shows the location of Santiago city, the capital and largest city in Chile.

Table 2: Years tracked by the two datasets

Chilean Region	*Dataset 1 (Harvest Tracking)*	*Dataset 2 (HPLC)*
Coquimbo	2018-21	2018-9
Libertador General Bernardo O'Higgins	2011,2015-21	2018-20
Maule	2011,2013-21	2018-20
Ñuble	-	2018-20
Región Metropolitana de Santiago	2011,2015-21	2018-20
Valparaíso	2011,2015-21	2018-20

Table 3: Baseline parameters Used in each model

Step in Model	Parameters	# Possible Links
1: Weekly Cumulative Soil Moisture	Altitude, soil composition (clay, silt, cfvo, sand), weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light)	11
2: Sugar Concentration	Sugar last week, week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light)	10
3: Acidity (pH)	Acidity last week (pH), sugar concentration, week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light)	11
4: DO 520	pH, sugar concentration, clone, pruning style (driving system), week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light), quality of crop being produced, rootstock	15
5: DO 280	pH, sugar concentration, clone, pruning style (driving system), week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light), quality of crop being produced, rootstock	15
6: Anthocyanin Concentration	DO520, DO280, pH, sugar concentration, clone, pruning style (driving system), week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light), quality of crop being produced, rootstock	17
7: Tannins Concentration	DO520, DO280, pH, sugar concentration, clone, pruning style (driving system), week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light), quality of crop being produced, rootstock	17
8: Flavanols Concentration	DO520, DO280, pH, sugar concentration, clone, pruning style (driving system), week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light), quality of crop being produced, rootstock	17
9. Phenols Concentration	DO520, DO280, pH, sugar concentration, clone, pruning style (driving system), week number (log), weekly cumulative soil moisture, Altitude, weekly and monthly weather (mean temperature, cumulative precipitation, cumulative light), quality of crop being produced, rootstock	17

Supplementary Formula 1

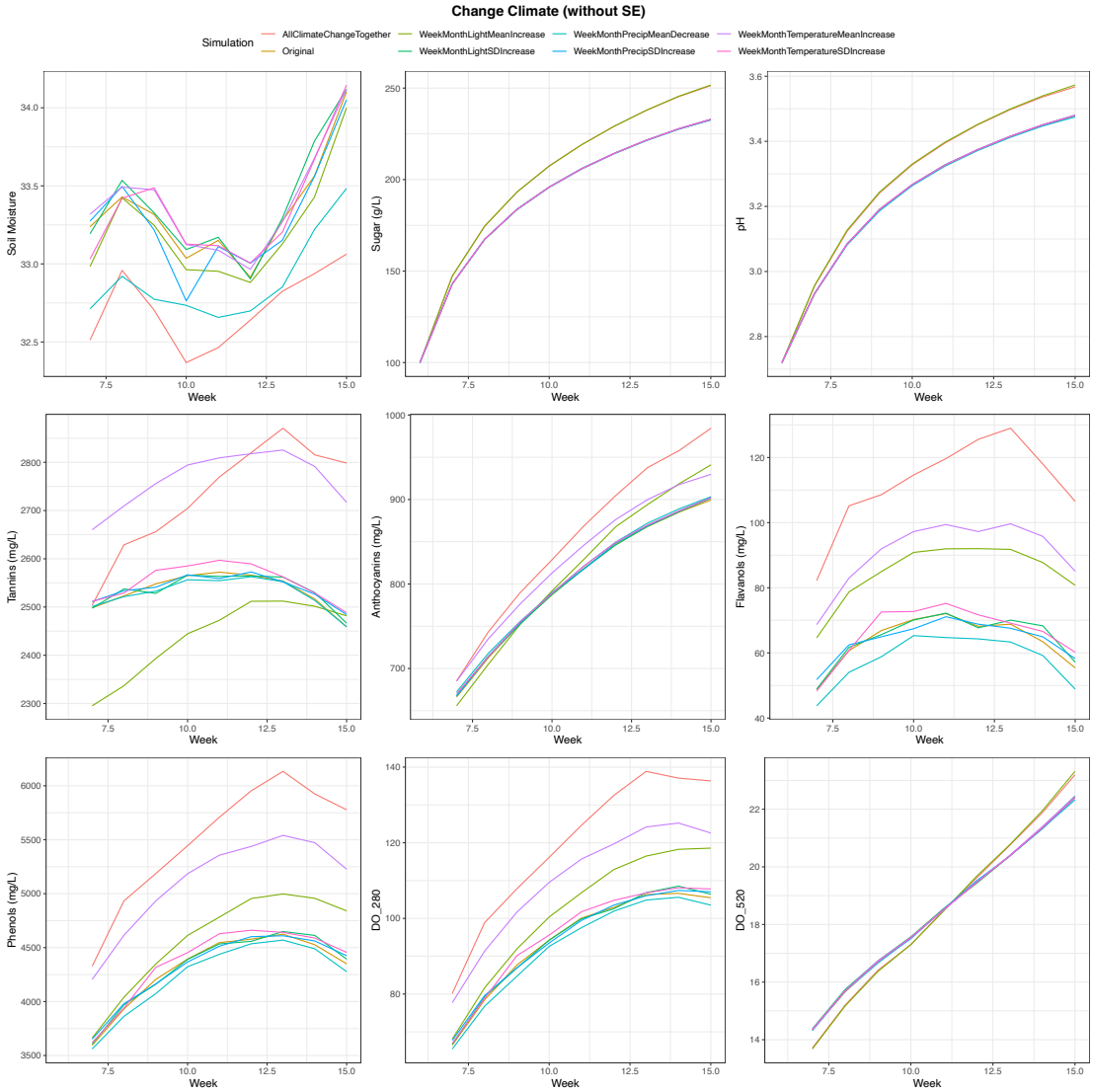
```
FullGLM <- glm(
                    formula = Output ~ Sugar +
                    pH + WeeklyMeanTemp + MonthlyMeanTemp +
      WeeklyCumPrecip + MonthlyCumPrecip +
      WeeklyCumLight + MonthlyCumLight +
      WeeklySoilMoisture + log(Week)+ Altitude + Clone + Quality +
      Rootstock+ DrivingSystem+ Age, family = gaussian(), data = data,
      na.action = "na.fail")
```

Supplementary Formula 2

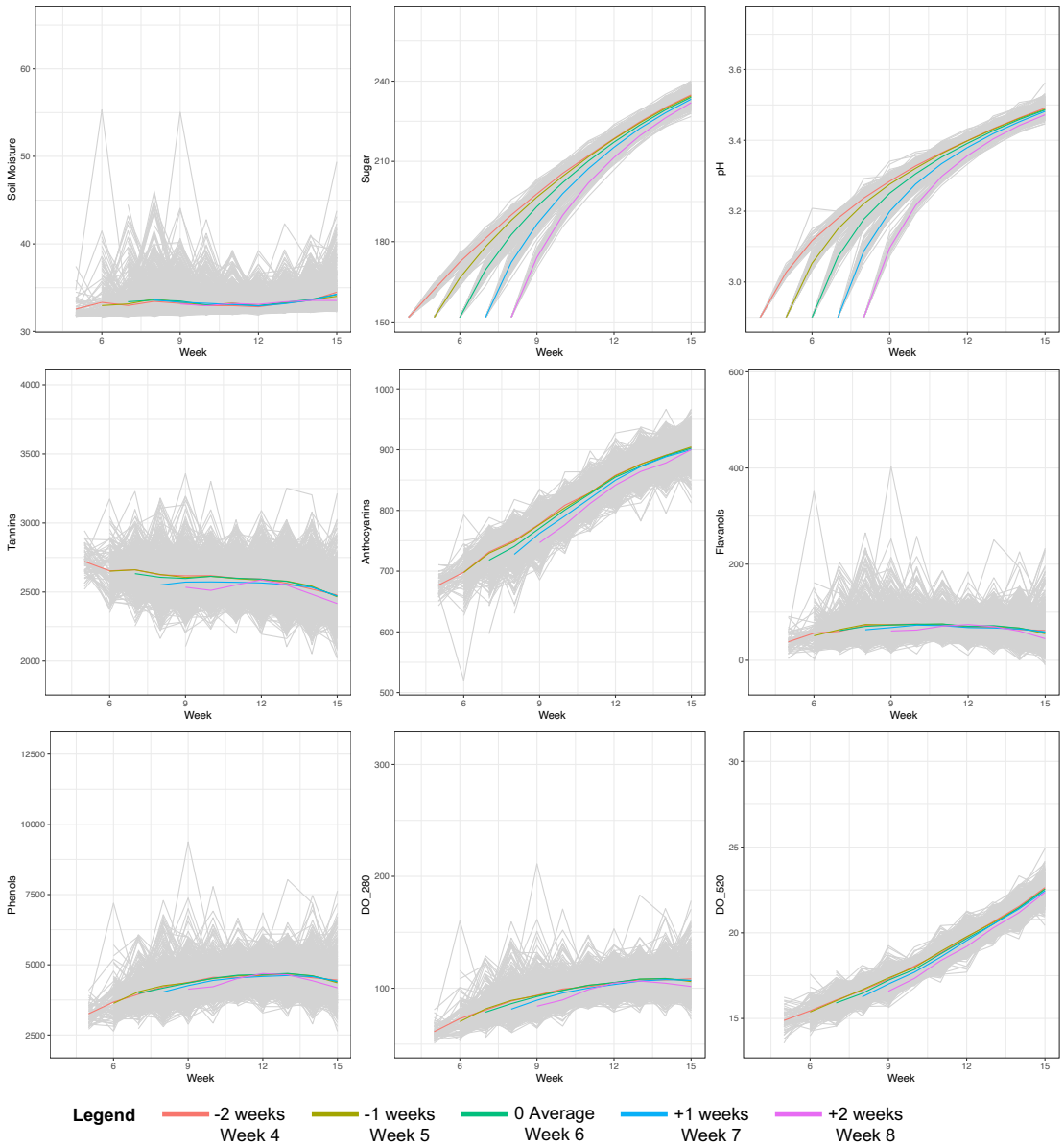
```
dredge(FullParameterGLM,
subset = (LightRollSumWeekly|LightRollSumMonthly) &&
       (TempRollWeeklyMean|TempRollMonthlyMean) &&
       (PrecipRollSumWeekly|PrecipRollSumMonthly))
```

Table 4: Models and their R^2 values

Model	AIC-Selected Model Formula	R^2 (2 sf)	Residual DF	# Variables
1	SoilMoistureRollSumWeekly ~ cfvomean + claymean + Altitude + LightRollSumWeekly + PrecipRollSumMonthly + sandmean + siltmean + 1	0.86	33875	7
2	log(SugarConc) ~ Altitude + LastSugar + LightRollSumMonthly + log(Week) + 1 + PredictedSoilMoisture	0.90	26742	5
3	pH ~ LightRollSumMonthly + PrecipRollSumMonthly + 1 + Altitude + LastpH + log(Week) + PredictedSoilMoisture + SugarConc	0.81	26738	7
4	log(DO_520) ~ DrivingSystem + Altitude + LightRollSumWeekly + SelectionClonal_Massal + SoilMoistureRollSumWeekly + 1 + Age + pH + SugarConc	0.51	230	8
5	log(DO_280) ~ DrivingSystem + Altitude + log(Week) + pH + PrecipRollSumMonthly + Rootstock + 1 + SugarConc + TempRollMonthlyMean	0.46	237	8
6	`TotalAnthocyaninsByAdams_(mg/L)` ~ PrecipRollSumMonthly + 1 + QualityLevel + DO_280 + DO_520	0.77	247	4
7	`TotalTanninsByAdams(mg/L)` ~ DO_520 + Altitude + LightRollSumMonthly + PrecipRollSumMonthly + 1 + Age + DO_280 + log(Week) + pH + SoilMoistureRollSumWeekly	0.79	247	9
8	`Flavonoles_totales_(mg/L)` ~ LightRollSumWeekly + pH + PrecipRollSumMonthly + 1 + Age + DO_280 + DO_520 + DrivingSystem + Altitude + SugarConc	0.72	242	9
9	`TotalPhenolsbyAdams(mg/L)` ~ QualityLevel + SoilMoistureRollSumWeekly + TempRollMonthlyMean + 1 + Age + DO_280 + DO_520 + pH	0.87	244	7



Supplementary Figure 2: Panel plot showing the impact of changes in mean and standard deviation of weather on the output variables in the simulation model.



Supplementary Figure 3: Panel plot showing the impact of changes in start date of the model on the output variables, with all runs completed shown as grey lines, and mean outputs shown in colour.

4

Determining the Optimal Temporal-Resolution of Temperature as a Predictor of Grape Harvest Dates

Words in Abstract: 149
Words in Chapter: 6504

Abstract

Changeability in phenological events is increasingly important with dramatic climate shifts leading to variation in quality and logistical problems. Previous climate forcing methods involve reliance on weather predictions to generate predictions of grape harvest dates. We utilise grape records for four different grape varieties from Germany and Champagne between 1950 and 2020 for competing supervised machine learning techniques to find the best way of predicting grape harvest date by variety. We use temperature at different temporal resolutions – daily, weekly, monthly, and annually, to determine the optimal temporal resolution. Using a monthly and weekly scale we find that prediction is possible for an 8- to 14-day window from as early as month 5 or 6 (May/June in Northern hemisphere), depending on grape variety. This leads to the potential for greater logistical preparedness in relation to the grape harvest and thus the ability to be better prepared for future harvest events.

Introduction

Phenology is the study of the timings of seasonal events. In grapes, it starts with budburst and progresses through leaf burst to flowering and then onwards to veraison (ripening), harvest and eventually leaf-fall[1]. The timings of such events are strongly affected by seasonal and inter-annual variation[1,2] and over extended periods of time have been shown to be associated with climate[3,4]. Viticulture is strongly reliant on phenology[5–7], with changes in the timings of harvests in particular changing logistics, flavours, and therefore affecting the quality of the wines. Changes in phenology have occurred across space and time, with Chuine et al (2004) showing that grape harvest dates (GHD) in Burgundy have advanced by an average of two weeks over the last 150 years[3]. Determining such harvest dates is a key area of viticultural management, with such dates determining labour and machinery costs, as well as the harvest quality of the grapes and hence the price of the wine[8–10]. Being able to better predict these harvest dates allows viticultural organisations to better plan their harvests, allows for more efficient utilisation of machinery, and thus have a better harvest – with cheaper costs and higher quality wines as the potential rewards.

Most current grape vine phenological models are stage based, and work to characterise the life cycle of the grape vine. The Baggiolini[11], Biologische Bundesanstalt, Bundessortenamt und CHemische Industrie (BBCH)[12,13], and Eichhorn and Lorenz Phenological (ELP)[14] scales each split the various stages of the grape growth into categories[15,16]. Such phenological models range in specificity with number of stages varying between 4 and 47[16]. Such forcing models are often simulated and predicted using accumulated temperature above (state-forcing, most famously Growing Degree Days, GDD) or below (chill-forcing, dormancy phase forcing) a temperature threshold, after which a phenological stage is triggered[17]. Most notable of these is Parker (2011)'s general phenological model[1], which was improved upon by Molitor et al (2014) to include 26 different phenological stages[18]. It also led to the Winkler scale which classifies wine growing regions by average GDD above 10 degrees celsius[19], as well as to the Huglin classification system which includes a latitude parameter as well as the GDD[20,21]. For cooling models, the two most famous models are the BRIN[22] and Caffarra-Eccel[23] models. They both use accumulated cooling to estimate aspects of phenology. These classifications and models work by accumulating daily temperature as heating or cooling units until the values reach a threshold, at which point a phenological stage is predicted to occur. For all stage-based phenological scales, higher indices indicate earlier phenological

stages. Such thresholds vary between varietals of grape and are often calibrated using site-specific observations and historical records[15,16,21,24,25]. Models which show the best performance have been found to be linear in form[26], despite other options being demonstrated as better predictors in other crops[27]. In Champagne these GDD models have led to the observational rule of thumb that harvest will occur 100 days post flowering. This rule of thumb is currently used by growers to plan harvest timings. But these models only consider thermal forcing, and consequently disregard other climatic factors which influence ripening[16].

Light and rainfall have historically been disregarded in phenology due to difficulties in their measurement and only small inter-annual variation being detected[28,29]. This has led to light and precipitation being unused for phenological prediction without a real examination as to why[1,19,30]. At a most fundamental level, light, water, and temperature are the three vital components of photosynthesis, and hence should be investigated for any plant-climate interactions and predictions. Further, increases in resolution due to high resolution datasets mean that small variations in precipitation variability can be detected, and correlations drawn if they exist. Water availability has also been shown to be important for harvest yield[31], and drought has been linked to earlier harvest dates[32]. The link between phenology and water is theoretically strong enough that historic drought reconstruction has previously been based upon local grape vine phenology[33]. Evapotranspiration rates have been used to help predict other aspects of vineyard phenology[34], but not yet harvest. Light has been shown to be important for grape berry growth and composition in both red[35] and white grapes[36]. Photoperiod has also previously been cited as important determinant of phenology in grapes[1,28,37–39], and canopy manipulation (including shoot and leaf removal) is a commonly used technique to manage light and heat availability to the grapes and impact ripening. Yet light is not often included in grape harvest phenological models, for similar detection issues to precipitation. However, the links between annual measures of light and water variability and phenological changes have not been examined to see how they compare to temperature as a correlative measure of phenological changes. Accordingly, viticultural knowledge gaps have been identified with respect to inter-annual variation due to weather as well as required reductions in physiological uncertainty to give higher precision in physiological predictions[5].

Difficulties in measurement and resolution with respect to global measurements have now been lessened due to global standardised, high-resolution weather records. ERA-5 land is a global re-analysis dataset, offering ~1km^2 resolution hourly weather records back to 1950[40].

It combines atmospheric data and mechanistic models of atmospheric physics to produce a globally complete and consistent weather dataset, from which standardised predictions can be made[40]. These weather records offer the potential to understand the impact of changes in weather on the changing dates of harvest by covering the whole globe, for every day of every year, since 1950. It is therefore possible to determine which weather factors are significant in the determination of harvest dates, and on what time scale they operate on. Temporal covariation in weather is not a new phenomenon[41–45] but determining on what scale to make predictions is important as it determines the utility of greater temporal resolution in future predictions of climate.

The Champagne region offers a good study area for understanding spatiotemporal variation in phenology. The Champagne region is a protected appellation in Eastern France consisting of 319 villages, each of which abides by the same specific regulations. These regulations cover the whole viticultural process, from planting, irrigation, canopy management, to harvest and vinification. Since 1989 these regulations have included the harvest dates for each village for each grape – Chardonnay, Pinot Noir and Pinot Meunier. The regulatory authority (CIVC - Comité Interprofessionnel du vin de Champagne), set this date by taking samples from 602 plots in the "Réseau Matu" network and then checking them for rate of colour change; average weight; estimated sugar and total acidity content; and for disease incidence such as grey rot[46]. When all these requirements are met, only then is the harvest date set and the grapes allowed to be picked. The German weather service (Deutscher Wetterdienst, DWD) operates a phenological research network (Deutscher Wetterdienst Phänologischer Dienst) which tracks the phenological stage of a diverse range of animals and plants, including crops like wine-grape vines. The network has approximately 1200 observers across the entire country across all species, with 441 locations used for wine grapes. These locations grow different varieties of grapes, including both late (Riesling) and early (Müller-Thurgau) harvesting varieties.

Machine learning (ML) offers the capabilities to improve predictions of grape harvest dates. ML is a sub-group of artificial intelligence techniques used to discover patterns in data and which can adapt and enhance their own predictive capacity without following explicit instructions. Supervised ML uses classification and regression to learn known patterns, unsupervised ML uses clustering and anomaly detection to learn unknown patterns. Machine learning has previously been utilised for crop phenology[47,48] and for vineyards[5] with

predictive capabilities being built into new vineyard management tools[34]. However, such approaches have not yet compared different uses of weather scales to predict harvest date phenology over multiple regions.

This paper sought to explore the potential of machine learning capabilities to predict the harvest date of grape vines. It used these supervised regression learning methods to not only improve the capacity of predictive capabilities across the whole year, but also to determine the earliest point of predicting the harvest window. This is a determination of the best and earliest method of predicting the harvest date, meaning that viticulturalists can have the longest time to logistically plan harvest – their most important day of the year.

Methods

This investigation used a supervised-regression machine learning approach to explore the link between aspects of seasonal weather and harvest date. It uses harvest date data from the Champagne region and from across Germany to correlate to annual light and precipitation and then daily, weekly, monthly, and annual mean temperatures. For each of these models, the years up to 2018 are used as training datasets, and the period 2019 to 2021 is used for testing data. The predictive capability of each set of models is compared using RMSE. Having selected the best performing models, we then systematically remove the last time-point for each year and retrain and test the model. This allows us to determine the optimal timing to predict the harvest date during the year, and on what temporal scale weather is required to be measured on.

Harvest Date:

Champagne grape harvest dates (GHD) for *Vitis vinifera var.* Chardonnay and Pinot Noir per village have been set and recorded by the champagne regulatory authority, the CIVC (Comité Interprofessionnel du vin de Champagne) and as such are a public record. They cover the start date of harvest for each of the 319 villages in the appellations of champagne since 1989. The location of each village is given in the Supplementary material and was extracted from OpenStreetMaps using the R package tmaptools[49] (latitude and longditude locations are given in the Supplementary). Data for *Vitis vinifera var.* Müller-Thurgau (early ripening grapes) and *Vitis vinifera var.* Riesling (late ripening grapes) were extracted from the Deutscher Wetterdienst Climate Data store for 441 locations and included location co-ordinates[50].

Weather Data:

Historical weather data were extracted from the ERA-5 land reanalysis weather dataset[40] for each location by using the *Krigr* package[51] and the Climate Data Store API. Daily mean temperature (K), sunlight (J m^3), and rainfall (m) were extracted for the first 300 days of the year on a 0.1° resolution at daily time intervals since 1st January 1950[40]. To create the weekly, monthly, and annual (whole growing season) values these daily values were then averaged by taking the mean, and the data cleaned to remove NA values. The Pearson, Spearman and Kendall correlation coefficients per day was taken for each location using the *stats* package in R.

Analysis:

Annual variation and trends were explored by fitting a quadratic regression line using the *lm* function from the stats package in R. This model explored the relationship between harvest date and year as a quadratic term. Correlations between annual weather and harvest day of year were analysed using linear models as well as Pearson's, Spearman's, and Kendall's correlation coefficients.

