Natural preconditioners for saddle point systems

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Abstract

The solution of quadratic or locally quadratic extremum problems subject to linear(ized) constraints gives rise to linear systems in saddle point form. This is true whether in the continuous or discrete setting, so saddle point systems arising from discretization of partial differential equation problems such as those describing electromagnetic problems or incompressible flow lead to equations with this structure as does, for example, the widely used sequential quadratic programming approach to nonlinear optimization.

This article concerns iterative solution methods for these problems and in particular shows how the problem formulation leads to natural preconditioners which guarantee rapid convergence of the relevant iterative methods. These preconditioners are related to the original extremum problem and their effectiveness—in terms of rapidity of convergence—is established here via a proof of general bounds on the eigenvalues of the preconditioned saddle point matrix on which iteration convergence depends.

1 Introduction

When a quadratic functional is minimized subject to linear(ized) constraints, Lagrange multipliers and stationarity conditions give rise to saddle point systems. When constraints are not exactly enforced or when a penalty, regularization or stabilization term is included, we obtain a generalized saddle point problem. Both standard and generalized saddle point problems are ubiquitous in scientific computing, with important applications including electromagnetics, incompressible fluid dynamics, structural mechanics, constrained and weighted least squares, constrained optimization, economics, interpolation of scattered data, model order reduction and optimal control [7, Section 2]. Thus, the numerical solution of standard and generalized saddle point problems, which we call saddle point problems for brevity, are of significant interest.

Certain saddle point problems are discrete in nature and lead directly to a linear system. In other applications, the original problem is continuous and must be discretized if it is to be solved numerically. In either case to obtain the solution to the saddle point problem (or an approximation to it in the case of discretization) we must solve the linear system

$$\underbrace{\begin{bmatrix} A & B^T \\ B & -C \end{bmatrix}}_{\mathcal{A}} \begin{bmatrix} u \\ p \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}, \tag{1}$$

where $A \in \mathbb{C}^{n \times n}$ is symmetric positive definite, $B \in \mathbb{R}^{m \times n}$, $m \leq n$ and $C \in \mathbb{R}^{m \times m}$ is symmetric positive semidefinite (and may be the zero matrix). The vector u is associated with the primal variables while p is related to the Lagrange multipliers. The standard conditions for invertibility of $\mathcal{A}$ in the common case $C = 0$ in fact only require that B has full rank and that A is positive definite on the kernel of B, but we will here consider only the usual situation that A is symmetric positive definite.

To highlight just how frequently saddle point systems appear, and their connection to constrained minimization (or maximization), let us highlight three simple applications. The first is the solution of Stokes equations in incompressible fluid dynamics, the second is related to interpolation on the sphere by a hybrid method that augments radial basis functions with polynomials while the third describes the flow of current in a closed electric circuit.

In their simplest form, the equations governing the velocity $u \in \mathbb{R}^d$, $d = 2, 3$, and pressure $p \in \mathbb{R}$ of a Stokes fluid in a bounded connected domain Ω with piecewise smooth boundary $\partial\Omega$ are [21, Chapter 5]:

$$-\nabla^2 u + \nabla p = 0 \;\; \text{in} \;\; \Omega,$$
$$\nabla \cdot u = 0 \;\; \text{in} \;\; \Omega,$$
$$u = w \;\; \text{on} \;\; \partial\Omega.$$

By examining the Stokes equations we see that they form a continuous saddle point problem: the velocity u is the primal variable while the pressure p is the Lagrange multiplier. Associated with this system we should expect to find a variational problem and indeed, the Stokes equations minimize the viscous energy subject to the incompressibility constraint and boundary conditions.

Interpolation on a sphere $\mathbb{S}^d \subset \mathbb{R}^{d+1}$ often involves scattered data. A particularly useful scheme when data is plentiful in some regions but sparse in others is the hybrid interpolation scheme [47, 53], which combines a local approximation (based on radial basis functions) with a global interpolant (that uses spherical polynomials). Assuming that the N data points are distinct, we can construct a radial basis approximation space $\mathcal{X}_N$ and a spherical polynomial approximation space $\mathcal{P}_L$, where $L \geq 0$ is the maximum total degree of the polynomials. To ensure that the interpolant is unique, the radial basis function component is constrained to be orthogonal to $\mathcal{P}_L$ with respect to the inner product associated with the radial basis functions (the native space inner product). We seek an interpolant of the form

$$u_{N,L}(\boldsymbol{x}_i) + p_{N,L}(\boldsymbol{x}_i) = f(\boldsymbol{x}_i),$$

where

$$u_{N,L}(\boldsymbol{x}) = \sum_{j=1}^{N} \alpha_j \phi(\boldsymbol{x}, \boldsymbol{x}_j) \in \mathcal{X}_N$$

is the radial basis function interpolant with strictly positive definite and radially symmetric kernel function ϕ and

$$p_{N,L} = \sum_{\ell=0}^{L} \sum_{k=0}^{M(d,\ell)} \beta_{\ell,k} Y_{\ell,k}(\boldsymbol{x}) \in \mathcal{P}_L$$

is the spherical harmonic interpolant with spherical harmonic functions $Y_{\ell,k}$ and where $M(d,\ell)$ is the dimension of the space spanned by the spherical harmonics of degree ℓ.

To recover the coefficients α_j and $\beta_{\ell,k}$ we must solve the saddle point system

$$\begin{bmatrix} A & Q \\ Q & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{f}_X \\ \boldsymbol{0} \end{bmatrix},$$

where $A \in \mathbb{R}^{N \times N}$ is a positive definite matrix associated with the radial basis function interpolant and $Q \in \mathbb{R}^{N \times M}$ is a matrix of spherical harmonics evaluated at $\boldsymbol{x}_1, \ldots \boldsymbol{x}_N$, with $M \leq N$. We note that the α_j are the primal variables and the $\beta_{\ell,k}$ are the Lagrange multipliers. In this setting the associated extremum problem is to minimise the error of the interpolant subject to the constraint.