As R^2 value was low (and RMSE high) for the annual rainfall model, the RMSE/R^2 of temperature and light about the same, and the correlation between daily temperature and daily light about 0.3, just temperature was chosen to be used in the supervised learning (ML) models[52]. A maximum-minimum normalisation was undertaken for both the temperature and the harvest day of the year using the general formula below and the specific formula found in Supplementary Formulas 1 and 2. The global maximum and minimum temperatures (all sites and all years) were used in the model, with the formula is as follows:

$$Normalised\ Value = \frac{x - \min(x)}{\max(x) - \min(x)}$$

Regression supervised learning methods:

We trained and compared 28 different forms of supervised regression-based machine learning techniques from the start of their dataset to the harvest in 2018. The models trained comprised of linear regression, Gaussian process regression, random forest decision trees (from fine to coarse), support vector machines, kernel regression, and deep and shallow neural networks. These algorithms were selected as together they capture a range of diverse

modelling approaches. Linear regression models were chosen as they describe a straightforward linear relationship; Gaussian process regression captures non-linear patterns and uncertainty; random forest decision trees offer ensemble learning capabilities; support vector machines are effective in high-dimensional spaces; kernel regression incorporates non-linear relationships through kernel functions; and deep and shallow neural networks allow for complex hierarchical feature representations. For the full list see Supplementary Table 1, with a description of each model trained. The MATLAB regression learner facilitated the training process, and we utilised 5-fold cross validation during the fitting process to ensure robustness and prevent overfitting. For each model the same data structure was passed to the model, and the fitting process used the default parameter choices. After the models were trained, they were tested against the harvest dates of 2019-2021. These models were compared by minimising the root-mean squared error (RMSE; in days) and by the best fitting predicted-actual plot which sat along the y=x line. This was carried out for daily, weekly, and monthly datasets. Plots can be seen in Supplementary Figure 3 for daily, Supplementary Figure 4 for weekly and Supplementary Figures 5 for monthly lowest best fit and Supplementary Figure 6 boosted trees respectively.

This model was then used as the basis of the chronological iterative removal of the last week or month from the models, and the retraining of the model. To understand when predictions could be made, months were removed one at a time from the model, before again being tested on three of the most recent years (2019-21). This allowed us to understand and measure the capacity of the model to predict from earlier points in the season, thus providing a better overall understanding of the model. For an overview see Figure 1 for a description of the methods.

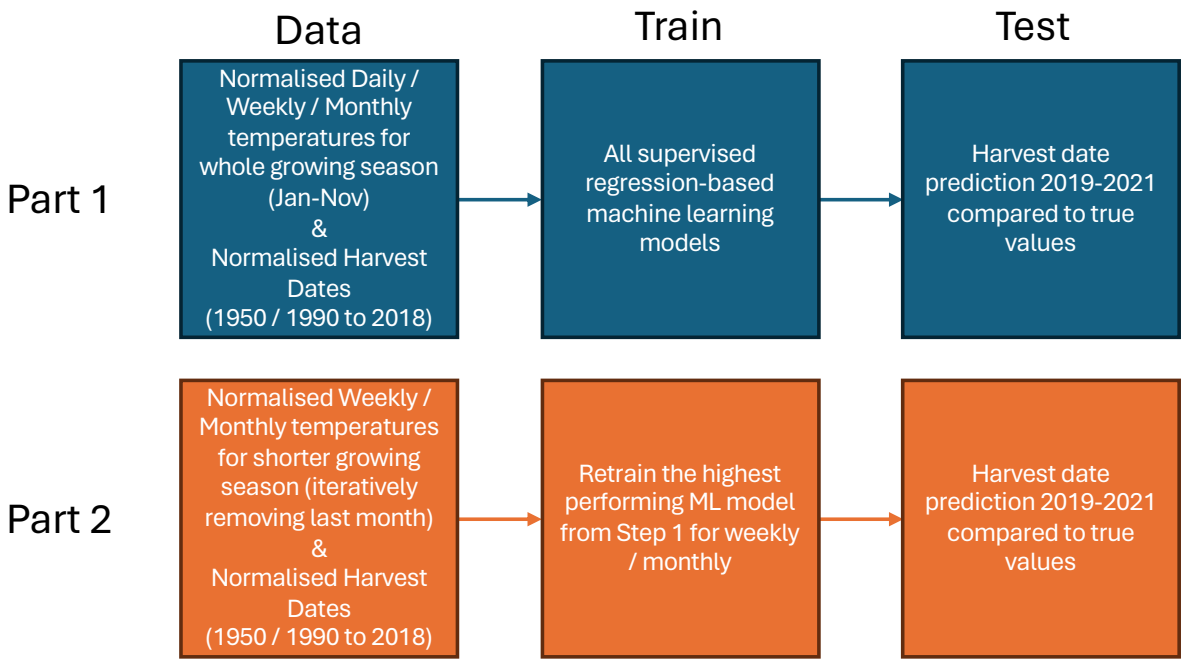


Figure 1: Summary of methods used.

Results

Over time and across both jurisdictions investigated, there is a trend for the date of harvest being earlier (Figure 2). This is more prominent, and the annual variation is greater, in the Champagne dataset (Chardonnay and Pinot Noir grapes). Quadratic advancement of harvest date over the period occurred faster for Pinot Noir and Chardonnay (0.58 and 0.50 days earlier per year respectively, see Supplementary Table 2) in Champagne than for Müller-Thurgau and Riesling (0.29 and 0.24 days earlier per year) in Germany. Over the 30 years in Champagne and 70 years in Germany this means that there is an average difference of between 21 and 15 days earlier than there was at the start of their data collection. For coefficients of quadratic models see Supplementary Table 2. The gold points denote years in which the scores from the wine critic Robert Parker are 95 points or above. Whilst for the Champagne grapes these appear to be years in which harvest occurs later than the quadratic average, for Germany the opposite appears true, with some earlier harvests having higher quality.

Rainfall, light, and temperature were all found to be correlated on a daily scale (Supplementary Figure 1). There is a strong seasonal trend, with light-temperature (L-T) and temperature-precipitation (T-P) trends reversing at around day 75. The magnitude of these correlations varies from -0.5 to +0.5 (L-T) and from +0.5 to -0.5 (T-P). This means that during the winter higher temperatures occur on wetter and darker days, a trend which reverses in the summer to have higher temperatures on drier and high light (sunnier) days. The correlation between light and precipitation (L-P) is constant throughout the year (-0.5), with higher precipitation occurring with lower light conditions. Due to this high correlation, this investigation chose to just use temperature to investigate the effect of changes in temporal resolution.

Annual means of temperature, precipitation, and light were used as predictors in linear models for harvest day of year (Supplementary Figure 2). For each grape, negative correlations were found for temperature and light, and small positive correlations for rainfall (Supplementary Table 3). The low mean R^2 value for temperature (0.26), light (0.25), and rainfall (0.07) and high test RMSE (8.33, 8.51, and 14.12 respectively) suggests that these models are a poor predictor of harvest date.

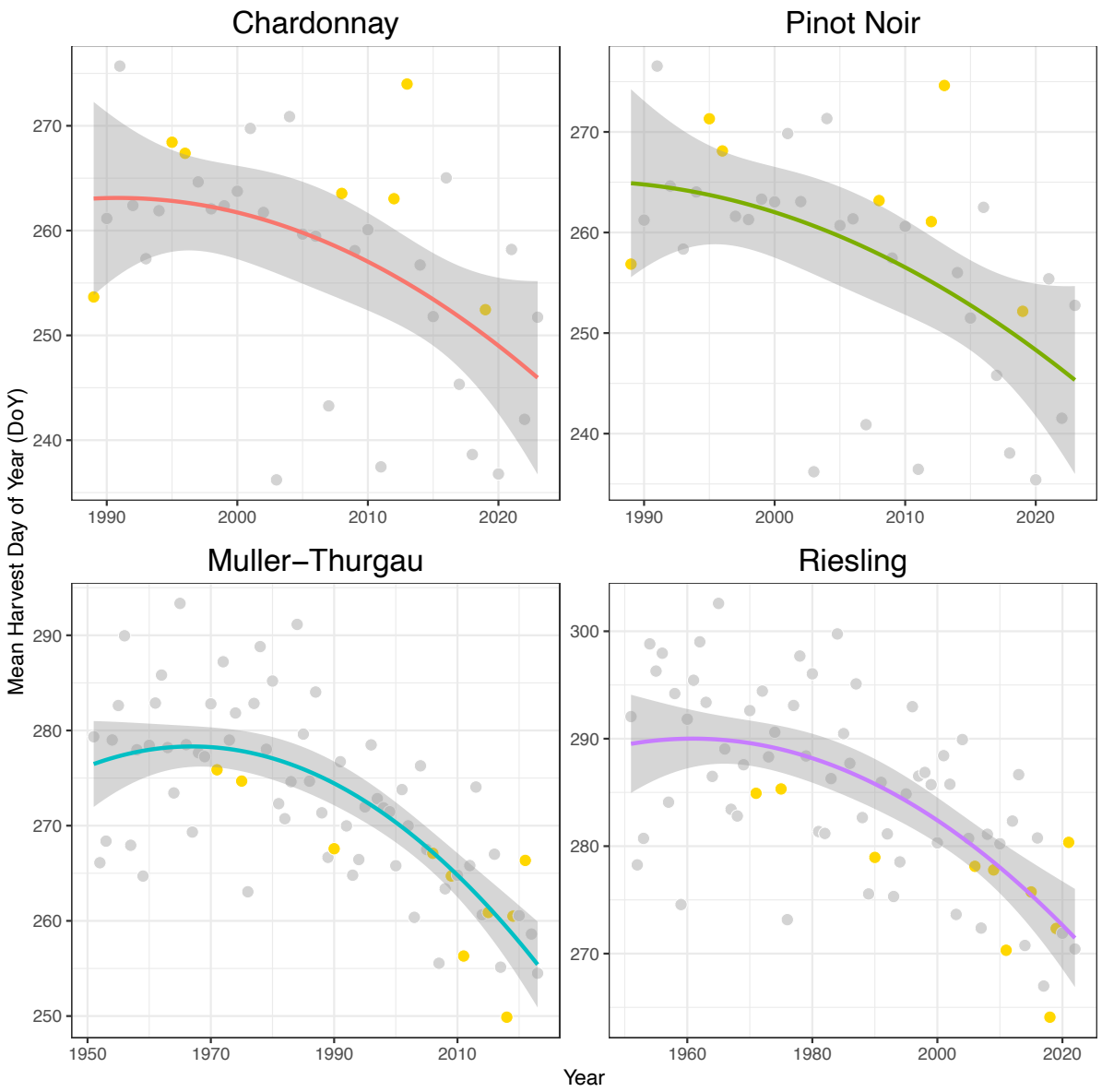


Figure 2: Panel plot showing the mean harvest dates for two varieties of grapes in the Champagne region of France (top row) and two varieties across Germany (bottom row). The gold dots denote years with a regional Parker score of 95 or above. Note that each panel is on its own axes.

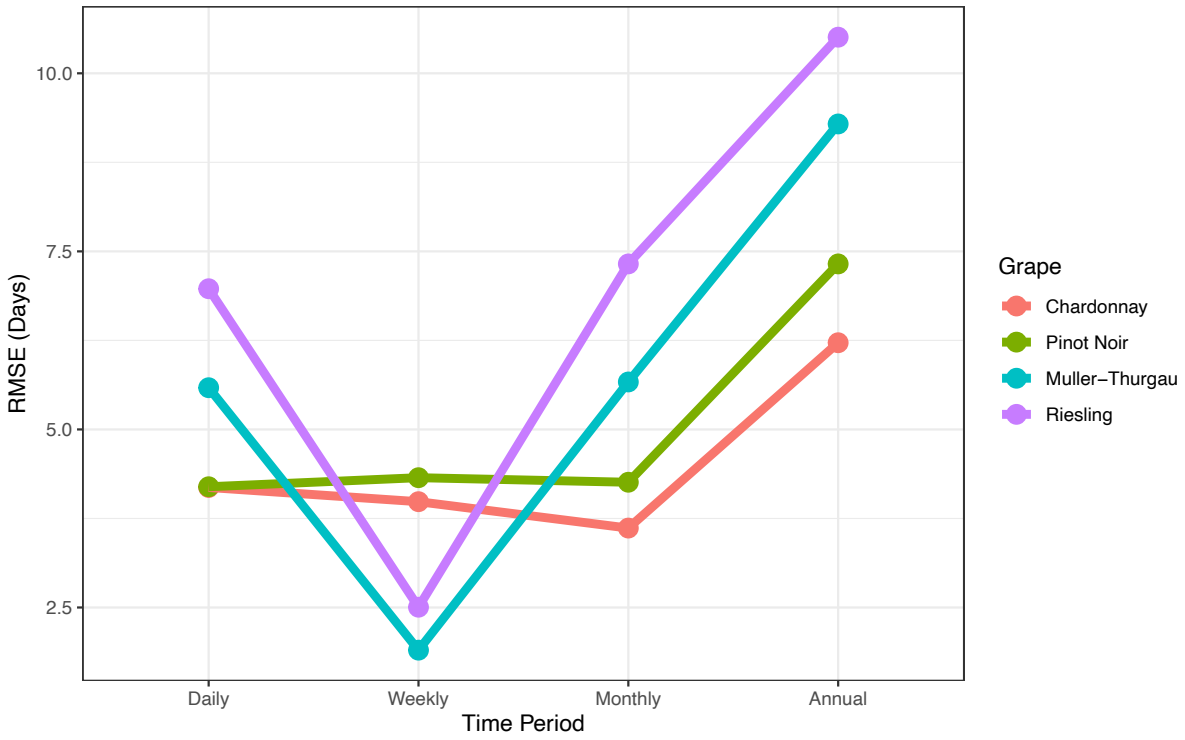


Figure 3: Daily, weekly, and monthly errors for the highest performing model fitted for temperature of each one.

For daily, weekly, and monthly temperatures 28 regression-based supervised machine learning models were built. The comparison between the best performing daily, weekly, and monthly models, as well as the annual linear models can be seen in Figure 3. For all models the worst performing model is the annual model (RMSE of test data C: 9.03, PN:9.61, MT:10.88, and R: 10.88). For the other time scales, there is only a small amount of difference between the error of prediction for Chardonnay grapes. The second highest error is for models using daily temperatures (RMSE 4.18), then for weekly temperatures (3.99), and then monthly temperatures (RMSE 3.62). For Pinot Noir the differences are still very small, but daily (RMSE 4.20) rises to weekly (RMSE 4.32) before falling to 4.26 days RMSE for monthly. In effect, each of these models has very similar predictive capacities, despite the large difference in temporal resolution between them, and information within them. Both Riesling and Müller-Thurgau have the same shaped trends, with high RMSE for daily (MT: 5.59, R: 6.98) and monthly (MT:5.67, R: 7.32) temperature resolutions, and lower errors for weekly temperatures (MT: 1.9, R: 2.5). See Supplementary table 5 for full comparison across all time scales.

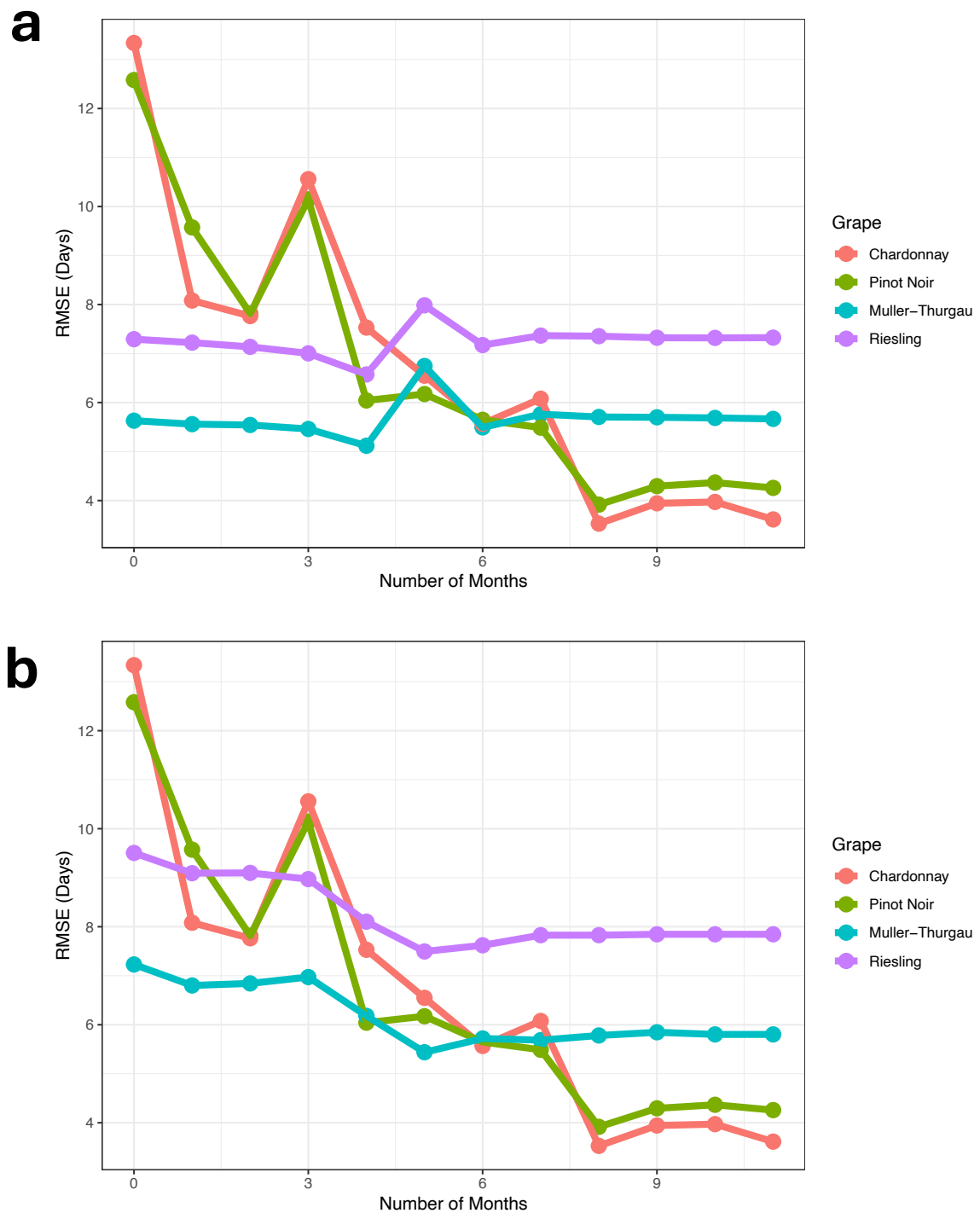


Figure 4: Error of models trained with an increasing quantity of data to determine the optimal time to predict the harvest date using either a) the best method possible (C: Boosted trees, PN: Exponential Gaussian Process Regression, MT: Linear SVM, R: Robust Linear Regression) and b) just boosted trees.

The chronological removal of months allowed for an understanding of when predictions could be made. For monthly predictions in Chardonnay and Pinot Noir there was a clear decrease in error as months are added to the model (Figure 4, both panels). The model predictions start of as quite inaccurate, at thirteen days RMSE. The error then declines sharply to eight days during February (month two), before rising to ten days in month three (March) and then declining to around seven days with four months in the model (April). This decline continues until month eight (August) when it plateaus at around 4 days for the rest of the growing season. This trend is the same for using both boosted trees and Exponential Gaussian Process Regression for Pinot Noir (Figure 4 comparing panels a and b). For Müller-Thurgau and Riesling the predictions are more stable, with the error generally at around a week, declining during the first part of the year to April, which is the lowest error for both grape varieties. There is a noticeable increase in error during May (month 5), after which the error is relatively stable until the end of the growing season. The main difference when using boosted trees to predict Riesling and Müller-Thurgau grape harvests (Figure 4b) is the magnitude of error has increased by approximately 2 days. The other difference is that instead of their being a peak during April and May, there is a decline, with May being the lowest error of prediction, and then it plateaus after this point.

When weeks are removed rather than months, there is a similar story as for months. Pinot Noir has a large peak during the first weeks of the year, before generally declining. There is a larger drop between weeks fourteen and fifteen of six days (between 11.27 and 5.75 days), after which it rises and falls to eventually reach a prediction only two-days more after 28 weeks. This trend of a high decline which declines to a plateau is common across all the grapes, as best seen in Supplementary Figure 7. Between weeks fourteen and fifteen is a common time for this decline to start to occur: a decline occurs between weeks fourteen and fifteen for Chardonnay, between thirteen and sixteen is Riesling, and the decline happens between weeks thirteen and eighteen in Müller-Thurgau. For Chardonnay this decline represents a six-day improvement in error, whereas for Müller-Thurgau and Riesling it represents about 0.3 days. Thus, in the German grapes there is very little improvement made on a weekly basis throughout the course of the year, instead the predictive ability is similar throughout the year.

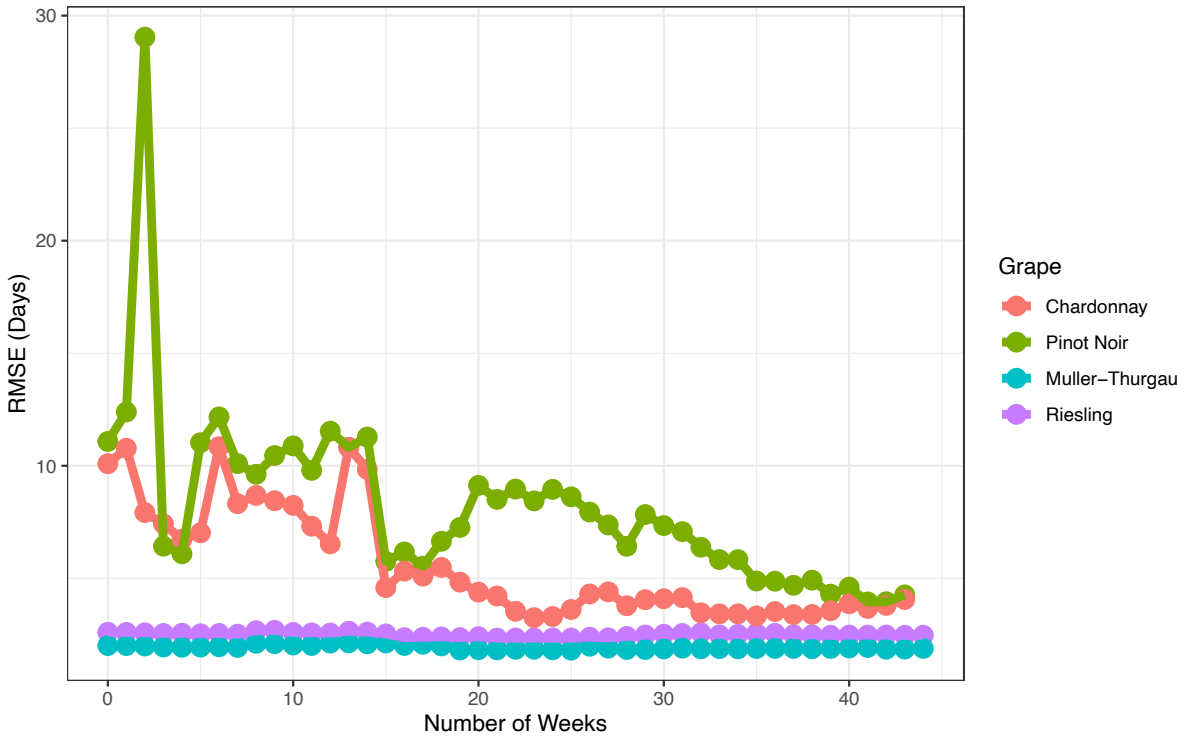


Figure 5: Error of models trained with a weekly increasing quantity of data to determine the optimal time to predict the harvest date.