Computing the flow of current in a closed electric circuit also leads to a saddle point system, albeit one that is inherently discrete, as we now show following the excellent description in Strang [49, Section 2.3][50]. Flow in a closed circuit is determined by Kirchoff's current law (KCL) and Kirchoff's voltage law (KVL), which force conservation of current and voltage, and Ohm's law, which relates drops in potential and current across a resistor. If the potentials and currents at a set of nodes in the circuit are placed in the vectors v and current i, respectively, then the application of these circuit laws leads to the discrete saddle point system

$$\begin{bmatrix} R & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} v \\ i \end{bmatrix} = \begin{bmatrix} f \\ g \end{bmatrix}.$$

Here R is a diagonal matrix containing the resistances of resistors in the circuit, B^T describes potential drops across these resistors and is determined by KVL and the vectors f and g contain the voltage and current sources, respectively. Perhaps surprisingly, KCL is enforced by B, i.e., the transpose of the potential difference matrix! The related variational problem is the minimization of potential energy subject to conservation of charge (described by KCL).

These applications raise two important points. The first is that physical systems often give rise to saddle point systems, since we are frequently interested in minimizing some energy functional subject to the conservation of a physical quantity. The second is that, although in some problems only the primal variables are of interest there are others, including the three given here, in which the Lagrange multiplier is important in its own right. Indeed, in the hybrid approximation application the interpolant cannot be recovered without the Lagrange multipliers. An advantage of the saddle point system is that both variables are simultaneously recovered.

When (1) is large and sparse, iterative methods such as Krylov subspace methods are particularly attractive. However, the convergence of these methods depends on the spectrum of the saddle point matrix—since it is real symmetric— and may be very slow. One issue is the indefiniteness of saddle point systems, which can delay the convergence of Krylov methods. Additionally, ab initio discrete problems may have poor spectra while problems that involve discretization usually give eigenvalues that vary with the discrete approximation.

These, and other, causes of slow convergence are typically remedied by preconditioning. We focus here on block diagonal preconditioners but note that many preconditioners for saddle point matrices have been proposed, such as

block triangular [12, 29, 31, 37], constraint [19, 20, 30, 35], augmented Lagrangian [9, 26] and splitting-based [6, 46] preconditioners. For more details we refer to Benzi, Golub and Liesen [7].

Many issues must be addressed when solving saddle point problems, including whether the problem has a unique solution, how to discretize a continuous saddle point problem, how to choose an appropriate preconditioner and how to predict the rate of convergence that can be expected from the preconditioned iterative method. It is somewhat surprising that for certain block diagonal preconditioners the answers to all of these questions are linked.

It is the aim of this manuscript to give an overview of the solution process for all saddle point problems, regardless of the particular application. We give conditions under which the original saddle point formulation is solvable and, if discretization is required, state an additional condition for the resulting finite dimensional problem. These conditions lead us to "natural" block diagonal preconditioners and allow bounds on the eigenvalues of the preconditioned matrix to be determined that can be used to estimate convergence of the resulting preconditioned system.

A wealth of literature on solving saddle point systems exists, much of it related to particular applications. Perhaps the most comprehensive work is the survey by Benzi, Golub and Liesen [7], which considers conditions under which the matrix formulation is solvable and block diagonal preconditioners but which has a focus on linear algebra. The conditions for a unique solution (often called Karush-Kuhn-Tucker or KKT conditions) are often discussed and can be found in, for example, the monograph by Nocedal and Wright [38] or, in the substantial area of PDEs, in Babuška [4] and Brezzi [14].

The "natural" block diagonal preconditioners we describe have been studied, largely in the context of PDEs, by Elman, Silvester and Wathen [21, Chapter 6], Hiptmair [27], Loghin and Wathen [34], Mardal and Winther [36], Vassilevski [51] and Zulehner [58]. Related preconditioners that are based only on a study of the eigenvalues of the preconditioned matrix have also been proposed [29, 32, 37]. Norm-based preconditioning also arises in particular applications in PDEs, such as in groundwater flow [12, 13, 18, 25, 42, 52], Stokes flow [16, 17, 22, 44, 55], elasticity [2, 15, 24, 31, 45], magnetostatics [40, 41] and in the hybrid interpolation scheme on the sphere [33]. We note that Arioli and Loghin [1] also use norm equivalence to investigate appropriate stopping criteria for iterative methods applied to mixed finite element problems; the aim here is to stop the Krylov subspace method when the error is commensurate with the discretization error.

Eigenvalue bounds for block diagonal preconditioned saddle point matrices are also prevalent in the literature. In certain cases (i.e., when the finite dimensional saddle point matrix is a standard saddle point problem), the bounds of Rusten and Winther [42] can be used. For generalized saddle point matrices, Elman, Silvester and Wathen [21] and Axelsson and Neytcheva [3] have bounds that are applicable.

The rest of the manuscript aims to unify this saddle point theory in an application-independent manner. In Section 2 we briefly describe saddle point problems and give conditions under which a unique solution exists. We discuss the discretization of continuous problems and the extra conditions that must be imposed on the discrete problem to ensure a unique solution. In Section 3 we describe the corresponding linear system that must be solved and show that the

conditions for a unique solution have linear algebra analogues that are useful when considering natural preconditioners and convergence bounds. Section 4 discusses the Krylov subspace methods that may be applied to these saddle point problems and describes the natural block diagonal preconditioner, while bounds on the convergence of the block diagonal preconditioned Krylov method are given in Section 5. Our conclusions are given in Section 6.

Throughout, we let x^T denote the conjugate transpose of the vector x and similarly for matrices. We use the Löwner ordering for symmetric matrices so that matrices $M_1, M_2 \in \mathbb{R}^{p \times p}$ satisfy $M_1 \succ M_2$ ($M_1 \succeq M_2$) if and only if $M_1 - M_2$ is symmetric positive definite (semidefinite).

2   Saddle point formulations

In this section we show how the saddle point formulation is obtained from a variational form with constraints, discuss generalized saddle point problems, and give conditions under which a unique solution to the standard and generalized saddle point problem exist.

2.1   Saddle point systems

Here we introduce a general framework for saddle point problems. Since some applications, such as partial differential equations, result in infinite dimensional problems, this discussion centres on bilinear forms in Hilbert spaces. However, we stress that the framework is equally applicable to problems that are ab initio discrete.

Let

$$a : \mathcal{X} \times \mathcal{X} \to \mathbb{R}, \ b : \mathcal{X} \times \mathcal{M} \to \mathbb{R}$$

be bounded bilinear forms acting on the real Hilbert spaces $\mathcal{X}$ and $\mathcal{M}$, so that

$$|a(v, w)| \leq C_a \|v\|_{\mathcal{X}} \|w\|_{\mathcal{X}} \ \text{ for all } v, w \in \mathcal{X}, \tag{2}$$

$$|b(v, q)| \leq C_b \|v\|_{\mathcal{X}} \|q\|_{\mathcal{M}} \ \text{ for all } v \in \mathcal{X}, q \in \mathcal{M}. \tag{3}$$

Let us additionally assume that a is symmetric and elliptic on $\mathcal{X}$ ($\mathcal{X}$-elliptic)[1], so that $a(v, w) = a(w, v)$ and $a(v, v) \geq \alpha \|v\|_{\mathcal{X}}^2 > 0$ for all $v, w \in \mathcal{X}$. The norms $\| \cdot \|_{\mathcal{X}}$ and $\| \cdot \|_{\mathcal{M}}$ are defined in the usual way in terms of the Hilbert space inner products $(\cdot, \cdot)_{\mathcal{X}}$ and $(\cdot, \cdot)_{\mathcal{M}}$. We stress that the Hilbert spaces may have finite or infinite dimension; the latter case is common in, for example, problems arising from partial differential equations while the former situation arises in, for example, optimization where $\mathcal{X} = \mathbb{R}^n$ and $\mathcal{M} = \mathbb{R}^m$ with $n \geq m$.

The variational problem we consider is to find

$$u = \arg \min_{v \in \mathcal{X}} J(v) = \frac{1}{2} a(v, v) - f(v) \ \text{ such that } b(v, q) = g(q) \text{ for all } q \in \mathcal{M}, \tag{4}$$

where $f \in \mathcal{X}'$ and $g \in \mathcal{M}'$ are bounded linear functionals.

Rather than solving the above problem directly, we can formulate an equivalent saddle point system by first introducing the Lagrange function

$$\mathcal{L}(v, q) = J(v) + [b(v, q) - g(q)], \ q \in \mathcal{M},$$

---

[1]If a is not elliptic we can consider, for example, an augmented Lagrangian formulation [23].

5

which coincides with J when the constraints are satisfied. Related to this Lagrange function is the following saddle point problem: find $(u, p) \in \mathcal{X} \times \mathcal{M}$ such that

$$
\begin{aligned}
a(u, v) + b(v, p) &= f(v) \quad \text{for all } v \in \mathcal{X}, \\
b(u, q) &= g(q) \quad \text{for all } q \in \mathcal{M}.
\end{aligned}
\tag{5}
$$

It is so named because any solution (u, p) also satisfies the saddle point property

$$
\mathcal{L}(u, q) \leq \mathcal{L}(u, p) \leq \mathcal{L}(v, p) \quad \text{for all } (v, q) \in \mathcal{X} \times \mathcal{M}
$$

and, crucially, the first component of a solution (u, p) is a minimizer of (4).

To this point, we have assumed that the constraint (4) is exactly satisfied. However, there may be reasons to relax this constraint or to apply a penalty term. Examples include nearly incompressible fluid flow [11, Chapter III, Sections 4 and 6], the regularization of an ill-posed problem [8] or in certain interior point methods [56, 57]. In these cases we obtain the generalized saddle point system: find $(u, p) \in \mathcal{X} \times \mathcal{M}$ such that

$$
\begin{aligned}
a(u, v) + b(v, p) &= f(v) \quad \text{for all } v \in \mathcal{X}, \\
b(u, q) - c(p, q) &= g(q) \quad \text{for all } q \in \mathcal{M}.
\end{aligned}
\tag{6}
$$

Here $c : \mathcal{M} \times \mathcal{M} \to \mathbb{R}$ is a third bilinear form that is assumed to be bounded, symmetric and nonnegative on M, so that

$$
|c(r, q)| \leq C_c \|r\|_{\mathcal{M}} \|q\|_{\mathcal{M}}, \quad \text{for all } r, q \in \mathcal{M},
\tag{7}
$$

$c(r, q) = c(q, r)$ and $c(q, q) \geq 0$ for all $r, q \in \mathcal{M}$. Associated with this generalized saddle point problem (6) is the functional

$$
\mathcal{L}(v, q) = \frac{1}{2} a(v, v) - f(u) + [b(v, q) - \frac{1}{2} c(q, q) - g(q)],
$$

and, analogously to the standard problem, solutions (u, p) of (6) satisfy the saddle point property

$$
\mathcal{L}(u, q) \leq \mathcal{L}(u, p) \leq \mathcal{L}(v, p) \quad \text{for all } (v, q) \in \mathcal{X} \times \mathcal{M}.
$$

Clearly, (5) is obtained from (6) by setting $c \equiv 0$. Consequently, the conditions under which both problems are uniquely solvable can be described by a single result [14],[58, Theorem 2.6]:

Theorem 1. *Let $\mathcal{X}$ and $\mathcal{M}$ be real Hilbert spaces with norms $\|\cdot\|_{\mathcal{X}}$ and $\|\cdot\|_{\mathcal{M}}$ induced by inner products $(\cdot, \cdot)_{\mathcal{X}}$ and $(\cdot, \cdot)_{\mathcal{M}}$. Let $a : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, $b : \mathcal{X} \times \mathcal{M} \to \mathbb{R}$ and $c : \mathcal{M} \times \mathcal{M} :\to \mathbb{R}$ be bilinear forms that satisfy (2), (3) and (7), respectively, and let a and c be symmetric, Let $f : \mathcal{X} \to \mathbb{R}$ and $g : \mathcal{M} \to \mathbb{R}$ be bounded linear functionals on $\mathcal{X}$ and $\mathcal{M}$, respectively. Then if*

$$
a(v, v) \geq \alpha \|v\|_{\mathcal{X}}^2, \quad \text{for all } v \in \mathcal{X},
\tag{8}
$$

$$
c(q, q) \geq 0 \quad \text{for all } q \in \mathcal{M}
\tag{9}
$$

and there exists a constant $\beta > 0$ such that the inf-sup condition

$$
\sup_{v \in \mathcal{X} \backslash \{0\}} \frac{b(v, q)}{\|v\|_{\mathcal{X}}} + c(q, q) \geq \beta \|q\|_{\mathcal{M}} \quad \text{for all } q \in \mathcal{M}
\tag{10}
$$

is satisfied, then there exists a unique pair (u, p) in $\mathcal{V} = \mathcal{X} \times \mathcal{M}$ that solves (6).