These results therefore suggest that weekly temperatures can be used to predict the harvest dates of wine grapes reasonably-accurately after just 15-20 weeks of the year. These results also suggest that weekly temperature weather is the best temporal predictor in more constant environments like Germany. In more rapidly changing environments like in Champagne these results suggest that monthly temperatures may be adequate to predict the harvest date to within a two-week period up to five months before the harvest takes place.

Discussion

This paper starts by discussing the changes in phenology which are occurring for wine grapes in the Champagne region of France and across Germany. It finds that they are experiencing different rates of phenological changes, with Germany varying less than Champagne in its harvest timing. This paper then uses linear models and correlation metrics to determine the suitability of three weather variables for the prediction of wine-grape harvest dates. These weather variables are the annual (whole growing season) mean temperature, light, and rainfall. Temperature and light are found to both be suitable candidates for the prediction of wine-grape harvest dates as they have similar predictive capability, and both perform much better than rainfall. Whilst these annual means were found to be poor at predicting the overall harvest date, these models demonstrate that there is a clear correlation between weather and harvest date, independent of location and site-specific factors.

Light and temperature are then found to significantly co-vary, and whilst either variable could have been selected, temperature was chosen to be used as it had slightly lower error, explained a higher proportion of the variance, and had higher field-applicability. Using the finer temporal resolutions of weekly, monthly, and daily temperature, supervised machine learning models were then used to predict the optimal harvest date. The models built suggest that in slower changing environments like Germany using weekly weather data is sufficient to predict harvest date to within a 5-day window (RMSE of 2.5 days), after approximately 15 weeks of the year. In the faster changing region of Champagne, the monthly data was better, and could predict to within an eight-day window (RMSE of 4 days) by month 5 of the growing season. This suggests a heterogeneity between regions in terms of their ability to be predicted by different modelling techniques and the different data requirements for each variety or region. These are all useful considerations when building a predictive model, especially as the earlier the prediction the better for logistics and business planning in the winery. We therefore suggest that this type of modelling would be helpful for wineries to employ in the future.

Our models also add to the ongoing debate concerning correlative versus mechanistic phenological models[42,45]. Mechanistic models that often use state forcing units (cooling for dormancy or heating for growing degree days (GDD)) are currently the most popular method of predicting phenology of grape vines[1,17]. They assume that accumulated temperature is the

main driver of phenological development[1,53,54]. The difficulty in utilising GDD for seasonal prediction lies in the uncertainty of predicting the weather. The benefit of using our machine learning techniques is they can utilise the covariance within the weather to better predict the outcome window from recent weather events[41–45]. The reason why predictions can be made so early in the year is that the non-linear relationships drawn by supervised machine learning models extract information that would be more challenging to draw out by an analyst working alone[41,45]. Accordingly, enough information can be drawn from the data by month 5 (or week 15) that the model can predict the harvest window to a range of approximately two weeks. This information is possible due to covarying nature of the temperature throughout the year – the temperature in one time unit is very closely related to the next and thus contains very little new information[45].

The potential for earlier prediction is a large potential benefit of correlative over mechanistic models. But predicting so early in the year does not mean short term variability will not impact the actual harvest dates. Extreme events that damage the crop: be that late frosts, high winds, or extreme disease outbreaks can all lead to a rushed harvest and a hastening of the harvest dates. Such events are not possible to be predicted in a framework such as this, and this can cause movement within and even outside of the expected prediction window. The greatest driver of this premature early harvesting is the onset of disease. This was the case in Champagne in 2021, when a year that was blighted with late frosts and mildew had the risk of grey rot (*Botrytis cinerea)* devastating the harvest and thus the harvest was moved earlier[55]. 2021 was part of the testing dataset for our model, and thus incidents like this led to greater uncertainty in our model predictions.

The use of correlative prediction models, especially those which allow for complex non-linear interactions such as ML methods, can implicitly account for these other factors like disease onset[45]. Whilst the black-box nature of the models can prohibit precise understanding of the factors driving the system[56], these correlative models will naturally consider any factors which lead to a change in harvest date. This is because the weather conditions that encourage it, such as warmer, wetter, autumns will be correlated as leading to an earlier harvest, as they have been used previously to predict disease outbreaks in grapevines[57]. The non-linear nature of the ML models we have utilised allows for these factors better than more determinable modelling approaches and thus can better capture all these dynamics, and thus produce a much better predictive tool.

A third advantage of using correlative over mechanistic models is the use of standardised data over accumulated climate forcing units. Accumulated units lose the information carried within each weather record, as it is simply calculated as a running total[53]. Thus, the impact of cold snaps or heatwaves, that occur at a particular time of year may have a differing impact depending on what time they affect the vine, in much the same way that they do quality[58]. This loss of information loses the nuance in the data, and thus potential predictive power.

It is also clear from a modelling perspective that preserving the right temporal-scale of information is important too. Daily data has the most information contained within it, but there also exists a large quantity of noise[41,45]. But conversely, annual data has had so much information removed from it, for each grape it was the least useful temporal scale to work on. We found that weekly data was an optimal outcome for the Müller-Thurgau and Riesling grapes within Germany. Weekly models also performed well for Pinot Noir and Chardonnay but were found to be equal to models made with monthly weather. This is useful for the creation of prediction tools as monthly weather models are much faster to run and require much less computing power to make the same level of prediction[42]. In the case of the German grapes, it was the case that the monthly data had had too much information removed from it to be useful. Getting the right level of information is clearly key.

This right level of information is also spatially important. The spatial extent of the data results in potential for cross-over of vineyards between close villages within each of the datasets. For each village and station only one location was used, and thus the accuracy of the predictions cannot be as precise either. It is possible to tie each individual plot to a weather location and then run the same analysis, but the potential for increase in temporal prediction is small. The benefit of this investigation is the possibility of early prediction of harvest windows. As harvest is the commencement of the winemaking schedule, it is important to have as much detail concerning the timings as they determine the logistics of the whole of winemaking, from people and machinery to fermentation and bottling.

These models are all possible due to the long-term datasets that are available for phenology. The advantage the systematic way in which the data is collected across the different DWD stations in Germany and Champagne's Résearch Matu network is that they give spatio-temporal resolution across the whole region. Such stringent regulation by the CIVC in terms

of controlling harvest dates and yields means that harvest dates can be taken as timings of peak ripeness and optimal quality per annum, akin to the same phenological time point used by the DWD stations.

This work also ties in the changes in phenology which are happening globally. The parabolic nature of the average harvest date suggests an increasing rate of harvest advancement in these areas. In doing so, our quadratic model agrees with the accelerating impact of climate change found by larger scale investigations of harvest dates[3,54,59]. This paper removes the requirement for the assumption of constant development and ripening rates over time[60], as the weather variable at each time point can link to the harvest date independently. In doing so it allows for the prediction and management of the advancement of harvest as a mitigation tool for dealing with climate changes in winegrowing regions. The variation in model and resulting specific outcomes mean that the erratic and extreme nature of predicted changes in winegrowing regions can be planned for by changing the harvesting timings to pick at the optimal maturity for the wine grape variety planted.

This investigation explores the predictability of the grape harvest. It uses supervised machine learning techniques to explore predictability of 4 different grape varieties in Champagne, France, and Germany between 1950 and 2021. As well as finding that harvests are predictable, it also underscores the potential for data-driven approaches to enhance viticulture practices. The findings have implications for precision viticulture and sustainable grape production, as well as developing our understanding of the phenological cycle, and how it is being impacted by changes in climate.

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Appendix For Chapter 4

Supplementary Table 1

Model Type	**Model Name**	**Description**
Linear Regression	Linear	The fitting of a linear equation to the observed data. The intention is to find the best-fitting line (or hyperplane in the case of multiple variables) that minimizes the sum of squared differences between the observed and predicted values of the dependent variable.
Linear Regression	Interactions Linear	The addition of interaction terms to the model which therefore adds the coupled effects of them together
Linear Regression	Robust Linear	Linear regression with down-weighting of outliers with large residuals to create more reliable estimates
Stepwise Linear Regression	Stepwise Linear	Linear regression which systematically selects and adds or removes variables based on certain statistical criteria (covariance, correlation coefficients etc.), iteratively refining the model to enhance predictive accuracy and interpretability.
Efficient Linear Regression	Efficient Linear Least Squares	Similar to standard linear regression but computationally less expensive. This version uses a gradient descent method which therefore minimizes the cost function by adjusting the model parameters in the direction of steepest descent.
Gaussian Process Regression	Squared Exponential GPR	GPR is a non-parameteric Bayesian approach which treats the relationship between y and x as a distribution over functions which takes a gaussian form. The kernel determines the smoothness and behavior of the modeled

		functions, in the case of squared exponential function it assumes smooth and continuous functions, making it effective for modeling data with underlying smooth trends.
Gaussian Process Regression	Matern 5/2 GPR	The Matérn covariance function is a function used in GPR and is defined by its flexibility, allowing for a range of smoothness levels in the modeled functions.
Gaussian Process Regression	Exponential GPR	Another function, the exponential decay function which assumes exponential decay in the correlation between data points, so makes it suitable for capturing trends with rapid changes.
Gaussian Process Regression	Rational Quadratic GPR	The presence of a rational quadratic term enables the modelling of both short-term and long-term dependencies in the data.
Tree	Fine Tree	All types of decision tree models, with varying levels of granularity. The model is a hierarchical tree-like structure consisting of nodes. Each node represents a decision or a test on a feature, and the branches emanating from a node represent the possible outcomes of the decision. The model makes decisions at each node by selecting the best feature to split the data based on certain criteria, in the case of regression this is mean squared error. A fine tree is a deeper structure with a large number of nodes and branches which generally exhibit high variance and have the potential to fit the training data very closely, which could lead to overfitting, especially if the dataset contains noise. Coarse trees are the opposite, with shallower structure and fewer nodes, but are less good at capturing data.
Tree	Medium Tree	
Tree	Coarse Tree	

Ensemble	Boosted Trees	Boosted Trees combines the predictions of multiple decision trees, sequentially correcting errors to enhance predictive accuracy.
Ensemble	Bagged Trees	Boosted Aggregate Trees builds multiple decision trees by training each on a bootstrapped subset of the data, reducing overfitting and improving generalization.
SVM	Linear SVM	Support vector machines for regression fit a linear tubular-shaped space around the data which encompasses as much of the data as possible. They differ from standard regression by using an epsilon-insensitive loss function, where deviations within a certain range (epsilon) are ignored. Data points falling within this range are considered correctly predicted, and deviations outside the range contribute to the loss. This loss function is linear in this instance, and there are no transformations applied
SVM	Quadratic SVM	For each of these there is a nonlinear transformation applied to the data before the SVM is trained, either quadratic or cubic in this instance.
SVM	Cubic SVM	
SVM	Fine Gaussian SVM	These models use a Gaussian Kernel to transform the data into a higher dimensional space. The Fine model makes finely detailed distinctions between classes, with kernel scale set to sqrt(P)/4, where P is the number of predictors. The medium model makes medium distinctions, with kernel scale set to sqrt(p) and coarse is sqrt(P)*4, again where P is the number of predictors.
SVM	Medium Gaussian SVM	
SVM	Coarse Gaussian SVM	
Efficient Linear Regression	Efficient Linear SVM	A linear SVM with a gradient descent method, as with the efficient linear least squares.

Kernel	SVM Kernel	These are kernel approximation models which approximate the transformed feature space by explicitly computing a lower-dimensional representation of the data. In this case SVMs or Least-squares regression is used to approximate the kernel.
Kernel	Least Squares Regression Kernel	
Neural Network	Narrow Neural Network	A neural network is composed of interconnected nodes, or artificial neurons, organized into layers - input, hidden, and output. The width (narrow, medium, or wide) of the network is a constraint on the number of internal nodes within the hidden layers of the network. Wider networks can capture more complex patterns, but can be prone to over-fitting of training data. The training involves adjusting the weight (strength of connection) and biases (additional hidden parameters) to best fit the data.
Neural Network	Medium Neural Network	
Neural Network	Wide Neural Network	
Neural Network	Bilayered Neural Network	The number of layers is the number of hidden layers within the neural network. Bilayered means just one layer of hidden nodes (like a sandwhich with input, hidden layer and output) and trilayered is two internal layers of hidden nodes (input, hidden layer 1, hidden layer 2, and output). Again, bilayered netural networks are simpler, but trilayered can capture more complex phenomena.
Neural Network	Trilayered Neural Network	

Supplementary Formula 1: Temperature

This is the full temperature standardisation, with 250K being the global minimum temperature, and 310K being the maximum temperature. This means that the formula can be written as follows:

$$Standardised\ Temperature = \frac{x - 250}{310 - 250} = \frac{x - 250}{60}$$

Where x is the daily/weekly/monthly temperature value for a single location to be standardised.

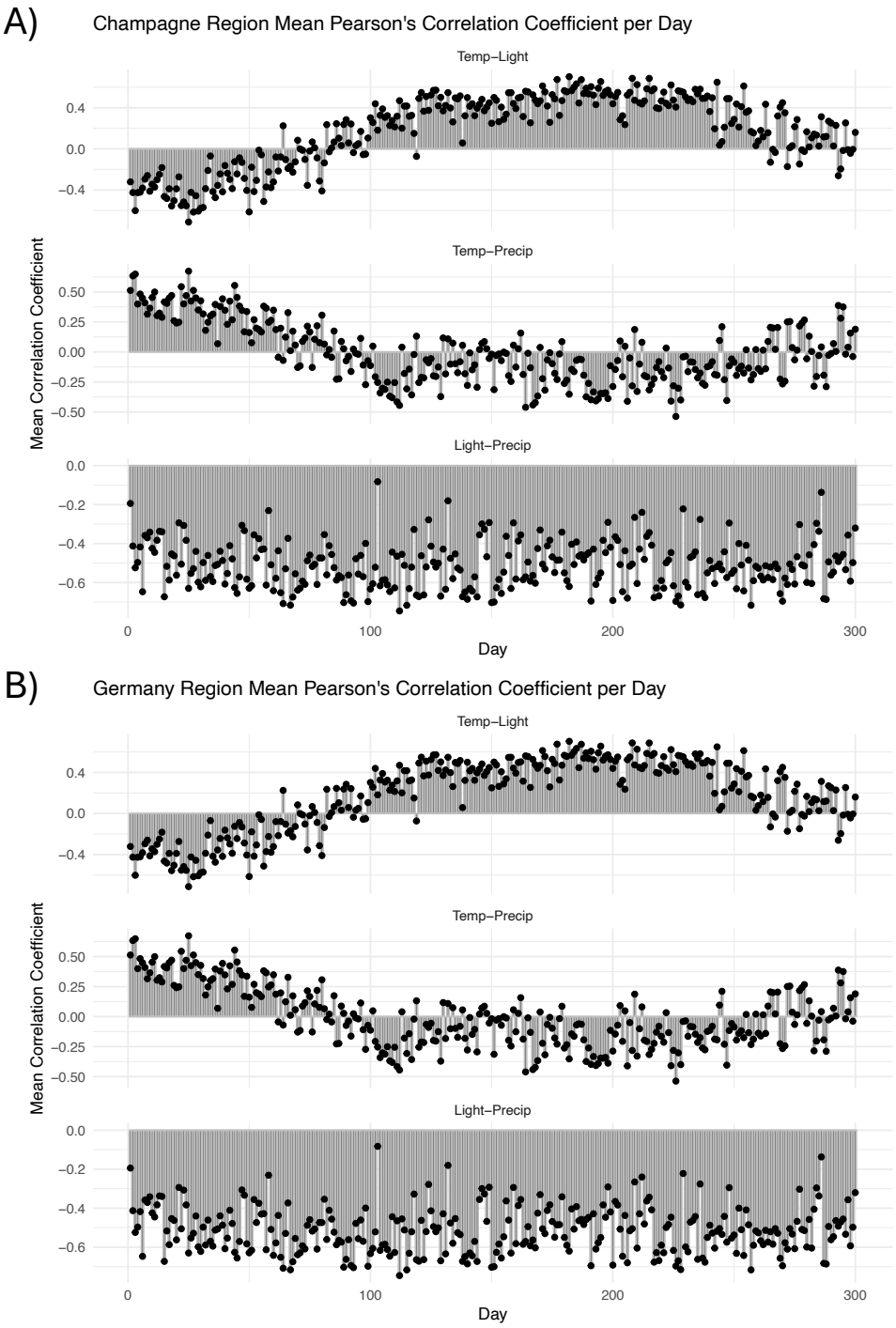
Supplementary Formula 2: Harvest Date

As for temperature, harvest date was also standardised using maximum minimum. The global maximum optimal day of harvest was day 300 and the minimum was 220, meaning the formula can be written as follows:

$$Standardised\ Harvest\ Day = \frac{x - 220}{300 - 220} = \frac{x - 220}{80}$$

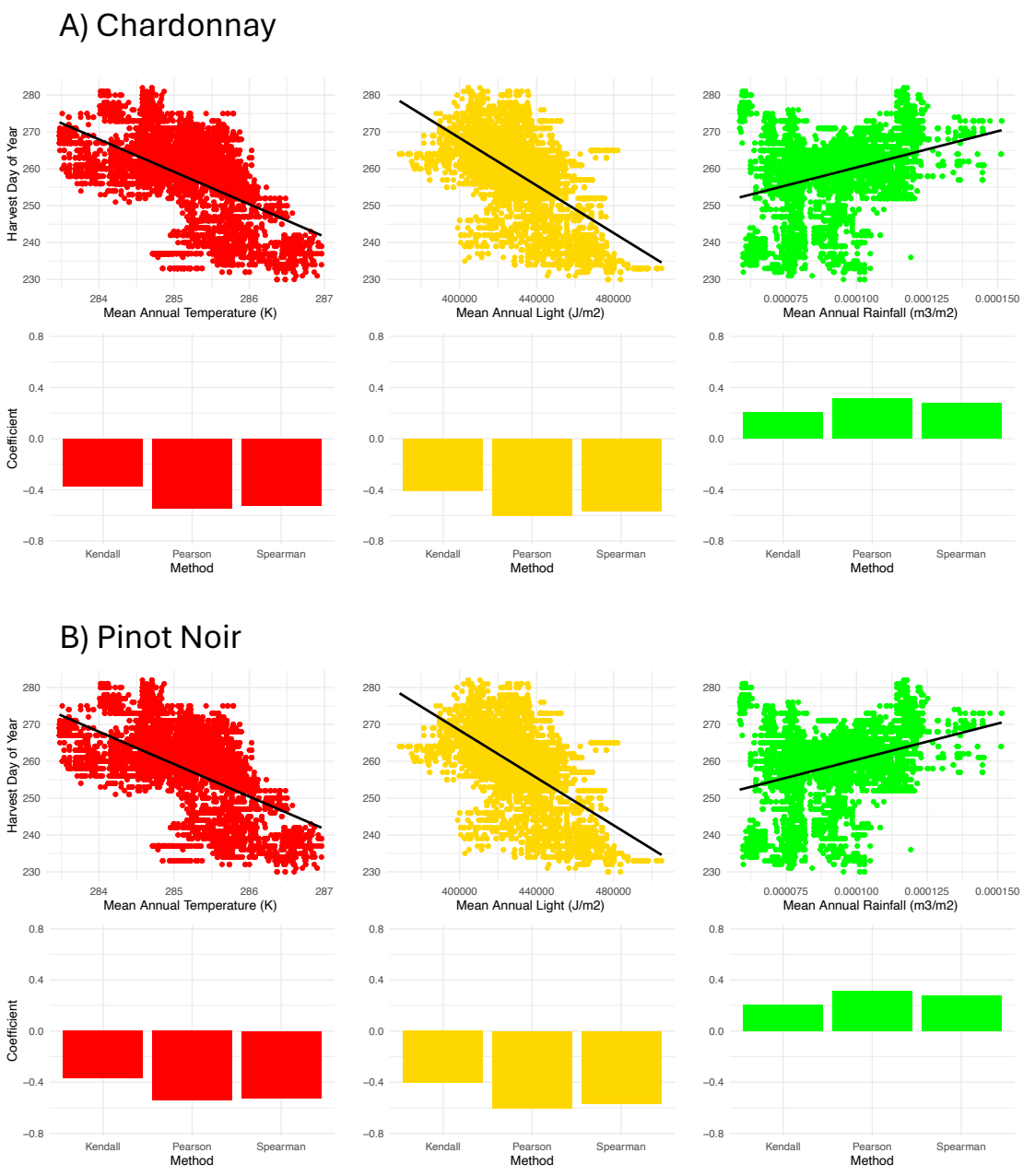
Where x is the optimal day of year to harvest the grapes.