Remark 1. The generalized saddle point problem (6) has a solution under weaker conditions but we do not consider these conditions here.

Remark 2. The boundedness and nonnegativity of c ensures that the generalized saddle point problem (6) has a unique solution whenever (5) has a unique solution [10, Theorem 1].

Theorem 1 shows that when a is elliptic on X and c is nonnegative, whether the generalized saddle point system (6) has a unique solution depends on the inf-sup condition (10). We also note that this is a general result that does not depend on the application; though it is well known in many continuous settings such as mixed finite element methods, it is equally applicable in discrete settings such as optimization.

Although Theorem 1 describes all conditions for an inherently discrete problem to be solved numerically, in the next section we will see that when $\mathcal{X}$ and $\mathcal{M}$ are infinite dimensional a discrete analogue of the inf-sup condition is essential. Additionally, in later sections we will use the conditions on a, b and c described here *that are necessary for a unique solution to the original saddle point problem*, to estimate the convergence of certain preconditioned iterative methods for the saddle point system.

2.2 Discrete saddle point systems

In some applications, such as certain optimization problems, the saddle point system (6) involves finite dimensional Hilbert spaces $\mathcal{X}$ and $\mathcal{M}$ and the linear system (1) can be obtained from the original problem. However, in other cases such as those involving partial differential equations, $\mathcal{X}$ and $\mathcal{M}$ may be infinite-dimensional, as we have already mentioned. If the infinite dimensional problem cannot be solved exactly, (6) is typically discretized in some fashion, perhaps by finite elements or radial basis functions, and a finite dimensional analogue of (5) is obtained. The discretization often depends on some parameter, such as the the mesh width or the number of interpolation points and we represent this dependence by a generic parameter N. We introduce families of finite dimensional subspaces $\{\mathcal{X}_N\}$ and $\{\mathcal{M}_N\}$ where $\mathcal{X}_N \subset \mathcal{X}$ and $\mathcal{M}_N \subset \mathcal{M}$ will generally depend on N. It is of course usually desirable that one has some approximability so that, for example, $\mathcal{X}_N$ becomes dense in $\mathcal{X}$ and $\mathcal{M}_N$ becomes dense in $\mathcal{M}$ as $N \to \infty$. Then an approximation of (6) is given by: find $(u_N, p_N) \in \mathcal{X}_N \times \mathcal{M}_N$ such that

$$\begin{aligned} a(u_N, v_N) + b(v_N, p_N) &= f(v_N) \ \ \text{for all } v_N \in \mathcal{X}_N, \\ b(u_N, q_N) - c(p_N, q_N) &= g(q_N) \ \ \text{for all } q_N \in \mathcal{M}_N. \end{aligned} \qquad (11)$$

Of course, the case that $\mathcal{X}$ and $\mathcal{M}$ are finite dimensional can be considered a special case of (11) in which $\mathcal{X}_N = \mathcal{X}$ and $\mathcal{M}_N = \mathcal{M}$ for all N.

A crucial issue arises when c in the continuous saddle point problem (6) is not uniformly positive, since the inf-sup condition (10) in Theorem 1 may not be satisfied in the subspaces $\mathcal{X}_N$ and $\mathcal{M}_N$, even though it is satisfied in $\mathcal{X}$ and $\mathcal{M}$. In this case, a unique solution to the discrete problem does not necessarily exist. This can be remedied by stabilization, that is, by modifying c or, in the case that $c \equiv 0$ in (6), by introducing a bounded, symmetric and nonnegative bilinear form c on $\mathcal{M}_N$ (see, for example, Elman et al [21, Chapter 5] in the

case of mixed finite element approximations of incompressible fluid dynamics problems).

Let us now focus in more detail on the conditions for a unique solution of the discrete system (11). Since a is positive definite on $\mathcal{X}$, it is automatically positive definite on $\mathcal{X}_N$. Similarly, the nonnegativity of c on $\mathcal{M}$ implies nonnegativity on $\mathcal{M}_N$. Thus, the only additional condition we are required to check is a discrete inf-sup condition [58, Theorem 2.6].

Theorem 2. *Let the conditions of Theorem 1 hold. If, additionally, there exists a constant β for which*

$$\sup_{v_N \in \mathcal{X}_N \setminus \{0\}} \frac{b(v_N, q_N)}{\|v_N\|_{\mathcal{X}}} + c(q_N, q_N) \geq \beta \|q_N\|_{\mathcal{M}} \quad \text{for all } q_N \in \mathcal{M}_N \qquad (12)$$

then there exists a unique solution $(u_N, p_N) \in \mathcal{V}_N = \mathcal{X}_N \times \mathcal{M}_N$ that solves (11).

Remark 3. The inf-sup condition and its discrete counterpart play an important role in mixed methods for PDE problems, such as those arising in fluid dynamics [21, Chapter 5] and solid mechanics [11, Chapter VI]. However, researchers have begun to appreciate the importance of inf-sup conditions in other applications, such as when developing hybrid interpolants on the sphere [33, 48].

Thus, if (6) is infinite dimensional, the way in which the finite dimensional spaces are chosen affects the additional discrete inf-sup condition (12) that must be satisfied. Certain choices may allow $c \equiv 0$ but for others it is necessary to include a stabilization term to ensure that (11) has a unique solution.

3 The matrix formulation

By selecting basis functions $\{\phi_1, \ldots \phi_n\}$ for $\mathcal{X}_N$ and $\{\psi_1, \ldots, \psi_m\}$ for $\mathcal{M}_N$, we can express the discrete generalized saddle point problem (11) in terms of the matrix equation (1) where

$$A = [a_{ij}], a_{ij} = a(\phi_i, \phi_j), \qquad B = [b_{kj}], b_{kj} = b(\phi_j, \psi_k),$$
$$C = [c_{k\ell}], c_{ij} = c(\psi_k, \psi_\ell),$$

$i, j = 1, \ldots, n$, $k, \ell = 1, \ldots, m$. The conditions on the bilinear forms a, b and c given in Section 2 ensure that $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite, $B \in \mathbb{R}^{m \times n}$, $m \leq n$ and $C \in \mathbb{R}^{m \times m}$ is symmetric positive semidefinite (and may be the zero matrix). However, $\mathcal{A}$ is always indefinite.

The choice of bases additionally facilitates the representation of norms on $\mathcal{X}_N$, $\mathcal{M}_N$ and the product space $\mathcal{V}_N = \mathcal{X}_N \times \mathcal{M}_N$ through the Gram matrices X, M and V. Specifically, we have that

$$X = [x_{ij}], x_{ij} = (\phi_i, \phi_j)_{\mathcal{X}}, \quad M = [m_{k\ell}] = (\psi_k, \psi_\ell)_{\mathcal{M}}$$

and

$$V = \begin{bmatrix} X & \\ & M \end{bmatrix}, \qquad (13)$$

where, as previously mentioned, $(\cdot, \cdot)_{\mathcal{X}}$ and $(\cdot, \cdot)_{\mathcal{M}}$ are the inner products on the Hilbert spaces $\mathcal{X}$ and $\mathcal{M}$.

These Gram matrices allow us relate the properties of a, b and c to properties of the matrices A, B and C and will prove useful when considering preconditioners. In particular, the ellipticity and boundedness of a, from (2) and (8), and boundedness and nonnegativity of c, from (7) and (9), imply that for any nonzero $v \in \mathbb{R}^n$ and $q \in \mathbb{R}^m$,

$$0 < \alpha \leq \frac{v^T A v}{v^T X v} \leq C_a \quad \text{for all } v \in \mathbb{R}^n \tag{14}$$

and

$$0 \leq \frac{q^T C q}{q^T M q} \leq C_c \quad \text{for all } q \in \mathbb{R}^m. \tag{15}$$

For the inf-sup condition (12), we first note that for any $q \in \mathcal{M}_N$,

$$\max_{v \in \mathcal{X}_N \setminus \{0\}} \frac{b(v,q)}{\|v\|_{\mathcal{X}}} = \max_{v \neq 0} \frac{q^T B v}{(v^T X v)^{\frac{1}{2}}} = \max_{w \neq 0} \frac{q^T B X^{-\frac{1}{2}} w}{(w^T w)^{\frac{1}{2}}} = (q^T B X^{-1} B^T q)^{\frac{1}{2}}$$

since the maximum is attained when w is the unit vector in the direction of $X^{-\frac{1}{2}} B^T q$.

Accordingly, as a consequence of (12) we have that for any $q \in \mathbb{R}^m$

$$\beta(q^T M q)^{\frac{1}{2}} \leq (q^T B X^{-1} B^T q)^{\frac{1}{2}} + (q^T C q)^{\frac{1}{2}}.$$

Since, for any nonnegative numbers d and e, $(\sqrt{d} + \sqrt{e})^2 \leq 2(d + e)$, we find that

$$\beta^2 \leq 2 \frac{q^T (B X^{-1} B^T + C) q}{q^T M q}. \tag{16}$$

The boundedness of b (see (3)) also ensures that

$$C_b \geq \max_{q \in \mathcal{M}_N \setminus \{0\}} \max_{v \in \mathcal{X}_N \setminus \{0\}} \frac{b(v,q)}{\|v\|_{\mathcal{X}} \|q\|_{\mathcal{M}}} = \max_{q \neq 0} \frac{\left(q^T B X^{-1} B^T q\right)^{\frac{1}{2}}}{(q^T M q)^{\frac{1}{2}}}.$$

so that for any $q \in \mathbb{R}^m$

$$\frac{q^T B X^{-1} B^T q}{q^T M q} \leq C_b^2. \tag{17}$$

We note that (14)–(17) give conditions for invertibility of the matrix $\mathcal{A}$. In particular, since A is positive definite, and C is semidefinite, a sufficient condition for invertibility is a matrix version of the inf-sup condition (12), i.e., $\text{null}(C) \cap \text{null}(B^T) = \{0\}$ [7, Theorem 3.1]. Of course, this condition is automatically satisfied if B has full rank.

4 Solution by iterative methods

In the previous sections we examined conditions for a unique solution of the discrete standard and generalized saddle point systems and showed that, by choosing basis functions for the finite dimensional spaces $\mathcal{X}_N$ and $\mathcal{M}_N$, we arrive at the symmetric indefinite matrix system (1). For an ab initio discrete problem this certainly carries through with $\mathcal{X}_N = \mathcal{X}$ and $\mathcal{M}_N = \mathcal{M}$ for all N.

When $\mathcal{A}$ is large and sparse it is common to solve (1) by a Krylov subspace method such as MINRES [39]. However, the convergence of Krylov methods

in the symmetric case is usually heavily influenced by the spectrum of $\mathcal{A}$. In applications involving discretization, convergence often depends on the parameter N and deteriorates as the approximation to (6) becomes more accurate. In the ab initio discrete case, poor convergence may be caused by the spectral distribution.

The effect on the spectrum can be mitigated by using an appropriate preconditioner $\mathcal{P}$. Conceptually we can consider solving the equivalent linear system $\mathcal{P}^{-1}\mathcal{A}x = \mathcal{P}^{-1}b$, although in practice we typically aim to preserve symmetry; this can certainly be achieved when $\mathcal{P}$ is symmetric positive definite in MINRES. Ideally, the preconditioner should be chosen so that convergence is independent of the parameter N and it turns out that this is at least theoretically possible when certain block diagonal preconditioners of the form

$$\mathcal{P} = \begin{bmatrix} P_1 & \\ & P_2 \end{bmatrix} \tag{18}$$

are applied with $P_1 \in \mathbb{R}^{n \times n}$ and $P_2 \in \mathbb{R}^{m \times m}$ symmetric positive definite. The matrices P_1^{-1} and P_2^{-1} represent symmetric positive definite isomorphisms that map $\mathcal{X}_N' \to \mathcal{X}_N$ and $\mathcal{M}_N' \to \mathcal{M}_N$ [29, 32, 33, 36, 37, 58]. We note that preconditioners $\mathcal{P}$ of this type may not be unique [36].