Supplementary Figure 1

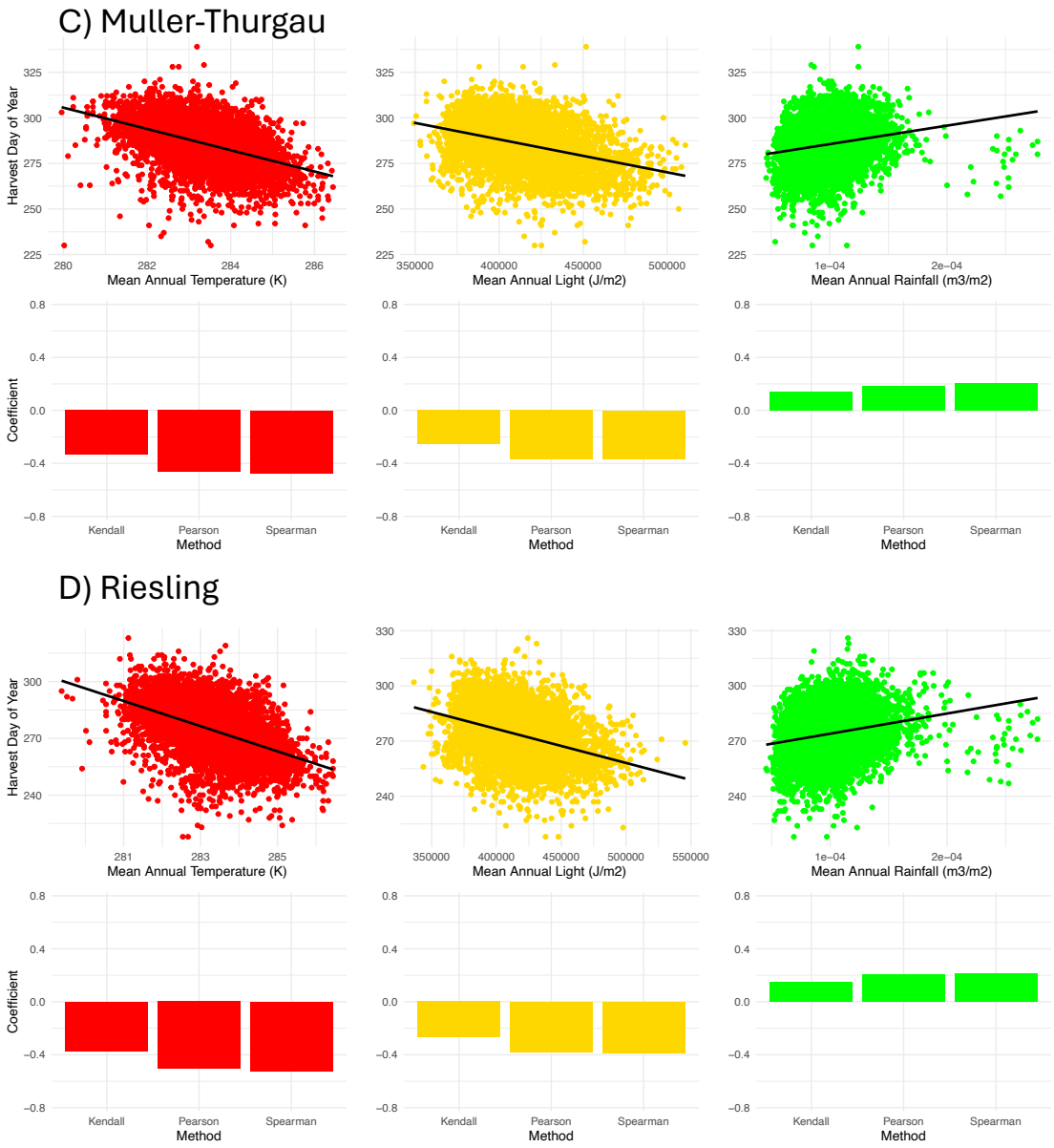


Supplementary Figure 1: Daily Pearson's correlation coefficient between each of the three climate variables – mean daily temperature, mean daily light and total daily precipitation for all locations in the Champagne region, France, and Germany.

Supplementary Figure 2

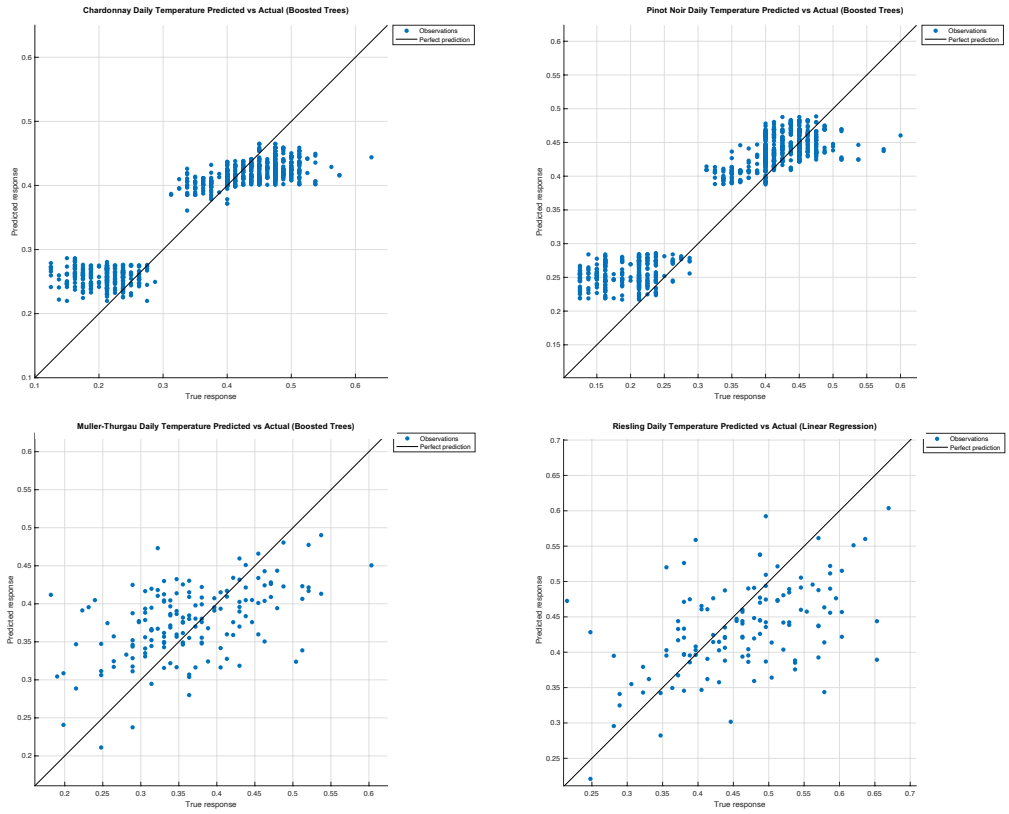


Supplementary Figure 2: Correlation between annual mean temperature, light and precipitation and the day of harvest for all locations in the Champagne region, France, and Germany. Correlation determined by Pearson's, Spearman's, and Kendall's correlation coefficients.



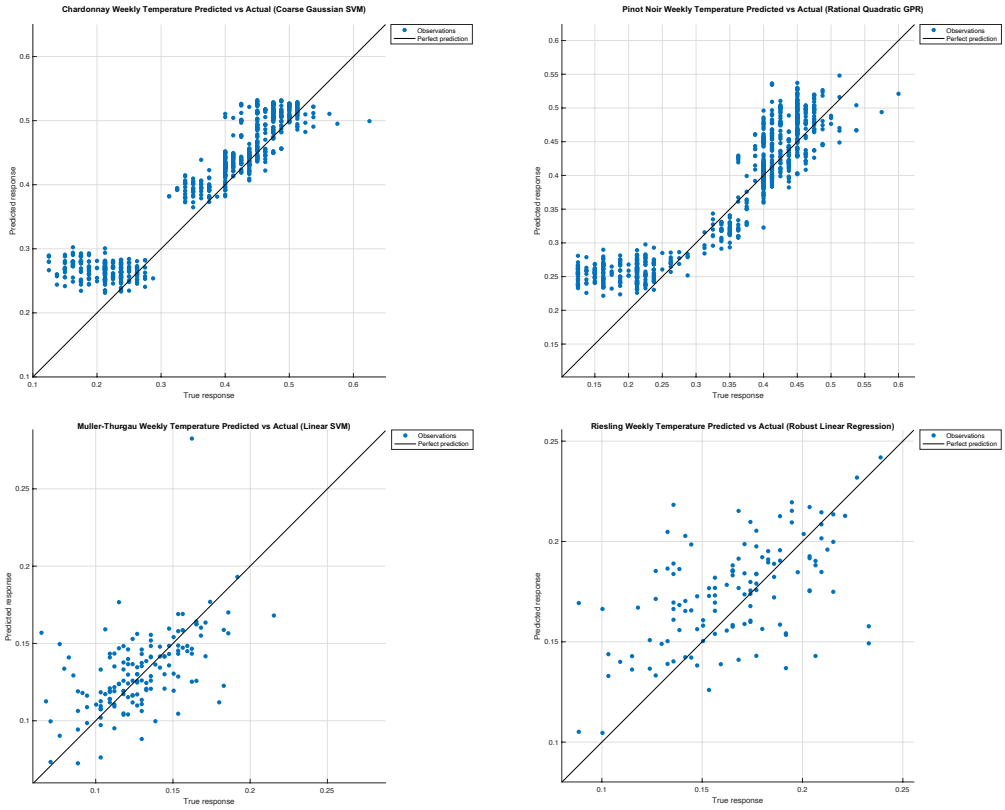
Supplementary Figure 2: Correlation between annual mean temperature, light and precipitation and the day of harvest for all locations in the Champagne region, France, and Germany. Correlation determined by Pearson's, Spearman's, and Kendall's correlation coefficients.

Supplementary Figure 3



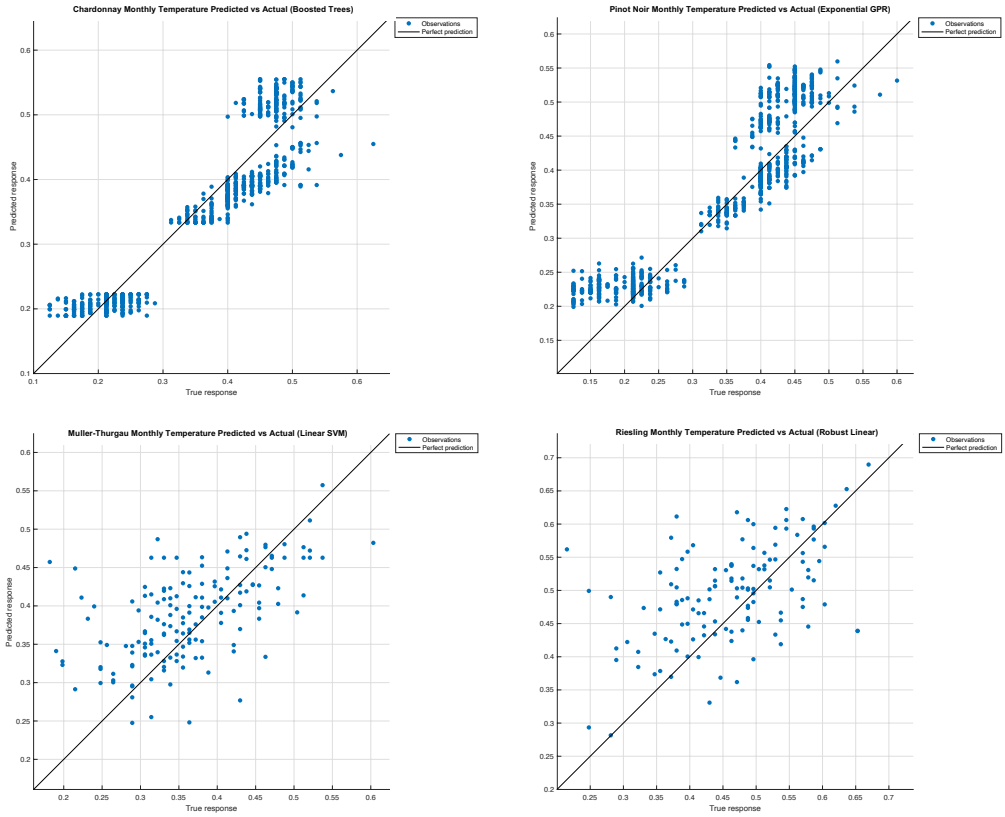
Supplementary Figure 3: Predicted vs Actual Plots for Daily Temperatures for test data set (2019-2021) for best prediction method (C: Boosted trees, PN: Boosted trees, MT: Boosted trees, R: Linear Regression)

Supplementary Figure 4



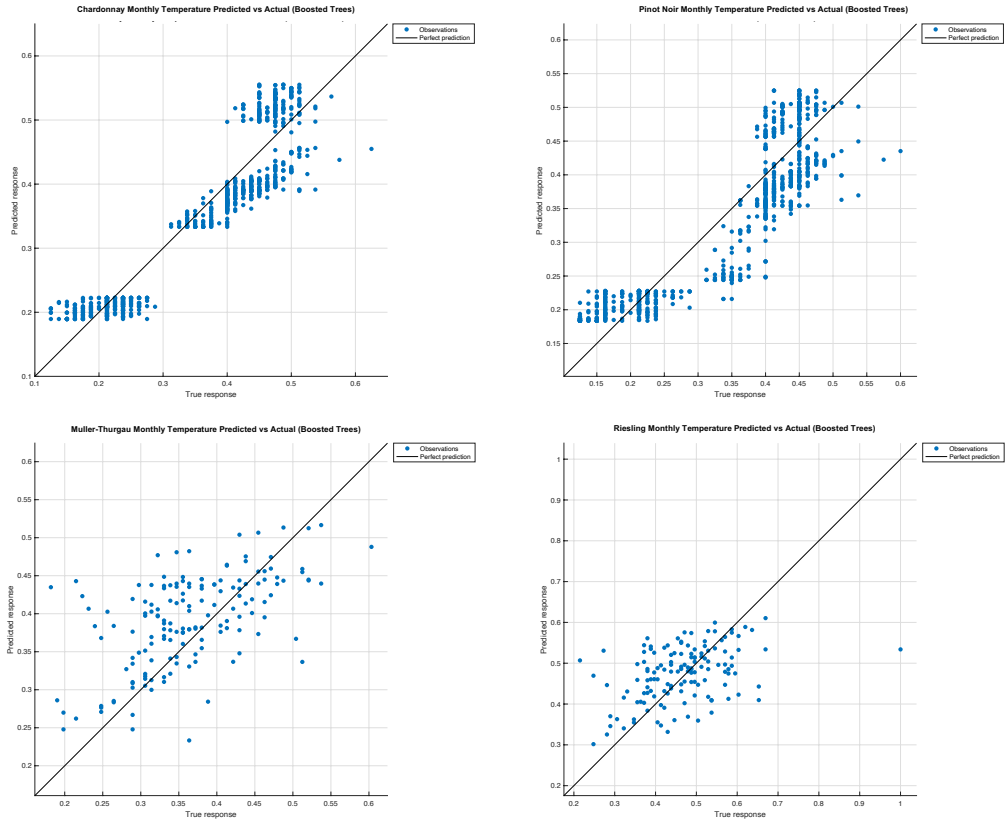
Supplementary Figure 4: Predicted vs Actual Plots for Weekly Temperatures for test data set (2019-2021) for best prediction method (C: Coarse Gaussian SVM, PN: Rational Quadratic Gaussian Process Regression, MT: Linear SVM, R: Robust Linear Regression).

Supplementary Figure 5



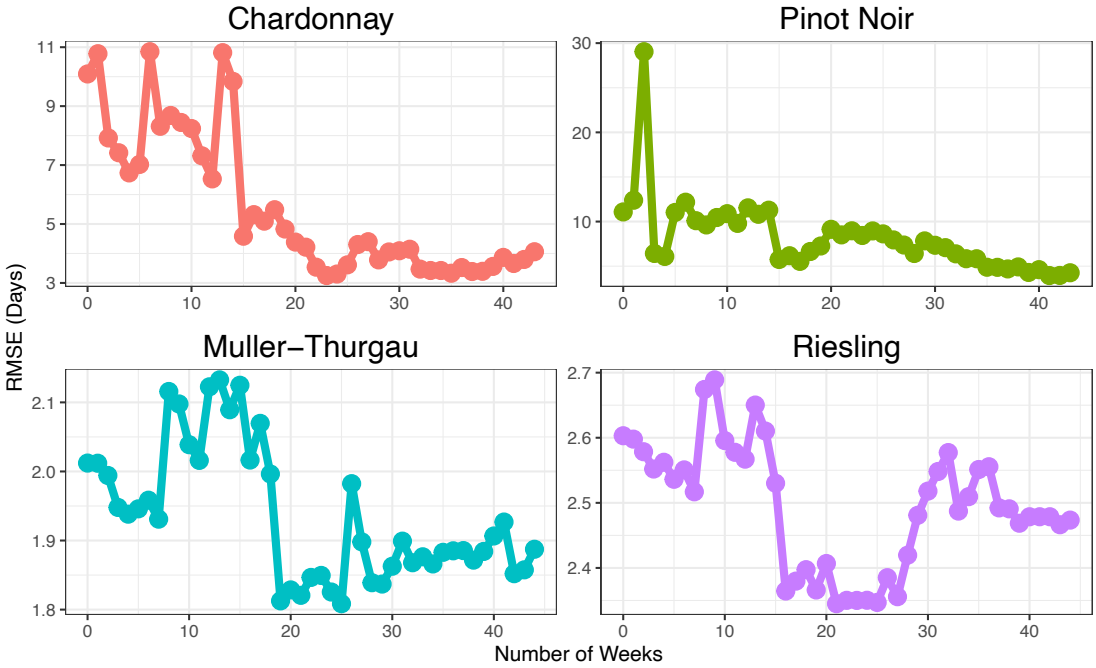
Supplementary Figure 5: Predicted vs Actual Plots for Monthly Temperatures for test data set (2019-2021) for best prediction method (C: Boosted trees, PN: Exponential Gaussian Process Regression, MT: Linear SVM, R: Robust Linear Regression).

Supplementary Figure 6



Supplementary Figure 6: Predicted vs Actual Plots for Monthly Temperatures for test data set (2019-2021) for boosted trees method.

Supplementary Figure 7



Supplementary Figure 7: Error of models trained with a weekly increasing quantity of data to determine the optimal time to predict the harvest date shown as individual plots.

5

Wine on the Move: Mapping the Shifting Terrains of Global Wine with Distribution Models

Words in Abstract: 147
Words in Chapter: 7987

Abstract

Climate change is expected to change the global distributions of wine growing regions. Regions vary in their quality, with variation in price resulting. We explore the predicted changes between different grape varieties at different price points. Our models predict that different priced wines of the same grape variety will respond differently under predicted changes in climate conditions. Three scenarios of range change are predicted: shift, contraction, and expansion (including persistence *in situ*). The predicted shifts raise potential challenges for some high-value wine producing areas (e.g. Napa and Sonoma). The poleward expansion into Northern Europe, South Central Chile, New Zealand, and Tasmania also raises possibilities for some burgeoning wine industries to rise further into the highest priced wines. Some persistence of current high-value regions (e.g. Bordeaux and Barossa) is also expected. Overall, this paper suggests a complex narrative when quality-through-price is considered in the ever-changing context of climate.

Introduction

Anthropogenic climate change is causing species distributions to shift primarily towards the poles[1–4]. This means there is a general trend that northern hemisphere species tend to move northwards, and southern hemisphere ones southwards[1-4]. However, more recent syntheses question the extent of this generality, with differences in rate and extent of movement being questioned[1,4]. Differential rates of species range expansion, contraction, and persistence suggests variation in the ranges of different organisms over time, and thus a necessity for specific models. This is particularly true for longer lived plants, whose ability to spatially move is restricted and persistence is key for longevity. Grape vines are one such heavily restricted plant, with vineyards requiring planting for multiple years before harvesting is possible, and higher quality grapes often coming from so-called "old vines" which can be anywhere between 30 and 400 years old[5,6,7].

There is a complex and multifaceted relationship between viticulture and anthropomorphic climate change. The forecasted increases in temperature are projected to have differing impacts on various parts of the world, with changes in land available for growing wine grape vines projected to decline between 18-65%, depending on severity climate projection and type of model used[8,9]. But the increasing temperature has also been predicted to increase quality[10] in some current areas of vineyards, and hence quality must be considered when predictions are being made. The quality and climate considerations are especially important given the global area under vine is currently declining[11]. This is not just because of climate change but also due to declines in consumption of wine leading to vineyards being replaced by other more profitable crops[12]. The change in trend means that there is an increased

preference for higher quality and thus more expensive wines. Accordingly, when models are being produced it is important to include the quality of the wine being produced. Wine quality can be measured in multiple ways, with critics scores[10], molecular concentration[13], and price[14] all demonstrating different aspects of quality.

Whilst quality varies by space and time, it also varies by grape variety, with each variety having its own recognised hallmarks of quality[5]. Whilst there are estimated to be 6000 grape varieties globally[15], it has been traditionally recognised that there are between 9 and 18 noble grape varieties[5]. International grape varieties are those varietals that are grown globally and have a reputation for making high-quality wines. The original 9 international varieties are Cabernet Sauvignon, Chardonnay, Chenin Blanc, Merlot, Pinot Noir, Riesling, Sauvignon Blanc, Semillon, and Shiraz (called Syrah in Europe), but more modern interpretations also include Muscat, Sangiovese, Viognier, Grenache, and Malbec[5].

Species distribution models seek to explore the range of spatial environments in which an organism can exist[16-18]. These spatial environments are predominantly characterised through their climatic conditions as climate envelope models but can also include any landscape factors from soil to biotic interactions[16-18]. Species distribution models are rarely built for agricultural species as agricultural systems are non-natural systems which are modified to control ideal growing conditions[19]. Vineyards are an exception to this, in which dry farming is widespread, especially in Europe, and local conditions make up the *terroir* which drives the flavour and quality of the wine.

This paper asked where the high- and low-quality wine growing regions for noble grape varieties would exist in 2100. It firstly used a distribution modelling approach to understand the meteorological (weather) and pedological (soil) relationships between vines and their immediate environment, and then projected this to a global scale to visualize and understand the current locations of producing wine. These relationships were then explored in a range of future climate scenarios by projecting the relationships forwards through climatic time. This was undertaken to understand the overall changes in global distributions of wines of varying quality with future climate change**.**

Accordingly, this paper uses price data derived from the LivEx wine price database (LWIN)[20] and explores the spatial distribution of prices in both the then-current and future predicted climates. It uses a species distribution modelling approach with climate and soil characteristics to explore the impact of changes in climate on the areas in which different qualities of wine could be produced, exploring how different intentions impacted the wine.

Methods

This investigation used a Species Distribution Model (SDM) approach to explore the impacts of changing climates on global wine quality. It used the mean price of individual wines sold over the last six months, bioclimatic weather variables, and clay and gravel contents of the soil to create maximum entropy (MaxEnt) models of wines of different grape varieties and quality levels. These niches were then forecasted into the future to create understandings of the changing niches of wines from now until 2100.