A preconditioner that is theoretically optimal may be too costly to apply in practice and may be replaced by a more computationally feasible alternative. A discussion of this topic can be found in Section 10.1.3 of Benzi et al [7], with particular reference to problems involving elliptic partial differential equations and interior point methods. Mardal and Winther [36] also discuss multilevel approximations in the context of mixed finite elements.

We expect that reasonable preconditioners that still provide N-independent convergence will satisfy the bounds

$$\delta \leq \frac{v^T P_1 v}{v^T X v} \leq \Delta \quad \text{for all } v \in \mathbb{R}^n \tag{19}$$

and

$$\theta \leq \frac{q^T P_2 q}{q^T M q} \leq \Theta \quad \text{for all } q \in \mathbb{R}^m \tag{20}$$

for positive scalars δ, Δ, θ and Θ. Better preconditioners are those for which Δ/δ and Θ/θ are small as we show in Section 5.

Importantly, if such bounds can be obtained for P_1 and P_2 then these, in conjunction with (14)–(17), allow us to bound the eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ and determine how convergence may be affected by the preconditioner. We quote just one convergence bound that shows the importance of these extreme eigenvalues. Let the eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ be contained in the intervals $[-\mu_m, -\mu_1] \cup [\nu_1, \nu_n]$ with $\mu_m - \mu_n = \nu_n - \nu_1$, so that the intervals are of equal length. Then after $2k$ steps of MINRES the residual $r^{(2k)} = b - \mathcal{A}x^{(2k)}$ satisfies the bound [21, Theorem 6.13]

$$\frac{\|r^{(2k)}\|_{\mathcal{P}^{-1}}}{\|r^{(0)}\|_{\mathcal{P}^{-1}}} \leq 2 \left(\frac{\sqrt{\mu_m \nu_n} - \sqrt{\mu_1 \nu_1}}{\sqrt{\mu_m \nu_n} + \sqrt{\mu_1 \nu_1}} \right)^k. \tag{21}$$

This bound can be pessimistic, particularly if the negative and positive eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ lie in intervals of significantly different lengths. However, it certainly shows that knowledge of the extreme eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ can provide useful information about the convergence of MINRES. (For more precise

bounds see Wathen *et al.* [54].) From the bound (21) we additionally discern that a sufficient condition for fast convergence is that μ_m/μ_1 and ν_n/ν_1 are small, since this will ensure that the eigenvalues are clustered away from the origin. The latter point is an important one since small eigenvalues can hinder the convergence of MINRES.

5 Bounds on the eigenvalues of the preconditioned matrix

Although several eigenvalue bounds for saddle point problems and preconditioners have been devised in various contexts, we now derive general bounds that explicitly make use of the important boundedness, coercivity and inf-sup constants of the original saddle point formulation (6). Specifically, we bound the positive and negative eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ using the bounds (14)–(17), that are related to the bilinear forms a, b and c, and (19) and (20), that depend on the preconditioner $\mathcal{P}$.

Crucial to our proof of these bounds is Schur's determinant lemma [5, 43], that relates the determinant of a block matrix to the determinant of the Schur complement. The lemma itself is easily understood given the following decomposition of a block matrix

$$\begin{bmatrix} E & F^T \\ F & -G \end{bmatrix} = \begin{bmatrix} I & 0 \\ FE^{-1} & I \end{bmatrix} \begin{bmatrix} E & 0 \\ 0 & -G - FE^{-1}F^T \end{bmatrix} \begin{bmatrix} I & E^{-1}F^T \\ 0 & I \end{bmatrix},$$

which holds whenever E is invertible. Since the determinant of a matrix product is the product of the determinants, we obtain Schur's result that

$$\det\left(\begin{bmatrix} E & F^T \\ F & -G \end{bmatrix}\right) = \det(E)\det(-G - FE^{-1}F^T).$$

Analogously, if G is invertible,

$$\det\left(\begin{bmatrix} E & F^T \\ F & -G \end{bmatrix}\right) = \det(-G)\det(E + F^T G^{-1}F).$$

Another important component of the proof is the equivalence of the maxima of certain generalised Rayleigh quotients, which we show here.

Lemma 3. *Let $B \in \mathbb{R}^{m\times n}$, $m \leq n$ have full rank and $X \in \mathbb{R}^{n\times n}$, $M \in \mathbb{R}^{m\times m}$ and $P_2 \in \mathbb{R}^{m\times m}$ be symmetric positive definite. Then*

$$\max_{x\neq 0} \frac{x^T B^T P_2^{-1} Bx}{x^T Xx} = \max_{x\neq 0} \frac{y^T B X^{-1} B^T y}{y^T My} \frac{y^T My}{y^T P_2 y}.$$

Proof. By the Courant-Fischer theorem [28, Theorem 4.2.11],

$$\max_{x\neq 0} \frac{x^T B^T P_2^{-1} Bx}{x^T Xx} = \max_{\widetilde{x}\neq 0} \frac{\widetilde{x}^T X^{-\frac{1}{2}} B^T P_2^{-1} B X^{-\frac{1}{2}} \widetilde{x}}{\widetilde{x}^T \widetilde{x}} = \lambda_{max},$$

where λ_{max} is the largest eigenvalue of $X^{-\frac{1}{2}} B^T P_2^{-1} B X^{-\frac{1}{2}} \in \mathbb{R}^{n\times n}$. Note that this matrix is symmetric positive semidefinite and so has real nonnegative eigenvalues. Moreover, B has rank m and so there are $n - m$ zero eigenvalues.

Since $X^{-\frac{1}{2}}B^T P_2^{-1} B X^{-\frac{1}{2}}$ and $X^{-1}B^T P_2^{-1}B$ are similar, λ_{max} is also the largest eigenvalue of $X^{-1}B^T P_2^{-1}B$ and there must be some nonzero vector $\hat{x} \in \mathbb{R}^n$ for which

$$X^{-1}B^T P_2^{-1}B\hat{x} = \lambda_{max}\hat{x}. \tag{22}$$

Note that if $\hat{x}$ is in null(B), the nullspace of B, the left-hand side of (22) is the zero vector. Since $\hat{x} \neq 0$, this implies that $\lambda_{max} = 0$ and that all eigenvalues of $X^{-\frac{1}{2}}B^T P_2^{-1}B X^{-\frac{1}{2}}$ are zero. However, we know that the largest eigenvalue must be positive and so we conclude that $\hat{x} \notin$ null(B).

Premultiplying (22) by $P_2^{-\frac{1}{2}}B$ gives

$$P_2^{-\frac{1}{2}}B X^{-1}B^T P_2^{-\frac{1}{2}}\hat{y} = \lambda_{max}\hat{y},$$

where $\hat{y} = P_2^{-\frac{1}{2}}B\hat{x}$ is nonsingular since P_2 is positive definite and $\hat{x} \notin$ null(B).

By again applying the Courant-Fischer theorem we see that

$$\lambda_{max} = \max_{\widetilde{y}\neq 0} \frac{\widetilde{y}^T P_2^{-\frac{1}{2}}B X^{-1}B^T P_2^{-\frac{1}{2}}\widetilde{y}}{\widetilde{y}^T\widetilde{y}} = \max_{y\neq 0} \frac{y^T B X^{-1}B^T y}{y^T P_2 y}$$

$$= \max_{x\neq 0} \frac{y^T B X^{-1}B^T y}{y^T M y} \frac{y^T M y}{y^T P_2 y}$$

which completes the proof. $\qquad\square$

We are now in a position to state the bounds. Note that these bounds appeared previously in Silvester and Wathen [44] in the particular context of mixed finite elements for Stokes equations.

Theorem 4. *Let $\mathcal{A}$ in (1) be preconditioned by $\mathcal{P}$ in (18) and let C_a in (2) and (14) be greater than or equal to one. Then, negative eigenvalues λ of the preconditioned matrix $\mathcal{P}^{-1}\mathcal{A}$ satisfy*

$$\lambda \in \left[-\theta^{-1}\left(C_c + \frac{C_b^2}{\alpha}\right), \frac{1}{2}\left(\frac{C_a}{\Delta} - \sqrt{\left(\frac{C_a}{\Delta}\right)^2 + \frac{2\beta^2}{\Theta\Delta}}\right)\right]$$

while positive eigenvalues λ satisfy

$$\lambda \in \left[\frac{\alpha}{\Delta}, \frac{1}{2}\left(\frac{C_a}{\delta} + \sqrt{\left(\frac{C_a}{\delta}\right)^2 + \frac{4C_b^2}{\theta\delta}}\right)\right].$$

Proof. Any eigenvalue λ of $\mathcal{P}^{-1}\mathcal{A}$ satisfies the equation

$$\det\left(\begin{bmatrix} A - \lambda P_1 & B^T \\ B & -(C + \lambda P_2) \end{bmatrix}\right) = 0. \tag{23}$$

Let us consider the cases $\lambda > 0$ and $\lambda < 0$ separately. If $\lambda > 0$, then $C + \lambda P_2$ is symmetric positive definite and by Schur's determinant lemma, (23) holds if and only if

$$\det\left((A - \lambda P_1) + B^T(C + \lambda P_2)^{-1}B\right) = 0.$$

Since the determinant of a matrix is the product of its eigenvalues

$$\lambda_{min}\left((A - \lambda P_1) + B^T(C + \lambda P_2)^{-1}B\right) \leq 0 \leq \lambda_{max}\left((A - \lambda P_1) + B^T(C + \lambda P_2)^{-1}B\right).$$

Note that $B \in \mathbb{R}^{m \times n}$ $(m \leq n)$ has rank at most m. It follows that the $n \times n$ positive semidefinite matrix $B^T(C + \lambda P_2)^{-1}B$ also has rank at most m and, therefore, a nullspace of dimension at least $n - m$. Associated with this nullspace are zero eigenvalues, so that $\lambda_{min}(B^T(C + \lambda P_2)^{-1}B) = 0$. This fact, combined with Weyl's inequality [28, Theorem 4.3.1] gives that

$$\lambda_{min}(A - \lambda P_1) \leq 0 \leq \lambda_{max}(A - \lambda P_1) + \lambda_{max}\left(B^T(C + \lambda P_2)^{-1}B\right). \quad (24)$$

From the lower bound in (24) and the Courant-Fischer theorem [28, Theorem 4.2.11] we find that

$$0 \geq \lambda_{min}(A - \lambda P_1) = \min_{x \neq 0} \frac{x^T(A - \lambda P_1)x}{x^T x}.$$

Thus, after multiplying by the positive quantity $x^T x / x^T X x$ for $x \neq 0$, we have that

$$\min_{x \neq 0} \frac{x^T A x}{x^T X x} \leq \lambda \max_{x \neq 0} \frac{x^T P_1 x}{x^T X x}$$

and, using (14) and (19), we obtain the lower bound for positive eigenvalues.

From the upper bound in (24), since $(\lambda P_2)^{-1} \succeq (C + \lambda P_2)^{-1}$, we find that

$$0 \leq \lambda_{max}(A - \lambda P_1) + \frac{1}{\lambda}\lambda_{max}(B^T P_2^{-1}B) = \max_{x \neq 0} \frac{x^T(A - \lambda P_1)x}{x^T x} + \frac{1}{\lambda}\max_{x \neq 0} \frac{x^T B^T P_2^{-1}B x}{x^T x},$$

where again we have used the Courant-Fischer theorem. It follows, by again multiplying by $x^T x / x^T X x$ and using (14) and (17), that

$$0 \leq C_a - \delta\lambda + \frac{1}{\lambda}\max_{x \neq 0} \frac{x^T B^T P_2^{-1}B x}{x^T X x}.$$

We want to bound the last term of this inequality. By applying Lemma 3, (17) and (19) we obtain the bound

$$\max_{x \neq 0} \frac{x^T B^T P_2^{-1}B x}{x^T X x} = \max_{y \neq 0} \frac{y^T B X^{-1}B^T y}{y^T M y}\frac{y^T M y}{y^T P_2 y} \leq \frac{C_b^2}{\theta}.$$

Thus, $\lambda^2 - (C_a/\delta)\lambda - C_b^2/(\theta\delta) \leq 0$, the solution of which gives the upper bound.