Mean Prices: The Liv-ex Wine Identification Number (LWIN) dataset provided global wine price data over the six-month period between May-November 2023 to create an accurate current price of each wine[20]. Liv-Ex draws price data from 620 merchants globally, and therefore comprises the largest real-time price dataset for wine[20]. In the last 6 months, 13124 wines from 7 international grape varieties had been traded, and the mean price for each wine was calculated. These grape varieties were Cabernet Sauvignon, Chardonnay, Muscat, Pinot Noir, Riesling, Sauvignon Blanc, and Shiraz. These grapes were then split into quality quartiles based upon their mean price during the last 6 months (and halves in the case of Muscat as there were many fewer wines).

Geospatial: Geospatial information was acquired through the Google Maps API using the *googleway* package in R[21]. This API provided the location of wineries, for which location specific data could then be ascertained. Bioclimatic weather variables were drawn from WorldClim: a partly spatially interpolated, global-gridded, and monthly climate dataset on a high resolution[22]. SoilGrids was used for soil data as it is

as a standard reference dataset of global soil information for multiple depths on the same gridded co-ordinate reference system as Worldclim. A 2.5 arc-minute resolution was chosen for both as it represents an area small enough that it can give precise information about the wine growing regions but is large enough to have a higher probability of including multiple vineyard plots as well as wineries[23].

Bioclimatic weather variables: Covariance analysis was conducted for each of the 19 bioclimatic variables and 6 soil variables (clay percentage of total soil, total nitrogen (cg/kg), gravel (cfvo, volumetric fraction) at 30-60cm and 100-200cm depth). In this analysis, each variable is plotted against each other and compared using Pearson's correlation coefficient. The threshold for keeping a variable was set at 0.5[24] to retain variables with the lowest covariance. In this way 5 variables were chosen to be used in the distribution models: Temperature Annual Range (BIO7), Mean Temperature of Warmest Quarter (BIO10), Annual Precipitation (BIO12), clay % between 30-60cm and gravel (Volumetric fraction of coarse fragments (> 2 mm)) between 100-200cm. These were plotted against each other to look for clustering and trends. We also used a linear model to examine the bioclimatic variables against each other with the quality quartile included. This enabled us to examine if higher qualities had a different statistical relationship with climatic variables or if we could use the same approach for all models.

The Species Distribution Models were built using a maximum entropy machine learning model (MaxEnt) function (*maxent*) in the package *dismo* (version 1.3-9)[25] using R statistical software (version 4.2.0)[26]. MaxEnt models use presence and pseudo-absence data to find the probability distribution of maximum entropy, given the constraints imposed by the environmental variables. The default hyperparameters

were used to give the most generalisable model across grape types and allow best comparison between grapes and models. MaxEnt was chosen over linear regression and general additive models (GAMs) as it can generate a tighter fit to the current wine regions whilst the regularisation parameters prevented overfitting.

To build the model, pseudo-absent points were generated by sampling three times the number of presence points from the background (i.e. non-winery locations). This was done using the spatSample function from the package terra (version 1.7-55)[27]. This is to ensure there are enough background points to form a suitable MaxEnt model[28,29]. These presence and pseudo-absence points were then used to create a MaxEnt model, with the default hyper-parameters. These MaxEnt models took the non-covarying variables and the occurrence/absence data for each quartile of each grape and fitted the optimal current climatic and pedological niche for each. 10833 samples in total were used for training, and 2291 were used for validation.

Once built, the models were validated by visually comparing to known current distributions. It was also possible to explore the relative contribution of each factor through their loading in the model. Then, to explore potential shifts in wine distribution under future climate, the same MaxEnt model was applied to future HADGEM climate predictions for three future 20-year periods (2040-60, 2060-80, 2080-2100) under a moderate climate change scenario (Shared Socioeconomic Pathway 1.26) [22]. This new climate data was on the same spatial scale and using the same bioclimatic variables as WorldClim[22]. In this pathway there are few challenges to mitigation and adaptation, and thus the impacts of climate change are less severe.

Three of the regions containing the most expensive wines per grape were chosen to be focused on for the main figures to illustrate three potential outcomes found in the

models. However, the global models have been made available via the accompanying shiny app. This shiny app viewer has been made whereby any point on the globe can be viewed for 20-year periods between current and 2100.

Results

The famous global wine areas of California, Europe, Australia, New Zealand, South America, and South Africa are well represented in the dataset (Supplementary Figure 1), In Supplementary Figure 2, two distinct global bands of high concentration of vineyards can be seen at around 50 degrees north and south of the equator. Within each continental wine area, famous wine growing regions are also possible to be determined, with clustering of different grapes in each of the regions – for example Riesling vineyards in both Mosel and Rheingau in Germany, or Chardonnay in Chablis, France and in Margaret River, Australia. It is worth noting that there are also exceptions in location to these major regions, with Mexican, Lebanese, and Chinese wines all being represented in the dataset.

The price of wines within the dataset approximately forms a normal distribution when plotted on a log-x-axis scale (Figure 1). The two most expensive wines in the dataset are from Riesling grapes, at around $150,000 a 6x75cl case (Table 1). This is followed by Cabernet Sauvignon, then Muscat, Chardonnay, and Shiraz. Pinot Noir and Sauvignon Blanc were found to have the smallest maximum price. Muscat and Shiraz are the least well represented in the database in terms of numerical quantities of wines. Each of the top two wines for each grape came from the same region, with Europe being the highest for 4 grapes (Cabernet Sauvignon, Chardonnay, Muscat, and Riesling), Australia and New Zealand for two grapes (Pinot noir and Shiraz), and North America one (Sauvignon Blanc; all as seen in Table 1). The mode of the whole dataset is $103 ($17.16 a bottle), and mean is $816.23 ($136 a bottle).

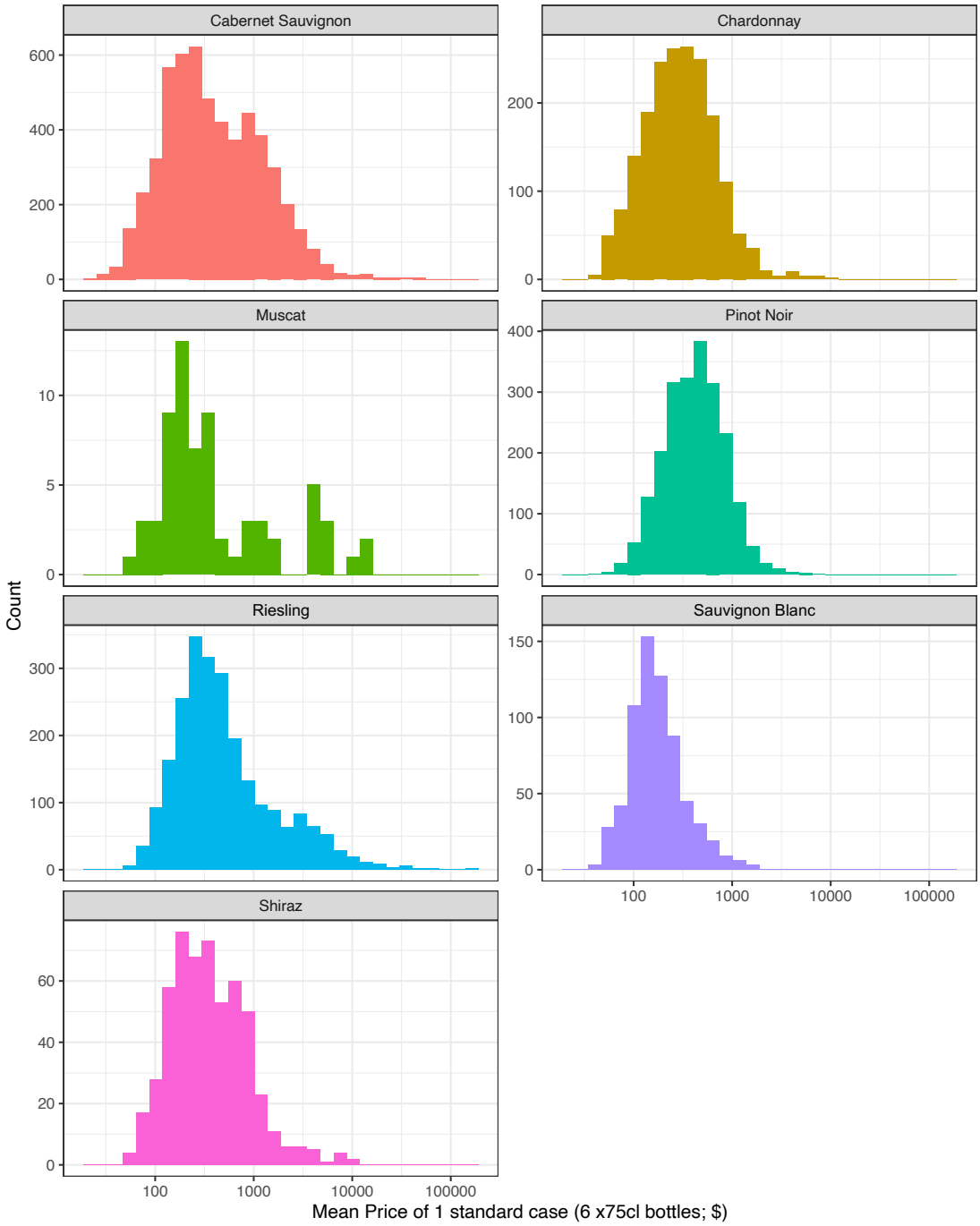


Figure 1: Price distributions of wines in the LWIN database split by grape variety

There is low covariance between the climatic and pedological variables selected (Supplementary Figure 3), the largest magnitude of the Pearson's correlation coefficient being 0.455 and the lowest 0.009. There is high overlap of the climatic niche for all wines (Supplementary Figure 4), with individual wines failing to cluster based on price bracket or grape variety. When the means of each group (grape and price quality quartile) are plotted there are some grape clusters which can be observed qualitatively (Supplementary Figure 5). Supplementary Figure 5 suggests that Shiraz grapes on average prefer lower rainfall and a hot, invariable, environment, whereas Riesling prefers cooler and drier. Price quartile does not generally correlate with any climatic variable in this instance. Examining the graph there is a qualitative appearance of a correlation between more extreme climate spaces (drier, hotter, more seasonal) and higher band of price, but this is not a true distinction and was found to not be a statistically significant relationship (Table 3).

The Maximum entropy models built are primarily driven by the two temperature climatic indicators to build the model (Temperature Annual Range (BIO7) and Mean Temperature of Warmest Quarter (BIO10)). These two factors had mean model loadings (the proportion variance explained by each variable) of approximately 40% each, and hence were found to best characterise the niche of each grape (Table 2). Precipitation (BIO12) was found to contribute just 8% of the variation by mean loading, and the clay and gravel compounds just 3 and 5% respectively.

Three distribution patterns emerge from the results. Firstly, and most commonly, a pole-wards shift which is seen in all models. Secondly, a range contraction disproportionately affecting higher or lower quality wines. Thirdly, there could be an

improvement in the growing conditions within and around a single location causing an expansion of the quality area.

The predominant predicted regional trend involves a shift toward the poles—north in the Northern Hemisphere and south in the Southern Hemisphere. This manifests as a higher probability of presence (higher greenness in the Figure) spreading towards the poles over time. This is present in every Figure but is most striking in Figure 2. The poleward shift suggests that the new future of Muscat may be further to the North-East, with strong increases in lands surrounding the Baltic Sea. There is also an increase in the intensity of potential for better wines across all nations of the United Kingdom and southern Scandinavia. These regions currently are viable for the growth of grapes but generally produce grapes which are not fully ripe, and consequentially do not necessarily produce the highest priced wines. The areas that remain or increase in suitability do so to a greater extent for high-price point muscat (Q2) than they do for cheaper muscat (Q1). In this instance, the higher priced wines will move northwards more than the cheaper priced wines. More broadly, the shift north for the Northern hemisphere wines can be further seen in Supplementary Figures 8, and 10 and for the Southern hemisphere in Supplementary Figures 6, 7 and 9.

As the future climate warms there is also predicted to be a contraction within the current winegrowing regions and a decrease in probability of presence. This can again be seen in Figure 2, with the decline in suitable areas for Muscat in the South of France, Spain, and the coastal regions of Italy. There are also declines in regions of Greece, Croatia, and the eastern regions of Crimea, Turkey, and Georgia. Crimea is where the most expensive muscat wines in the database are from, and strong declines

are expected over the north of the region with the predicted outcome by 2100 being just a small coastal region around the current winery location left.

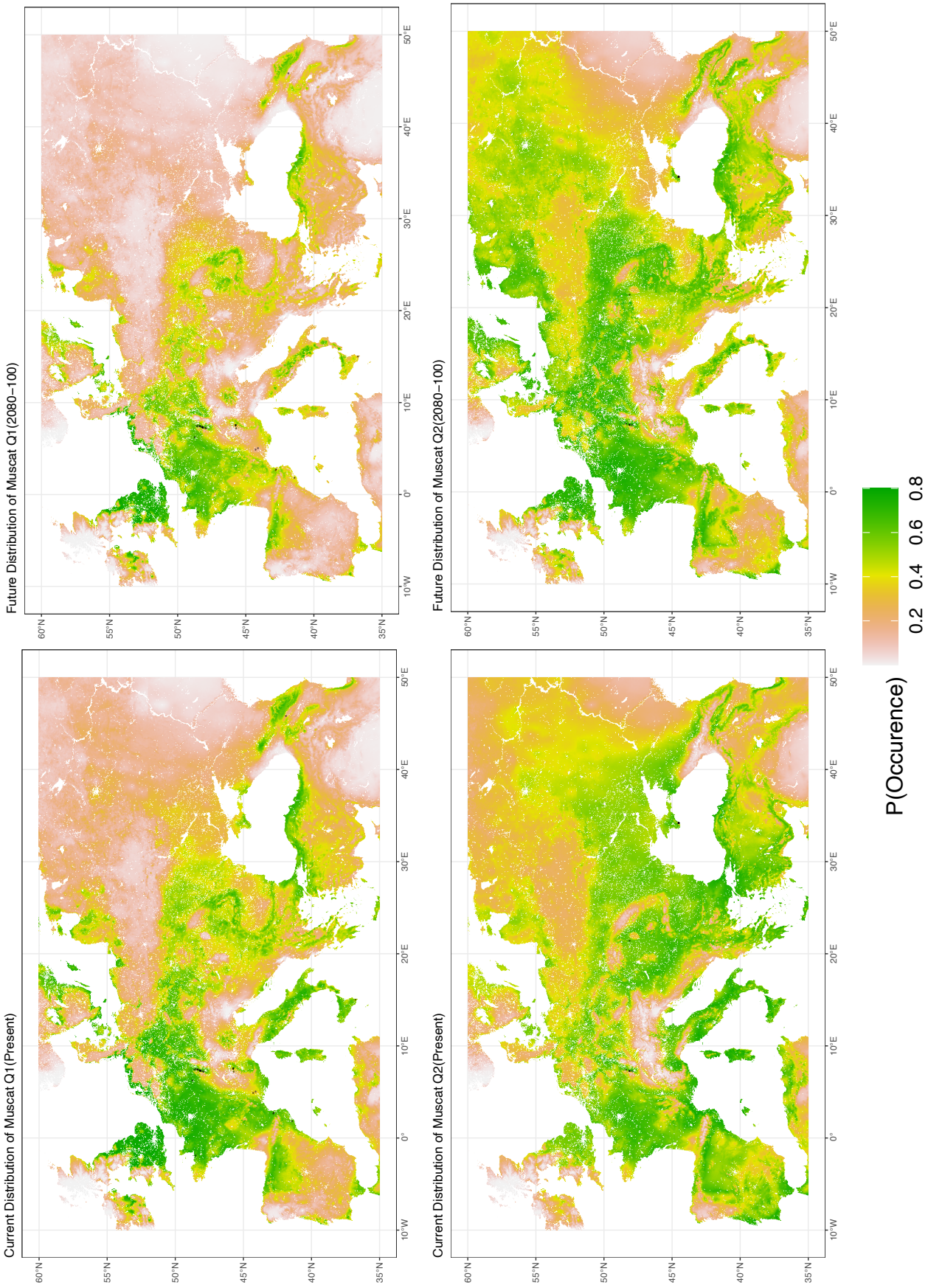


Figure 2: Current and future (2100) European distributions of low (Q1) and high (Q2) quality Muscat wines (HADGEM Predicted climates under SSP 1.26)

At the very extremes, this second scenario of a predicted range contraction can lead to the prediction for a complete disappearance of suitability for growing the same value grapes in a wine region. This can be seen in Figure 3 where the central valley of California is predicted to completely lose all suitability. This prediction therefore suggests the complete loss of grape suitability for parts of the Napa and Sonoma valley wine regions. The predicted declines in the more coastal regions are also dramatic, with most of the current high-quality wine regions contracting to just the very coastal areas of California and more southerly regions being lost completely. Whilst the current distribution of Sauvignon Blanc is higher in Western United states for more expensive (Q4) wines than it is for cheaper wines (Q1), both are predicted to have a very similar fate in terms of the loss of the central valley (Figure 3). In contrast to European Muscat (Figure 2) where there is a differential response for quartiles, both expensive and cheaper wines for Sauvignon Blanc in Western America are predicted to lose most of their range. Both wines price bands are predicted to be in regions of low suitability by 2100.

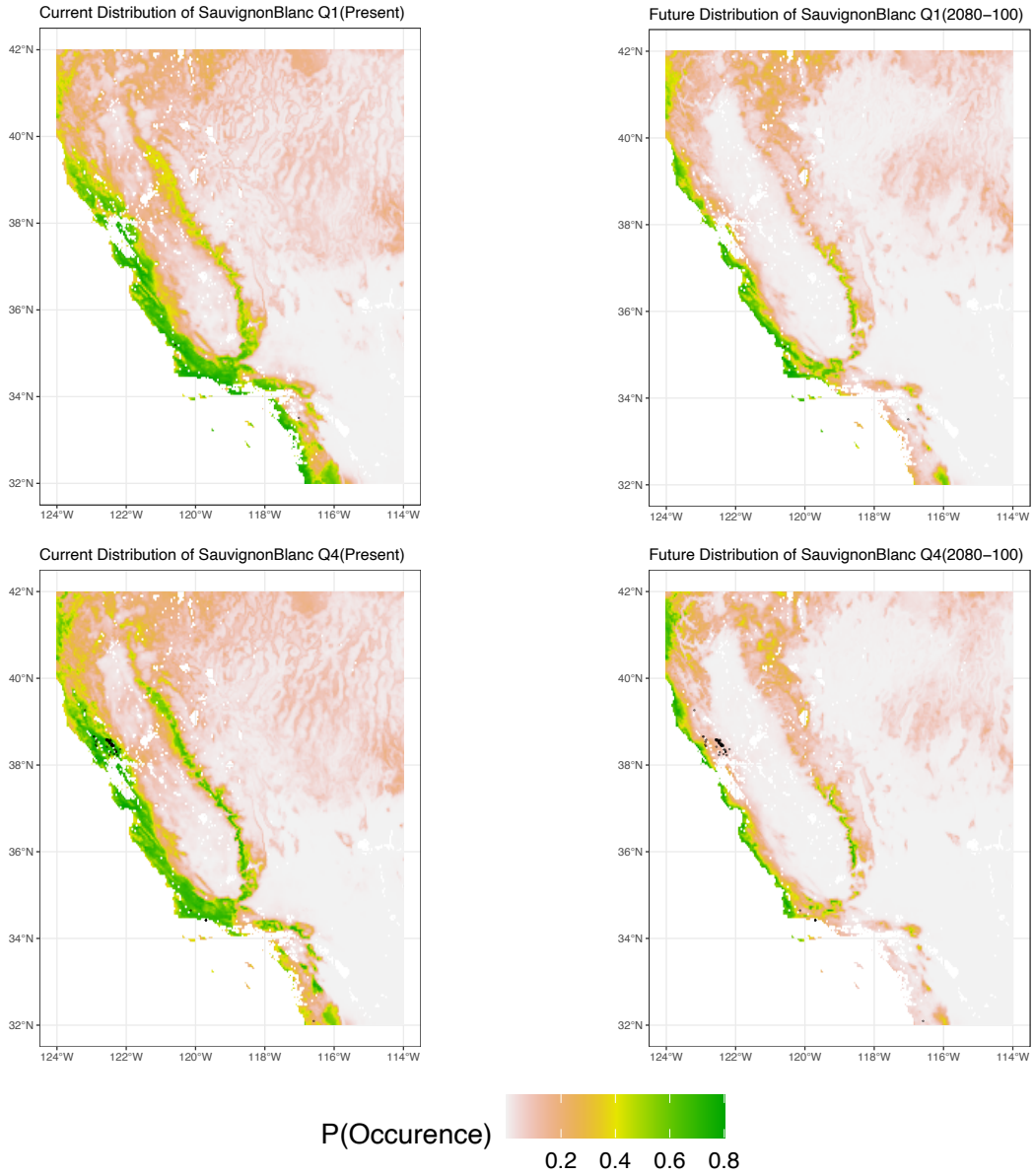


Figure 3: Figure 2: Current and future (2100) West American distributions of low (Q1) and high (Q4) quality Sauvignon Blanc wines (HADGEM Predicted climates under SSP 1.26)

The third scenario is that of a predicted range expansion, which generally includes a persistence *in situ* as well as a poleward shift without a dramatic contraction on the equatorward side. This is the case for Cabernet Sauvignon in Europe, as in Figure 4. For Cabernet Sauvignon it is predicted that Bordeaux as an appellation will continue to remain suitable for both high- and low-priced wines. There are only a few wine regions whose predicted suitability for Cabernet Sauvignon declines in Europe. These are mainly Bordeaux's southerly compatriots in Nouvelle-Aquitaine of Gascogne, Armagnac, and around Cahors. Some areas across Northern Spain and Italy will also be affected, and some areas between Slovenia, Croatia and Hungary which currently form a triangular wine producing area. This is still quite a large area, but what is striking about Figure 4 is the huge swathe of Europe for which suitability remains or increases. Suitability increases in Rhone, Burgundy, Champagne, and the Loire of France; there is higher suitability in Greece, Germany, and Poland (as well as wrapping around the Baltic Sea), and across the Alps of Switzerland and Austria. Turkey retains some suitability too, and the remnants of a highly suitable area run along the central spine of Italy. In short, with a few caveats, the range of Cabernet Sauvignon in Europe will change from Bordeaux, Northern Italy, and Central Europe to the whole of Europe from North to South. This is a dramatic potential for expansion in range.