Let us now consider $\lambda < 0$. With this choice, $A - \lambda P_1$ is symmetric positive definite and (23) is equivalent to

$$\det\left((C + \lambda P_2) + B(A - \lambda P_1)^{-1}B^T\right) = 0.$$

Again we infer that

$$\lambda_{min}\left((C + \lambda P_2) + B(A - \lambda P_1)^{-1}B^T\right) \leq 0 \leq \lambda_{max}\left((C + \lambda P_2) + B(A - \lambda P_1)^{-1}B^T\right)$$

so, using Weyl's inequality, we must have that

$$\lambda_{min}(C + \lambda P_2) + \lambda_{min}\left(B(A - \lambda P_1)^{-1}B^T\right) \leq 0 \leq \lambda_{max}(C + \lambda P_2) + \lambda_{max}\left(B(A - \lambda P_1)^{-1}B^T\right).$$

Since $A^{-1} \succeq (A - \lambda P_1)^{-1}$, the upper bound gives that

$$0 \leq \max_{y \neq 0} \frac{y^T(C + \lambda P_2)y}{y^T y} + \max_{y \neq 0} \frac{y^T B A^{-1}B^T y}{y^T y}.$$

Multiplying by the positive quantity $y^T y / y^T M y$ for $y \neq 0$ and applying (15) and (20) gives that

$$0 \leq C_c + \theta\lambda + \max_{y \neq 0} \frac{y^T B A^{-1} B^T y}{y^T M y}.$$

For any $x \in \mathbb{R}^n$, we have that $\alpha x^T X x \leq x^T A x$ from (14). Combining this with (17), we find that

$$0 \leq C_c + \theta\lambda + \frac{1}{\alpha} \max_{x \neq 0} \frac{y^T B^T X^{-1} B^T y}{y^T M y} \leq C_c + \theta\lambda + \frac{C_b^2}{\alpha}.$$

Thus, $\lambda \geq -\theta^{-1}(C_c + C_b^2/\alpha)$, which is the lower bound for negative eigenvalues.

For the upper bound on negative eigenvalues, we find that

$$0 \geq \min_{y \neq 0} \frac{y^T(C + \lambda P_2)y}{y^T y} + \min_{y \neq 0} \frac{y^T B(A - \lambda P_1)^{-1} B^T y}{y^T y}.$$

From (14) and (19) we find that, for any $x \in \mathbb{R}^n$, $x^T(A - \lambda P)x \leq (C_a - \lambda\Delta)x^T X x$ and so

$$0 \geq \min_{y \neq 0} y^T(\lambda P_2 + C)y + \frac{1}{C_a - \lambda\Delta} \min_{y \neq 0} y^T B X^{-1} B^T y$$

$$\geq \min_{y \neq 0} \lambda y^T P_2 y + \frac{1}{C_a - \lambda\Delta} \min_{y \neq 0} y^T (B X^{-1} B^T + C)y,$$

using the assumption that $C_a \geq 1$. From (16) and (20) we obtain $\lambda\Theta + \beta^2/2(C_a - \lambda\Delta) \leq 0$, the solution of which gives the upper bound on negative eigenvalues. $\square$

Remark 4. As has been shown previously [21, Theorem 6.6]) the upper bound on positive eigenvalues can be made simpler, although less sharp, by completing the square of the term under the square root sign. Doing so gives the bound for positive eigenvalues $\lambda \in [\alpha/\Delta, C_a/\delta + C_b^2/(\theta C_a)]$.

Through (21), the bounds of Theorem 4 can be used to infer information about convergence of MINRES applied to $\mathcal{P}^{-1}\mathcal{A}$. In the ideal case that $\delta = \Delta = \theta = \Theta = 1$, the bounds reduce to

$$\lambda \in \left[-\left(C_c + \frac{C_b^2}{\alpha} \right), \frac{1}{2} \left(C_a - \sqrt{C_a^2 + 2\beta^2} \right) \right] \cup \left[\alpha, \frac{1}{2} \left(C_a + \sqrt{C_a^2 + 4C_b^2} \right) \right].$$

Thus, ensuring that the eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$ are clustered away from the origin reduces to ensuring that α, the coercivity constant for a, and β, the inf-sup constant, are not too small, and that the boundedness constants C_a, C_b and C_c are not too large. As the ratios Δ/δ and Θ/θ get larger, so too do the intervals in Theorem 4 that contain the eigenvalues of $\mathcal{P}^{-1}\mathcal{A}$. Since Δ/δ and Θ/θ determine how well P_1 and P_2 approximate X and M, it is desirable to have preconditioners that that approximate these Gram matrices well.

6 Conclusions

In this manuscript we have described the necessary components for solving standard and generalized saddle point problems by iterative methods, irrespective of the application. In particular, we have given conditions for the unique solution of the saddle point problem, and shown that a sufficient ingredient is fulfillment of an inf-sup condition. When the saddle point problem requires discretization, another inf-sup condition must be satisfied on the finite dimensional discretization space.

To numerically solve the saddle point system we must solve a linear system involving a saddle point matrix, and conditions for its invertibility follow straightforwardly from those of the saddle point problem. Moreover, the spaces on which the saddle point problem are posed provide guidance for choosing a suitable block diagonal preconditioner. We have given bounds on the eigenvalues of the block preconditioned saddle point matrix and have indicated how they can be used to estimate the convergence rate of the MINRES Krylov subspace method applied to the linear system. These bounds show that coercivity and boundedness constants, as well as the inf-sup constant, are important not only for determining when the saddle point problem can be solved. Instead, these constants are integral to the whole solution process and, in conjunction with suitable bounds on the preconditioner blocks, provide valuable information about the solution of the linear system by preconditioned iterative methods.

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