Whilst for many regions one aspect of expand, contract, or shift is predicted to dominate the future changes; all regions exemplify each of the three distribution scenarios to varying degrees. In the case of New Zealand and Australian Pinot Noirs all three factors are seen in our predictions (Supplementary Figure 6). West Australian Pinot Noir wines are predicted to suffer a fate like the central valley of California's Sauvignon Blanc (Supplementary Figure 6 and Figure 3 respectively) - a dramatic

range contraction. But movement south is predicted to occur for both low- and high-priced wines too, with the Barossa Valley forecasted to remain good for high priced wines whereas the Adelaide hills instead are projected to become less suitable for high priced but still highly suitable for lower value wines. Here again the shift in niche is expected to be different for each price point. Some areas however are still predicted to be suitable. Victoria is estimated to remain a highly suitable area for Pinot Noir of all qualities, and it is predicted that both price points of Pinot Noir will be able to be grown on Tasmania. The greatest increase in location suitability is projected to be in New Zealand. Significant increases in probability of high suitability are forecasted to occur on New Zealand's North Island and along near most the entire eastern coast of the South Island. In the case of this grape in this place, there is a balance between all the potential outcomes.

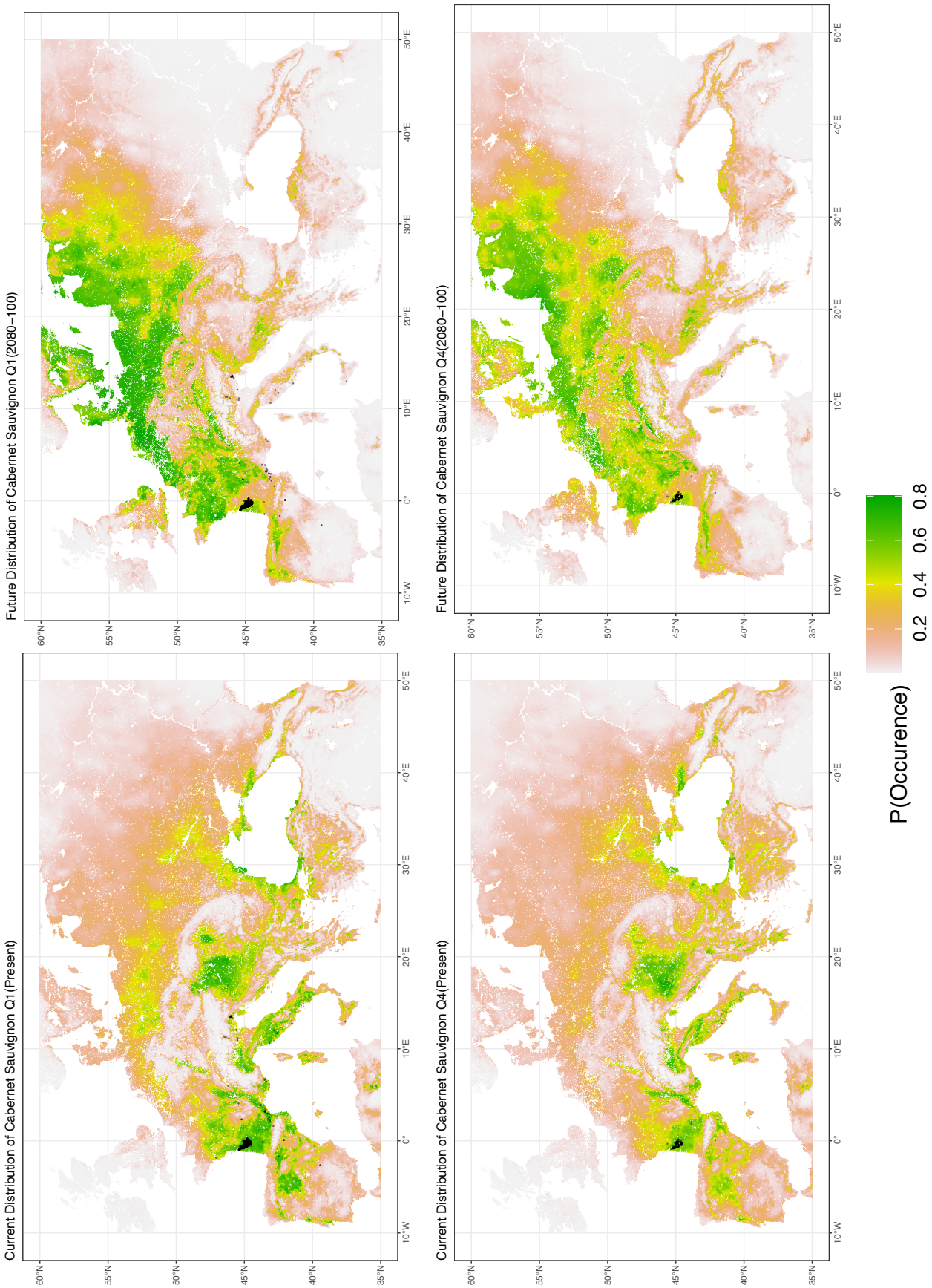


Figure 4: Current and future (2100) European distributions of low (Q1) and high (Q4) quality Cabernet Sauvignon wines (HADGEM Predicted climates; SSP 1.26)

Discussion

This paper considers the changes that are predicted to occur to winegrowing regions globally over the next 80 years. It finds that there are three types of change that are predicted to occur to areas within the global winegrowing regions. These changes can be simply described as expand, contract, and shift. They manifest to varying degrees for different price quartiles in each of the regions worldwide. Ranges were found to expand to fill whole regions or contract until the whole area has disappeared; or somewhere in between. Range shifts were found to move different price bands to different extents globally, with variation between all localities and grape varieties.

Global poleward shifts for future climates have long been predicted in viticultural literature[1,3,8,30–32]. We found them to be present in all regions, varieties, and price bands investigated, however they varied in their extent and directionality. Moriondo et al (2013) previously suggested a north and north-westerly shift in the growing regions for European wines[30]. Whist we agree with the former, we suggest that there are also easterly regions for which we predict there will be an increase in suitability (Figure 2 is the most striking example of this). It has previously been suggested that grapes in such new areas would become lesser in quality[33]. We find this not to be true, with vast swathes of land predicted to be able to produce high priced wines during this period. Previous predictions have also suggested that South American wines will need to increase in altitude to attain the same quality as current wines[34], a prediction our projections disagree with as the forecasted lands instead reach southerly (Supplementary Figure 7).

Global declines in extent of suitability of winegrowing areas were also expected as they had again been widely predicted in the literature[8,9,33]. We concur with such declines in terms of general *in situ* current suitability. We find across broad swathes of current production land on all continents areas that are predicted to be unsuitable for viticulture in 2100. The Central valley of California is one such example, with our predictions correlating with those that suggest that 81% California's winegrowing regions may be lost by 2100[33,35], including 51% of current acreage in Napa and Santa Barbara counties [35]. More recent studies have found that this decline could be rapid, with a 42% loss by 2050[36]. These studies suggest that this is due to lack of water and higher temperatures, the two model variables which drive our species distribution models. Our models suggest widespread loss of Californian suitability, with suitability retreating towards the coast and dramatically southwards towards Bakersfield (Figure 3).

In Europe, there has been widespread suggestion in the literature of declines in suitability for both Bordeaux and central Spain due to forecasted changes in the Gulf Stream[8,33,37]. Our predictions suggest that these two areas may not have the same fate. Our predictions suggest that whilst the central region of Spain and the south-west of France may generally decline in suitability, the high value areas close to the city of Bordeaux will retain their suitability for Cabernet Sauvignon. In South Australia, we concur with previous forecasts that the Murray River may become less suitable for high quality grape production in the future[37], although we predict it is more likely to maintain the suitability for lower-priced wines. We also disagree that McLaren Vale as a region will decline in suitability for high-priced wine production[38], and we predict that for all price points the wine will continue to be viable *in situ*. Pinot noir and Shiraz in South Australia and New Zealand, Chardonnay across much of Europe,

and Riesling in Germany (Supplementary Figures 6, 9, 10, and 8 respectively) are all predicted by our models to have some constancy in their production. But these suggestions of persistence *in situ* for some regions is a phenomenon of islands of constant quality in an ever-present and turbulent sea of change.

The areas which are predicted to be disproportionately affected are those which are on the edges of wine producing regions. For some, like the central valley of California or Nouvelle-Aquitaine in France, this prediction is of a complete loss of suitability for some types of grapes and quality levels. For others, like much of England in the United Kingdom, this may well be a dramatic increase in climate suitability. All our predictions have an implicit assumption that locations do not themselves move between price brackets (e.g. from Q1 to Q2 or vice versa), and that the price bands themselves do not change. It's possible, for example, that an additional bracket that cannot be reached now (due to lacking climatic conditions) exists which makes even better wine, and this would not be possible to be modelled using our approach. Consequently, whilst some areas may be seen as shifting out of a quality bracket, it is not possible to state if this is upwards or down.

This paper has also demonstrated that different grapes may move to different extents. This concurs with a broader framework of differential range shifts across species and populations[1]. This variation in rate and extent was seen in all grape cultivars, and this understanding that different cultivars react differently matches Morales-Castilla et al. (2020) in their findings that different varietals can replace each other in the movement of climate space[39-42]. This variation contrasts with a rule of thumb that was developed by Kenny and Shao (1992) that a 1 degree rise in temperature is a 1 isotherm poleward movement[46]. This isothermal rise was shown as a global trend by Jones and

Alvez (2012) and suggests a reasonably uniform global change in the general climate zones for the global wine growing region[31]. We find this not to be completely valid, and we find there not to be a uniform change for different grape varieties -rather they all move independently. Our new predictions, like all global scale predictions[8], do not consider land use in their future predictions, and thus the local situation may well be unsuitable for wine growing as it may be anything from an urban area to a national park. As with all future predictions, our models are reliant upon the accuracy of the future climate forecasts, as well as having the assumptions built into them of stationarity in the underlying soil data sets.

Across the global landscape, our predictions indicate that the areas for producing different price bands of wines also move. This occurs most strikingly in our predictions for Muscat where the niche for the more expensive wines moves northwards more than the niche for cheaper wines (Figure 2). This is not what is suggested in previous literature, with the outcome of increased climate effects suggested as a switch to lesser quality[33,34]. This is because of the assumption that lower priced wines are made in a less climatically suitable niche. These niches are thought to be larger with any climate change as the niche can be non-optimal for multiple factors and thus the wine is highly likely to be affected[33,40]. Any change in climate will therefore automatically lead to a lower quality wine being produced. But our results suggest a different outcome. They suggest that Muscat is currently less climatologically restricted, and instead there are other factors like vineyard management strategies which are important for the development of these higher-priced wines.

The niches characterised and utilised in this paper were found to be primarily driven by climate. The low model loadings (the relative contribution to the output predictions for each variable) for soil and precipitation suggest that generally grape locations are driven by temperature, which may lead to some over-prediction especially in the future scenarios. However, each variety had very different loadings, with up to 20% variation per variable showing that each variety has very different factors by which it can be characterised. This differential loading suggests different factors which need to be mitigated for, each with different consequences. Moderate dry-farming temperature and irrigation concerns can often be mitigated by changes in watering practises (either addition or restriction), but at more extreme temperatures the controls are often expensive and difficult to manipulate. The model currently does not account for watering practises, and availability of irrigation may be a moderator of these results.

It is also important to consider the local viticultural factors which can lead to changes in microclimate. These mitigation strategies can potentially provide some respite from increased temperatures and the large-scale changes which are predicted to occur. There is also the potential to adjust to new climate regimes through changes in phenology and adjusting ripeness levels[42-44]. The resulting wine that comes from facing these challenges may pose a threat or change to the identity of many wines – with wines becoming generally stronger with hotter climates[31,43-45], but it may then be possible for value to be retained or enhanced in many vineyards.

This paper encapsulates the interplay of climate and vine and speaks to the ever-evolving story unfolding in vineyards globally. Our investigation suggests that bio-envelope models can be built for wine grapes, and thus suggests that there is a role for

using distribution modelling approaches as agricultural modelling tools to explore the impact of climate on crop outputs. The price-identified regions of wine production have been predicted to shift globally, but with variation occurring between varieties and qualities. The predicted redistribution of wine price-quality regions may be better for some regions and worse for others. The predicted shifts raise potential challenges for some high-value, well-established, and well-renowned wine producing areas like Napa and Sonoma in California. But the poleward expansion into Northern Europe, Central Chile, New Zealand, and Tasmania also raises possibilities for some burgeoning wine industries to rise further, with expansion of high value wines into these regions. The noteworthy persistence of certain areas like Bordeaux and Barossa indicates a complex interplay between changing climate and grape niche, with some regions able to persist *in situ*. The climate-linked changes raise the potential need for mitigation in some areas of the world, but also the lesser need for it in others. This paper also predicts new areas for wine to increase in quality in, and thus allow for planning of future increases too. Combined, these changing price-linked wine grape niches offer insight into the ever-shifting terroir of global wine.

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Appendix For Chapter 5

Table 1: Most Expensive Wines Per Grape

Wineries with the highest mean price sold between May-November 2023, registered with LWIN (Liv-Ex), price standardised by 6x75cl bottles

LWIN	Grape	Wine Name	Lat	Lon	Price ($)	Region	Years Covered	Number
1011074	Cabernet Sauvignon	Chateau Gruaud Larose 2eme Cru Classe, Saint-Julien	45.14	-0.75	54776	Europe	1825-2022	115
1011872	Cabernet Sauvignon	Chateau Lafite Rothschild Premier Cru Classe, Pauillac	45.22	-0.77	53581	Europe	1806-2022	118
2483252	Chardonnay	Maison Pierre Overnoy, Chardonnay Savagnin, Arbois Pupillin	46.88	5.76	11830	Europe	1999-2007	2
2164221	Chardonnay	Domaine des Murmures, Chardonnay, VdF	44.07	5.19	9199	Europe	2016-2018	2
1330500	Muscat	Massandra, White Muscat Gurzuf, Crimea	44.52	34.20	13763	Europe	1924	1
1330454	Muscat	Massandra, Pink Muscat Alushta, Crimea	44.52	34.20	13757	Europe	1924	1
1253700	Pinot Noir	Bass Phillip, Reserve Pinot Noir, Gippsland	-38.56	145.88	8239	Aus/NZ	1997	1
1874109	Pinot Noir	Willi Opitz, Pinot Noir Eiswein, Burgenland	47.76	16.80	5952	Aus/NZ	2021	1
1089945	Riesling	Egon Muller, Scharzhofberger Riesling TBA, Mosel	49.65	6.61	151039	Europe	1976-2018	10
1378405	Riesling	Egon Muller, Scharzhofberger Riesling TBA Goldkapsel, Mosel	49.65	6.61	144514	Europe	1990-2001	2
1879700	Sauvignon Blanc	Checkerboard, Estate Sauvignon Blanc, Napa Valley	38.56	-122.55	1641	North America	2020	1
2815598	Sauvignon Blanc	Honig, Sauvignon Blanc Late Harvest, Rutherford	38.47	-122.41	1476	North America	2019	1
1375606	Shiraz	Chris Ringland, Ranges Shiraz, Barossa Valley	-34.56	138.96	10527	Aus/NZ	2008-2013	3
1854718	Shiraz	Penfolds, Bin 111A Shiraz, South Australia	-34.48	138.99	10000	Aus/NZ	2016	1

Table 2: Table Of MaxEnt Model Loadings

Model Name	Training Sample Size	Loading in MaxEnt Model (%)				
		cfvo	clay	bio_7	bio_10	bio_12
Cabernet Sauvignon Q1	972.00	8.92	0.43	39.91	42.45	8.29
Cabernet Sauvignon Q2	993.00	8.24	0.23	36.99	41.86	12.68
Cabernet Sauvignon Q3	1099.00	2.35	0.33	37.04	46.03	14.25
Cabernet Sauvignon Q4	1078.00	4.81	0.89	42.10	37.25	14.95
Chardonnay Q1	426.00	4.55	0.52	49.02	45.12	0.79
Chardonnay Q2	422.00	2.98	0.73	44.57	50.96	0.75
Chardonnay Q3	438.00	4.34	0.74	41.77	52.32	0.82
Chardonnay Q4	417.00	4.14	0.56	44.04	44.89	6.37
Muscat Q1	31.00	1.34	3.57	49.37	18.77	26.94
Muscat Q2	31.00	4.44	0.34	29.98	49.45	15.79
Pinot Noir Q1	474.00	2.94	1.46	46.75	48.34	0.52
Pinot Noir Q2	491.00	3.90	3.35	44.45	48.17	0.14
Pinot Noir Q3	508.00	1.90	4.18	44.91	48.83	0.18
Pinot Noir Q4	465.00	1.31	0.16	44.73	51.28	2.52
Reisling Q1	490.00	0.97	5.30	40.08	39.85	13.80
Reisling Q2	493.00	2.24	8.34	37.31	36.59	15.51
Reisling Q3	488.00	6.53	7.91	34.35	37.75	13.46
Reisling Q4	474.00	5.72	7.41	36.38	37.46	13.03
SauvignonBlanc Q1	153.00	3.80	3.89	41.39	46.49	4.43
SauvignonBlanc Q2	144.00	2.67	1.73	42.43	51.49	1.67
SauvignonBlanc Q3	143.00	8.95	1.11	34.17	47.36	8.41
SauvignonBlanc Q4	139.00	7.76	0.83	43.44	44.76	3.21
Shiraz Q1	122.00	7.03	1.02	55.20	35.24	1.50
Shiraz Q2	112.00	4.29	4.94	42.45	42.93	5.39
Shiraz Q3	116.00	6.59	7.08	41.72	31.70	12.90
Shiraz Q4	114.00	8.88	15.87	38.55	26.97	9.74
Mean	**416.65**	**4.68**	**3.19**	**41.66**	**42.47**	**8.00**
Max	**1099.00**	**8.95**	**15.87**	**55.20**	**52.32**	**26.94**
Min	**31.00**	**0.97**	**0.16**	**29.98**	**18.77**	**0.14**

Table 3: Linear Model Outputs

Table 3a: Model 1 (bio7 ~ bio12 + Quartile)

Term	estimate	std.error	statistic	p.value
(Intercept)	22.71	2.11	10.76	0.00
meanBio12	0.00	0.00	1.10	0.28
Quartile2	-0.06	0.65	-0.10	0.92
Quartile3	-0.46	0.70	-0.65	0.52
Quartile4 (Expensive)	0.38	0.70	0.54	0.60

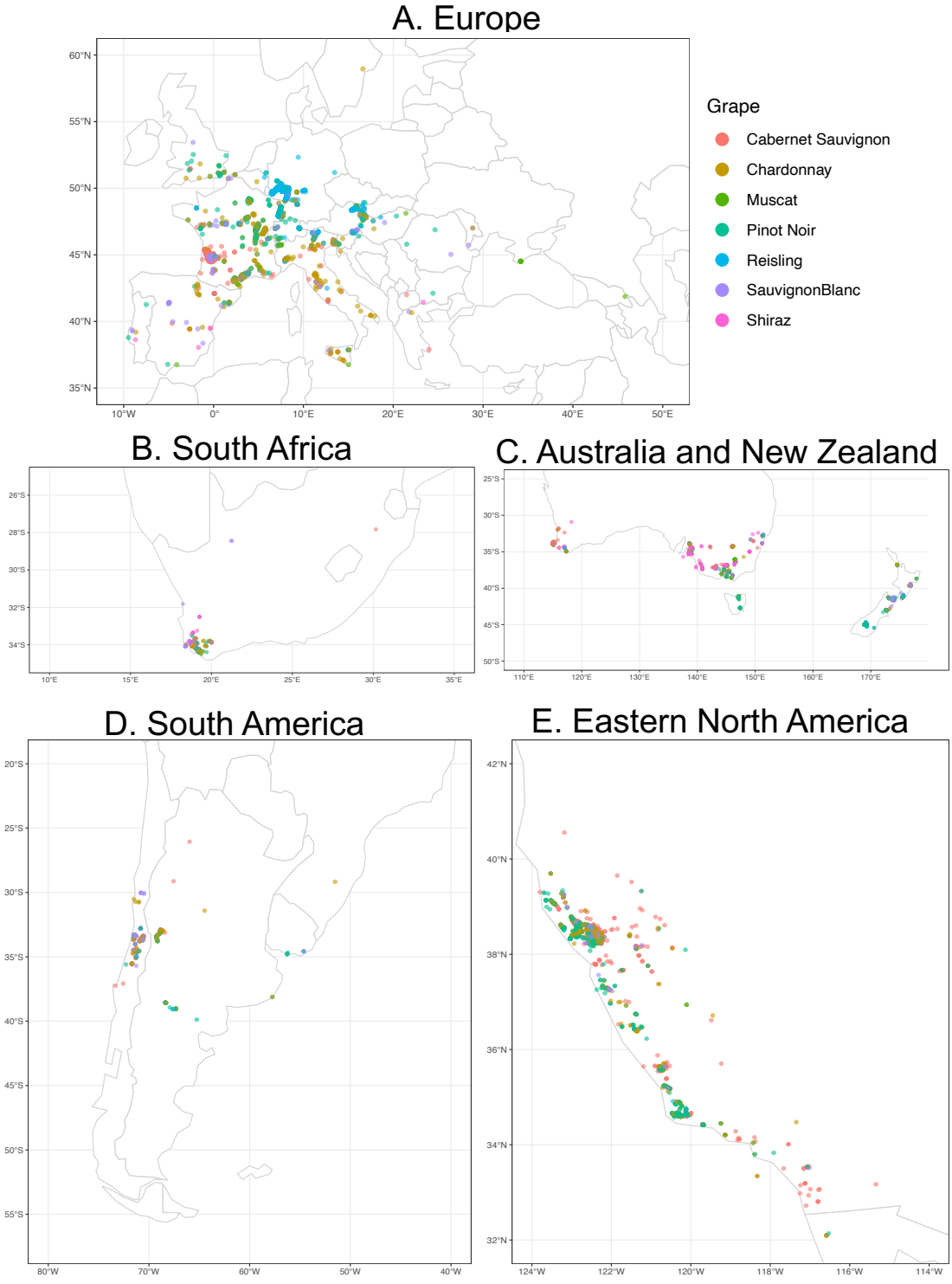
Table 3b: Model 2 (bio7 ~ bio10 + Quartile)

Term	estimate	std.error	statistic	p.value
(Intercept)	24.67	4.94	4.99	0.00
meanBio10	0.02	0.25	0.06	0.95
Quartile2	-0.01	0.67	-0.01	0.99
Quartile3	-0.26	0.71	-0.36	0.72
Quartile4 (Expensive)	0.57	0.70	0.82	0.42

Table 3c: Model 3 (bio10 ~ bio12 + Quartile)

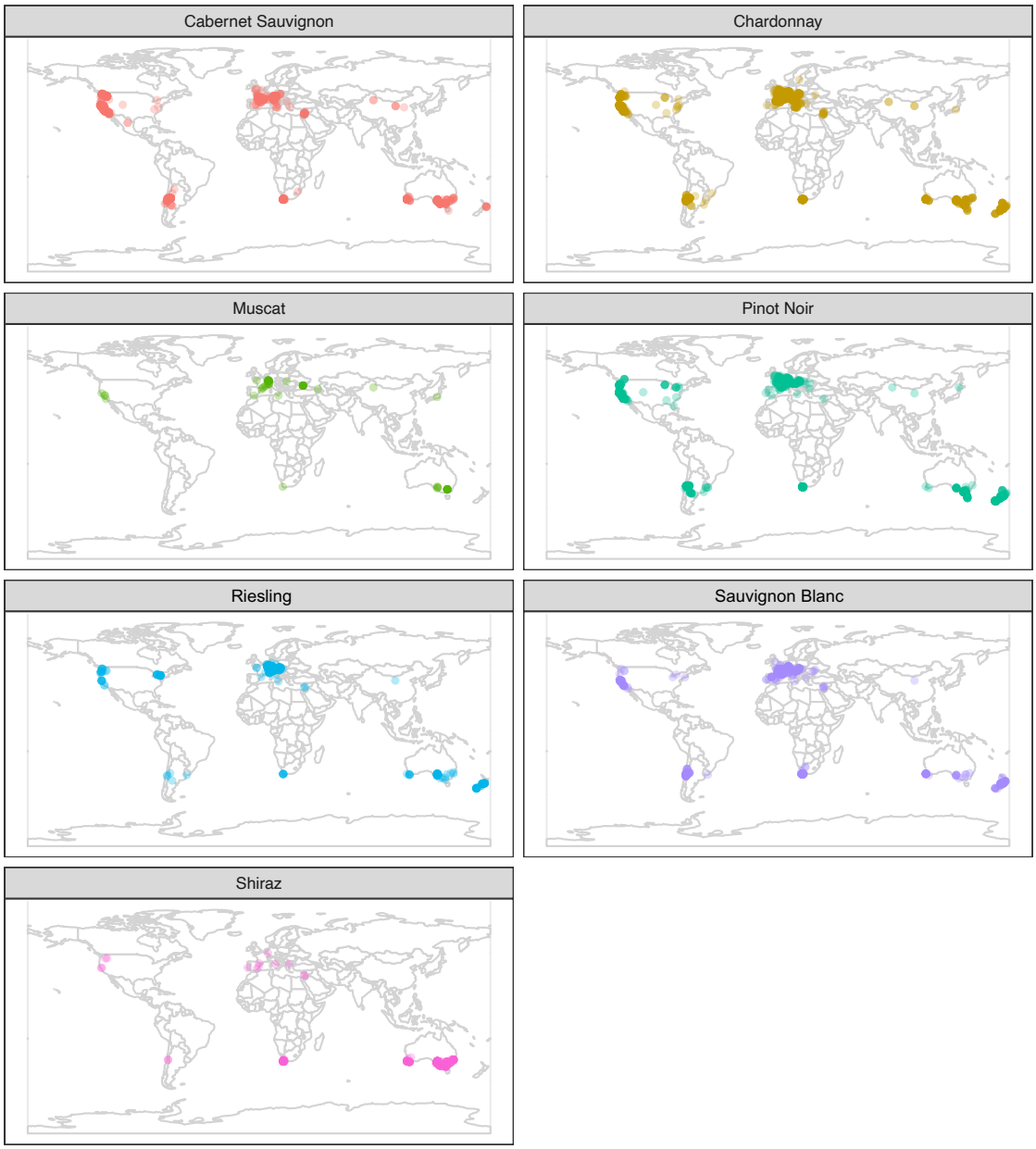
Term	estimate	std.error	statistic	p.value
(Intercept)	21.78	1.83	11.88	0.00
meanBio12	0.00	0.00	-1.18	0.25
Quartile2	-0.04	0.57	-0.08	0.94
Quartile3	-0.26	0.61	-0.43	0.67
Quartile4 (Expensive)	-0.05	0.61	-0.08	0.94

Supplementary Figure 1



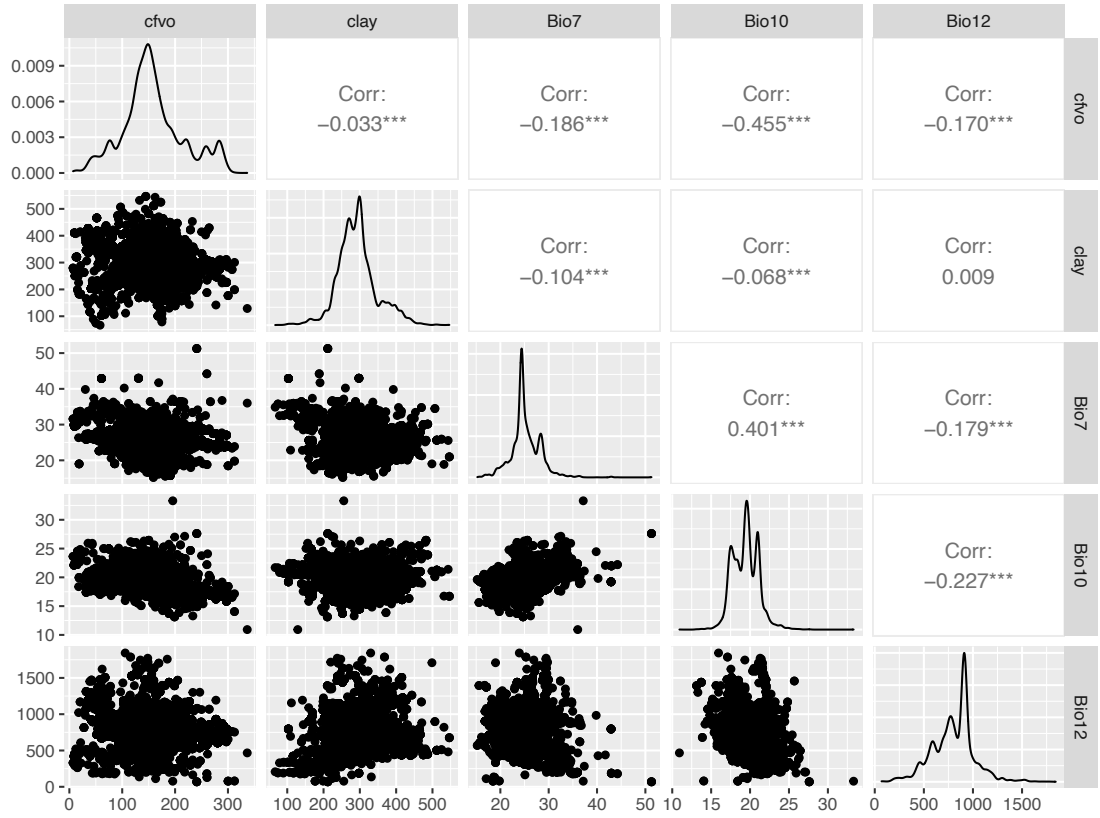
Supplementary Figure 1: Global distribution of wines by continent

Supplementary Figure 2



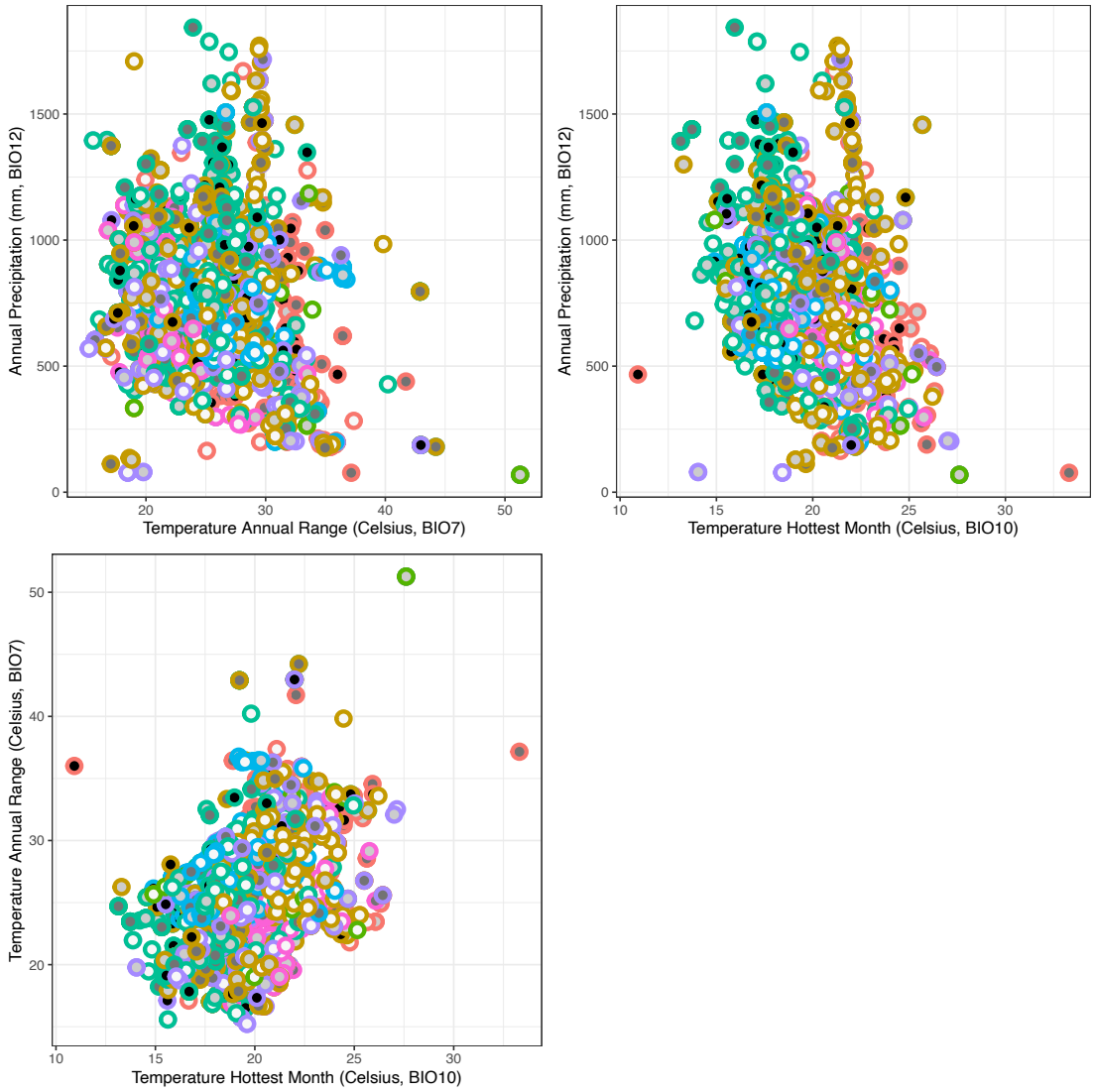
Supplementary Figure 2: Global distribution of wines by variety of grape

Supplementary Figure 3



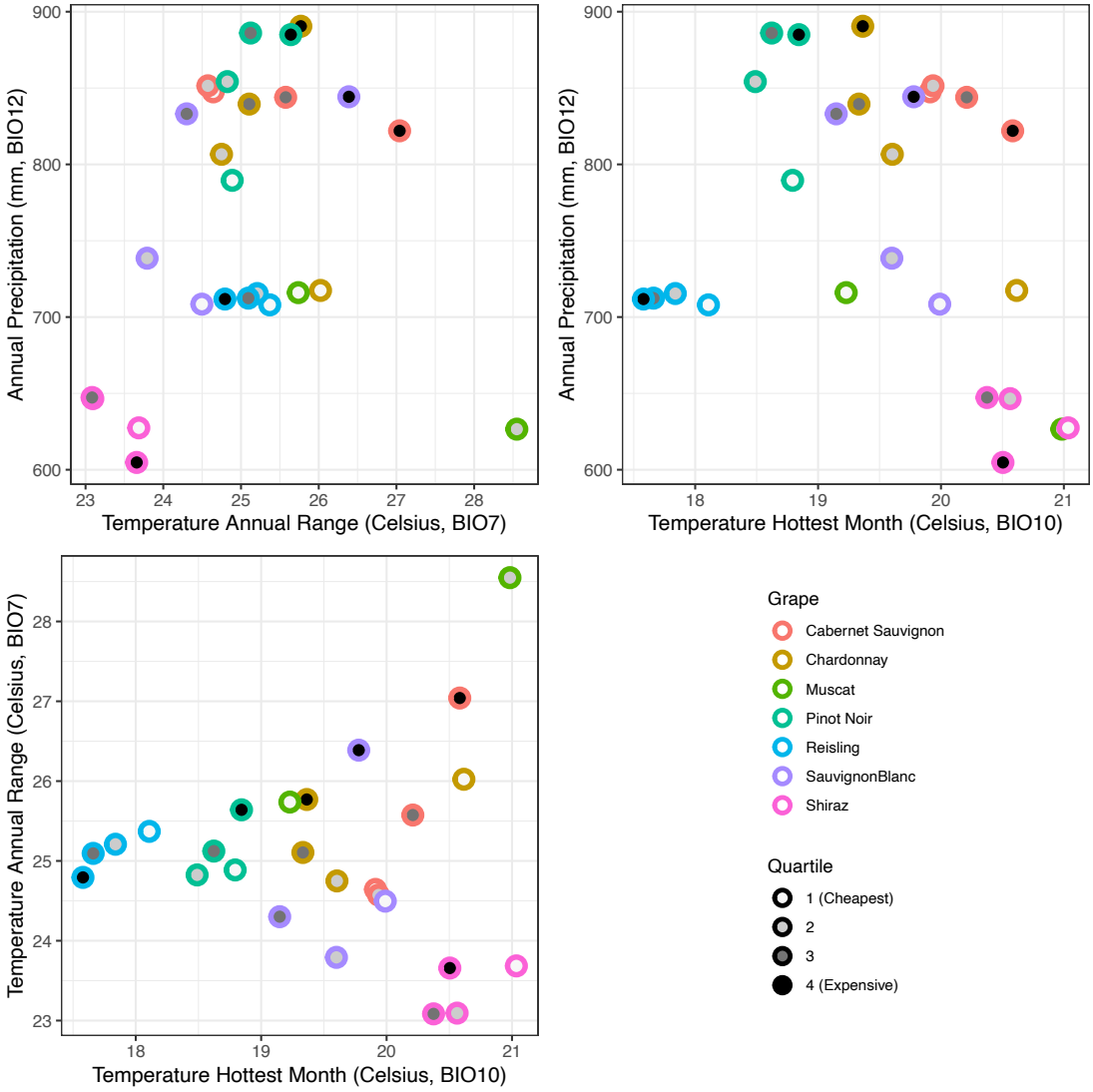
Supplementary Figure 3: Correlation plot of chosen bioclimatic indicators and soil composition. Values are Pearson's correlation coefficient for each indicator. Bio 7: Temperature annual range; Bio 10: Mean temperature of warmest quarter; Bio12: Annual precipitation; clay: Proportion of clay particles (< 0.002 mm) in the fine earth fraction (g/kg) 30-60cm deep; cfvo: Volumetric fraction of coarse fragments (> 2 mm) between 100-200cm deep .

Supplementary Figure 4



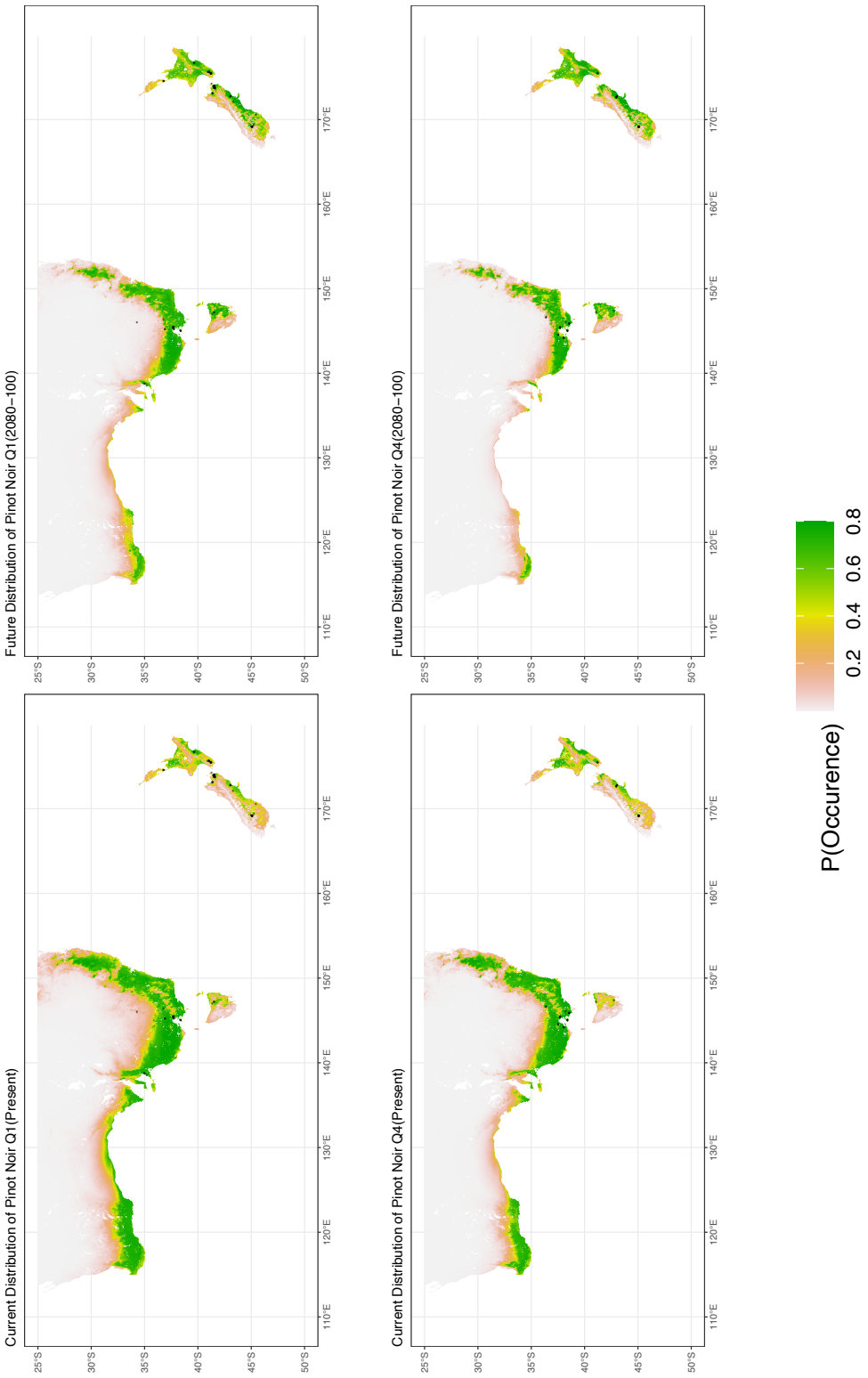
Supplementary Figure 4: Scatter plot of weather variables for all wines. Bio 7: Temperature annual range; Bio 10: Mean temperature of warmest quarter; Bio12: Annual precipitation.

Supplementary Figure 5



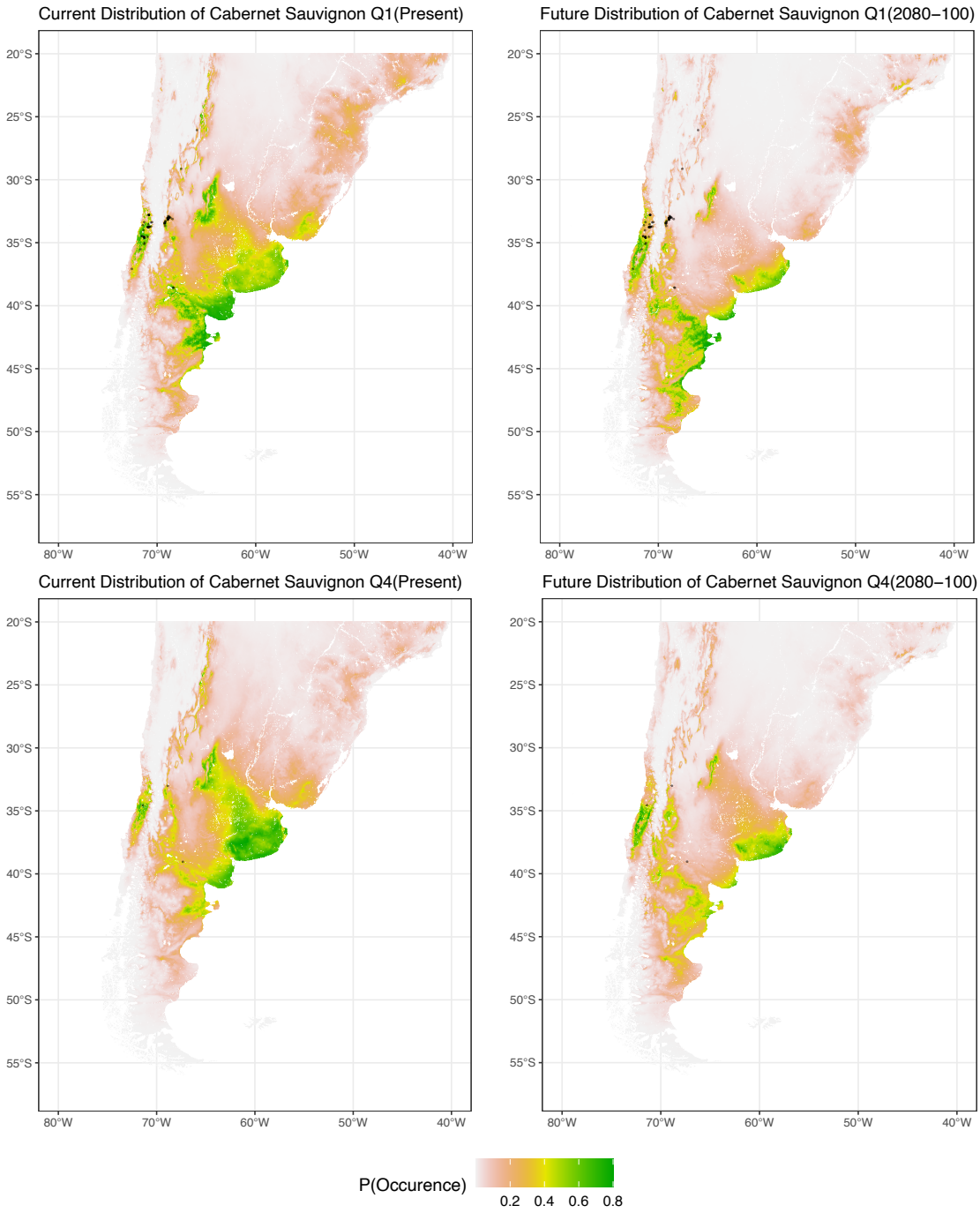
Supplementary Figure 5: Scatter plot of weather variables for wines grouped into variety-quartiles. Bio 7: Temperature annual range; Bio 10: Mean temperature of warmest quarter; Bio12: Annual precipitation.

Supplementary Figure 6



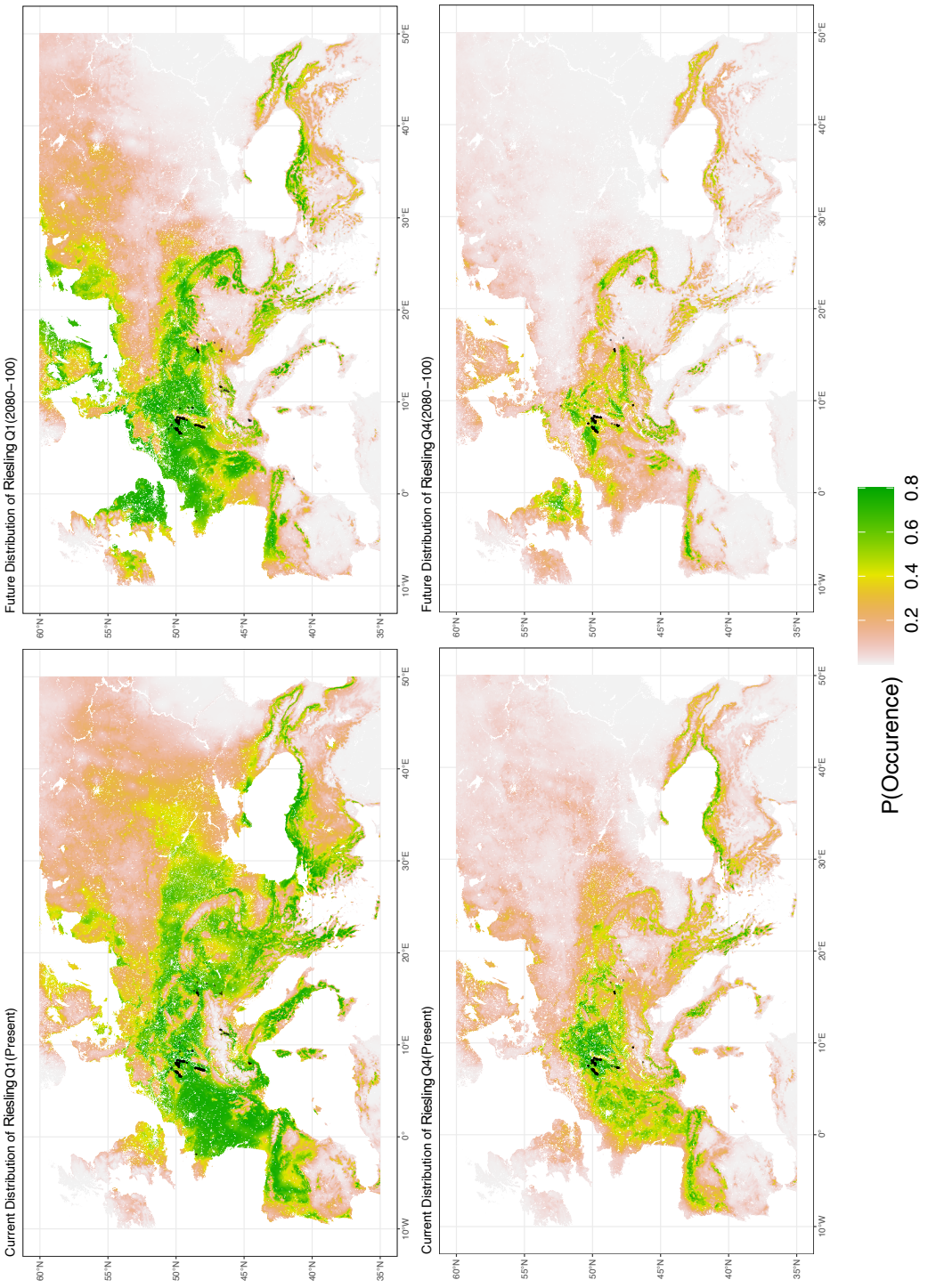
Supplementary Figure 6: Current and future (2100) Australasian distributions of low (Q1) and high (Q4) quality Pinot Noir wines (HADGEM Predicted climates under SSP 1.26)

Supplementary Figure 7



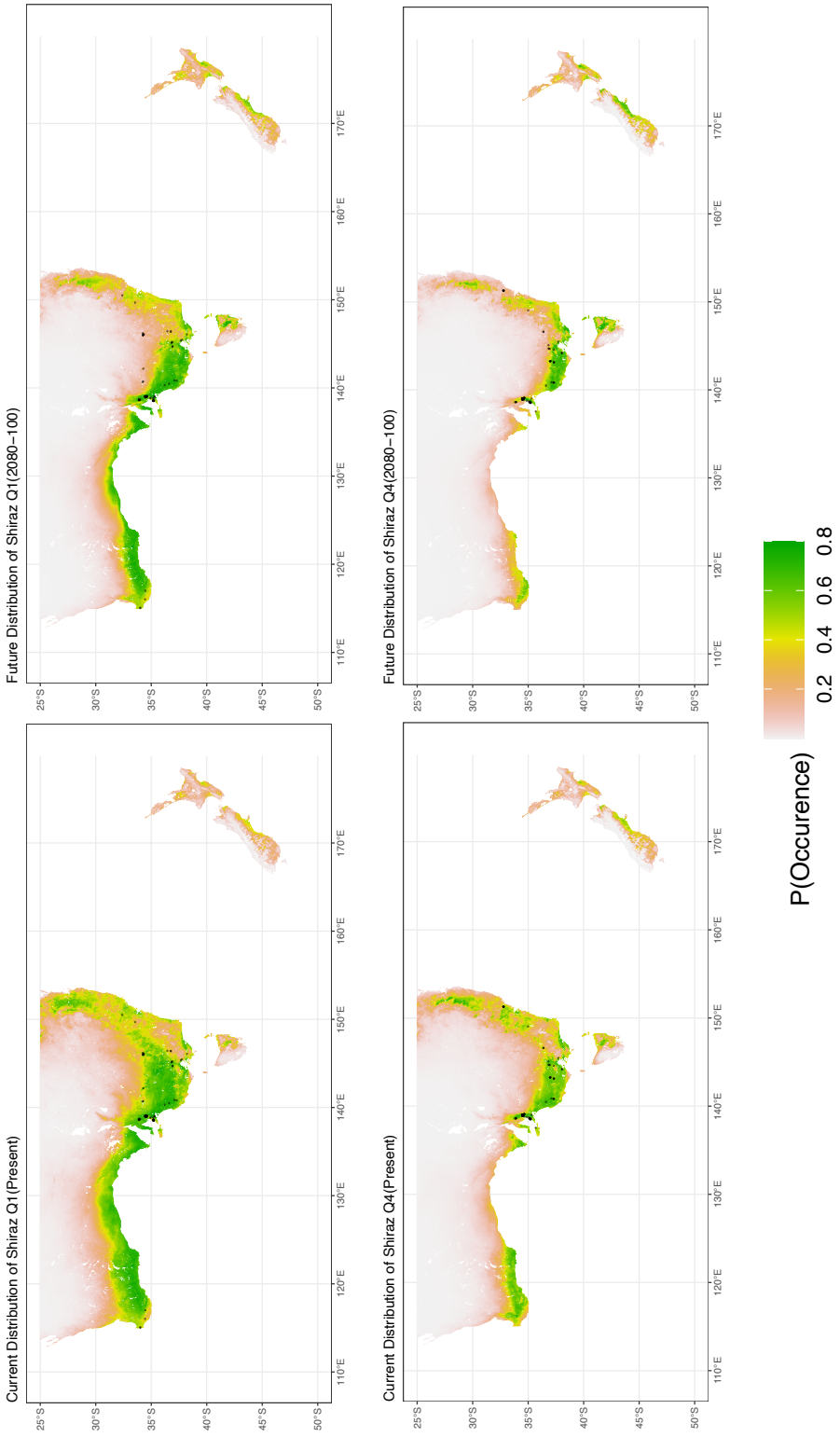
Supplementary Figure 7: Current and future (2100) South American distributions of low (Q1) and high (Q4) quality Cabernet Sauvignon wines (HADGEM Predicted climates under SSP 1.26)

Supplementary Figure 8



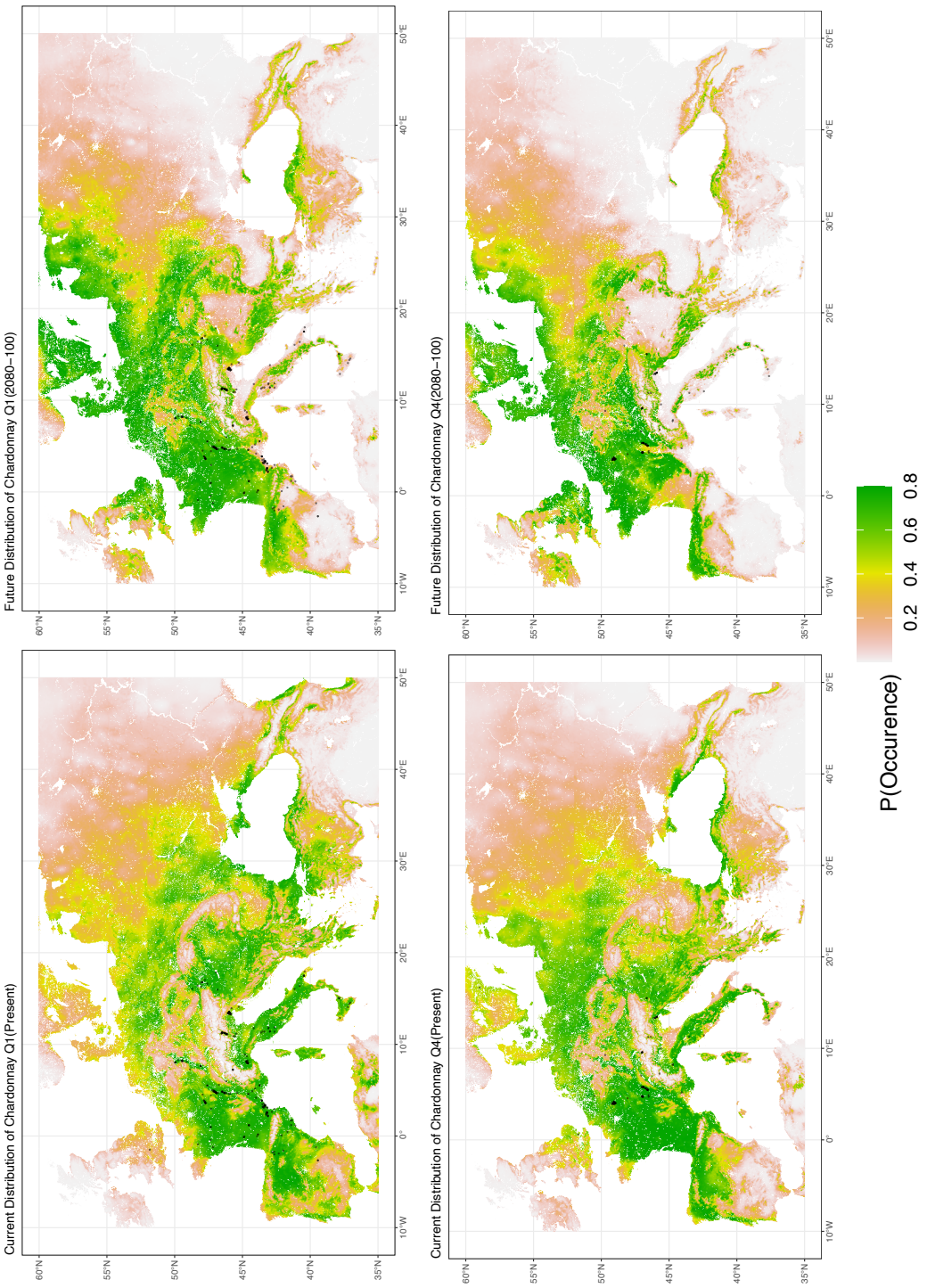
Supplementary Figure 8: Current and future (2100) European distributions of low (Q1) and high (Q4) quality Riesling wines (HADGEM Predicted climates under SSP 1.26)

Supplementary Figure 9



Supplementary Figure 9: Current and future (2100) Australasian distributions of low (Q1) and high (Q4) quality Shiraz wines (HADGEM Predicted climates under SSP 1.26)

Supplementary Figure 10



Supplementary Figure 10: Current and future (2100) European distributions of low (Q1) and high (Q4) quality Chardonnay wines (HADGEM Predicted climates under SSP 1.26)

6

In Conclusion...

Words in Chapter: 2102

In Conclusion...

This thesis has sought to explore the impact of climate change on the quality of wine. It has done so through examining wine quality through a variety of different measures and quantitative techniques. These measures have included wine critics scores (Chapter 1), metabolic indicators of quality (Chapter 2), the harvest dates (Chapter 3), and finally price (Chapter 4). The first half of the thesis uses classical frequentist statistics in the form of generalised linear models and coupled linear models (to form a path model) to seek to understand the drivers of wine quality, be that the contribution of temperature, rainfall, and appellations (Chapter 1) or the more multifactorial analysis including soil, management, grape clone, rootstock, and a range of weather over different time scales (Chapter 2). In the second half of the thesis, I use machine learning techniques to seek to understand the predictability of wine harvests and distributions. In this I endeavour to understand not why the models are predicting as they are, rather I am seeking to make the best predictions possible concerning the future of wine harvests and distributions.

Table 1: Table of Methods Used In Thesis

Method Used	Wine Critics Scores	Metabolic Indicators	Harvest Dates (Phenology)	Wine prices
Classical Frequentist Statistics	Chapter 1 (primarily GLMs)	Chapter 2 (Path model with LM, GLMs, GLMMs)	Chapter 3 (linear models)	Chapter 4 (In data preparation)
Machine Learning			Chapter 3 (Trees, SVMs, neural networks)	Chapter 4 (MaxEnt)

In its first case, chapter 1, this thesis finds that there is a distinct weather pattern which gives the highest quality wine. It then finds that this pattern can be derived through both seasonality and through seasonal blocks of time. In doing so it offers a granular view of the interplay between temperature, rainfall, and appellations. This thesis then suggests that in regions which have not yet reached their physiological maximum such as Central Chile, the predicted future climate changes will lead to a higher concentration of many of the compounds which denote quality (Chapter 2). It also explores the role of other factors, broadening the interplay between weather and wine grape to also include management and genetics of both scion and

rootstock. The changing timing of such optimal quality is then the subject of chapter 3, with the chapter developing and comparing the predictability of said quality optimum point with different machine learning methods. The final chapter seeks to explore the future distribution of wine, finding the patterns that different qualities of wine will take and where the noble grape varieties may be able to be grown in the future. These machine learning techniques add a predictive dimension to the thesis, with the techniques used demonstrating the anticipatory capabilities to predict future harvests and global distributions in the context of changing climatic conditions.

The clear extension to chapters 1, 2, and 3 is to extend the local findings out to a global or regional scale. The other clear extension is to extend the findings to other grape varieties, and to find the generality across grape varieties. Delving further into the mechanism as to why vines develop at the times that they do would extend these works from correlative to causative. The development of viticultural tools to be used in the field is also another potential next step. Chapter 4 could be further developed by exploring the outcomes of the models and adding further independent variables – most likely other soil characteristics or other areas of terroir such as slope aspect and light characteristics. Part of this extension is in customisation of the models for individual winemaking styles. Making a dry Riesling is very different to making a Bordeaux-style Cabernet Sauvignon blend, and so the quality markers change too. Thus, the molecular models should be extended so that they include both the constituent molecules that make up the compound groups (like flavanols and tannins), but also those that are important for flavours of wines – a large and diverse range depending on the wine[1]. Each wine style can and should be modelled separately, and will react to climate change outcomes differently.

There also exists the very long-term effects of climate change. This thesis only considers, at the maximum, effects which occur over the monthly timescale. But wine grapevines can live for a very long time, with the oldest vines thought to be around 400 years old and still producing grapes[2,3]. Thus, there exists a large question over the multi-year effects of climate change on the quality of a grape in years to follow. Does, for example, a heatwave last year impact the quality of grapes the following year? Or does a drought make this year better but next year, or the year after, or three years hence, worse? As the bud formation on a grapevine takes multiple years (with a minimum of one-year old canes producing buds)[3–5], it could

potentially be hypothesised that impacts on bud formation would follow through to grape development.

These chapters have all been purposefully designed to use data-rich environments and thus make the use of any large datasets that are available. In this way this thesis sees quality as an analytical trait that is directly related to the composition of the grape, itself a function of the environment in which it grows. It therefore suggests that it is possible to analyse critics scores, to look at prices, as well as the underlying plant physiology and link them and the weather that makes them so. In this way the thesis relates back to the works of Ashenfelter (1995) and his price-based Bordeaux equation[6], but also more recently to the works of Coombe and Iland (2004), Jones et al. (2005), Ramirez (2008), Poni et al (2018), and Kurtural and Gambetta (2021), all of which have been cited multiple times throughout this thesis[7–11]. What these papers do is to draw links between quality and weather, looking either through observation or metric at the changes associated between quality and the changing weather of the world. This thesis builds from these ideas, seeking to explore and predict the real-world impacts of climate change which will have dramatic consequences for winemakers globally.

This thesis also uses a range of methods to explore these different techniques. The challenge with large datasets is using the appropriate methodology for the task at hand. There is a tendency in some areas of ecology and data analysis to move towards models with a complexity commensurate with the phenomena itself[12,13]. But excessive complexity in models begets unintelligibility in the outcome; hinders understanding of processes; and obscures causality in effect. It also leads to HARKing, a term coined to refer to "**H**ypothesizing **A**fter **R**esults are **K**nown"[14]. The risk is that if analysts create and publish models with incorrect complexity, we diminish the impact of all models. It has therefore been argued that model building requires more "hard thinking" *a priori* to first determine the true aims of the model[15]. This "hard thinking" refers to the design of candidate models before construction based on justification from relevant literature[15]. In short, the argument has been made for less application of new techniques just for the sake of it, and more thinking about construction of better scientific questions through meaningful hypotheses and hence meaningful models.

This thesis is built on these axioms. Each chapter of the thesis was planned before it was written and had different outcomes desired. Levins (1966) remarked upon the impossibility of achieving generality, realism, and precision simultaneously[16]. He thus argued that different models are built depending upon which outcomes are to be maximised[5]. For the first two chapters of the thesis, I chose to seek to try and understand the underlying factors and hence I chose to maximise generality and maintain realism but have larger errors and hence have less precision. For chapters 3 and 4 I primarily wanted to make accurate predictions. In doing so I chose therefore to use modelling approaches which were more complex (based on machine learning) and thus sacrifice generality in favour of precision and realism.

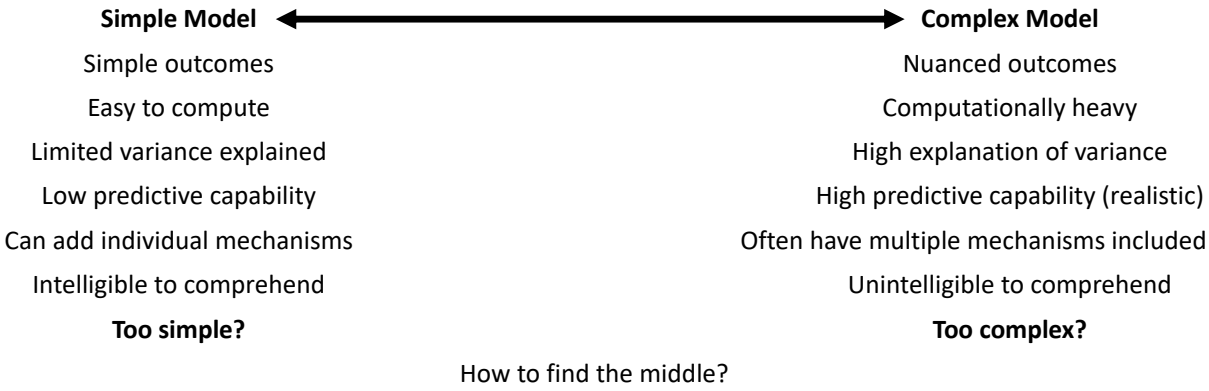


Figure 1: "The Complexity Spectrum": Simple and complex modelling approaches can be thought of as two ends of a spectrum within which all models lie. Choosing the right complexity of modelling approach is key to building the right model.

This thesis highlights the importance of increasing our understanding of how global processes shape the quality of wine. It demonstrates that wine quality is a highly analytical trait which can be analysed from multiple different angles. It also suggests that there is a generality in quality outcomes which occur across time and space with respect to weather and soil. The amalgamation of statistical and machine learning methodologies in this thesis provides a comprehensive and practical framework for comprehending the intricate relationship between climate change and its impact on wine production. By employing classical statistical analyses in the initial phases, the thesis identifies significant drivers of wine quality, laying the groundwork for subsequent machine learning applications. Temperature on a monthly scale repeatedly emerges throughout the thesis as a good predictor of multiple aspects of quality.

The insights derived from these methodologies present a nuanced understanding of the evolving landscape of wine production in the face of climate change. Practical implications and the basis for prediction tools emerge as key contributions, with the findings serving as a valuable resource for the wine industry. This thesis goes beyond theoretical discussions, with the applied outcomes offering actionable insights that can inform strategic planning and decision-making within the sector. As climate dynamics continue to shift, the industry faces the imperative to anticipate and adapt to these changes. The integration of statistical and machine learning approaches equips stakeholders with a robust toolkit for proactive decision-making.

That wines change with weather is not a new thing and underpins the concept of a vintage wine[6,17–19]. But with the increased effects of climate change being felt globally, an increased understanding of the precise effect of weather on wines is pivotal. This means that developing understanding is not just a curiosity or interesting prospect but a practical necessity in navigating the complex interplay between changing climate dynamics and the pursuit of high-quality wine. As the wine industry looks to the future, the insights presented in this thesis serve as a pragmatic guide for fostering resilience, ensuring the continued production of exceptional wines in a changing climate.

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