

# **Receive array magnetic resonance spectroscopy: Whitenened Singular Valued Decomposition (WSVD) gives optimal Bayesian solution**

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## Abstract

Receive array coils play a pivotal role in modern magnetic resonance imaging. Magnetic resonance spectroscopy can also benefit from the enhanced signal-to-noise ratio and field of view provided by a receive array. In any experiment using an  $n$ -element array,  $n$  different complex spectra will be recorded and each spectrum unavoidably contains an undesired noise contribution. Previous algorithms for combining spectra have ignored the fact that the noise detected by different array elements is correlated. We introduce here an algorithm for efficiently, robustly and automatically combining these  $n$  spectra using noise whitening and the singular value decomposition ("WSVD") to provide the single combined spectrum that has maximum likelihood in the presence of this correlated noise. Simulations are performed that demonstrate the superiority of this approach to previous methods. Experiments in phantoms and *in vivo* on the brain, heart and liver of normal volunteers, at 1.5T and 3T, using array coils from 8 to 32 elements, and with  $^1\text{H}$  and  $^{31}\text{P}$  nuclei validate our approach, which provides SNR improvements of up to 60%. The WSVD algorithm becomes most advantageous for large arrays, when the noise is markedly correlated, and when the signal-to-noise ratio is low.

**Keywords:** MR spectroscopy, array, combination, WSVD.

## Introduction

Magnetic resonance (MR) spectroscopy provides unique insights into the chemical composition of a subject in a completely non-invasive manner. For example, chemical shift imaging (CSI) and single voxel spectroscopy (SVS) allow measurement of the concentrations of metabolites containing nuclei such as  $^1\text{H}$  and  $^{31}\text{P}$ , offering a window into biochemical processes occurring *in vivo*. Nevertheless, constraints on the signal-to-noise ratio (SNR) obtainable with current technology are one of the primary factors limiting clinical applications of MR spectroscopy. We report our recent work to alleviate this SNR limitation through an improved method for combining the data gathered from receive array coils.

Receive array coils have a long history in the magnetic resonance imaging community following the work of Hyde (1) and Roemer (2). By replacing the single radiofrequency receive coil in an MR scanner with an array of smaller coils (“array elements”), improvements in SNR are obtained. The smaller size of each of these elements makes it couple more strongly with the magnetisation in the subject under examination, giving stronger signals and hence a larger SNR than with a single element coil. Furthermore, although each element has a smaller field of view, the field of view covered by *at least one* coil may be very large. Thus when the signals from each element are combined appropriately, a receive array provides data of significantly enhanced SNR that cover a wider field of view. Roemer’s founding paper (2) on receive array MR imaging introduced a widely accepted model of the array detection process, which we use here to allow a unified description of existing methods for receive array combination in MR spectroscopy.

When dealing with MR spectroscopy data, processing inevitably begins by decoding the spatial information encoded by the pulse sequence applied in order to obtain effectively one free induction decay (FID) per voxel from each array element. These FIDs must then be reconciled to give a single FID (or spectrum) per voxel. Fig. 1 illustrates Roemer’s model of this process applied to a single voxel. The concepts apply equally well to single voxel spectroscopy, or 2D or 3D CSI when the voxels are analysed sequentially. Once the radiofrequency pulse sequence has been applied, the nuclear spins in the voxel precess producing a transverse magnetic field which couples with the elements of the array. In general the magnitude and phase of the signal received by each element differs: the signal  $\overline{s}_{i,k}$  received at time  $t_k$  from the  $i^{\text{th}}$  element is

$$\bar{s}_{i,k} = \bar{\alpha}_i q_k + \text{noise} \quad [1]$$

where  $q_k$  is the transverse magnetisation of the sample, *i.e.* the “perfect” free induction decay;  $\bar{\alpha}_i$  is a complex number representing the sensitivity and phase shift for the  $i^{\text{th}}$  element; and the noise is partially correlated. These values depend on the position of the excited voxel with respect to that element, on the design of the array, on the geometry and dielectric properties of the sample, and on the gain of that receiver channel. An equivalent relationship holds in the frequency domain

$$\bar{S}_{i,k} = \bar{\alpha}_i Q_k + \text{noise} \quad [2]$$

where  $\bar{S}_{i,k}$  is the  $k^{\text{th}}$  spectral component detected by the  $i^{\text{th}}$  element and  $Q_k$  is the corresponding spectral component of the sample magnetisation. Coil combination algorithms aim is to use data  $\bar{S}_{i,k}$  or  $\bar{s}_{i,k}$  from the receive array to recover  $q_k$  or  $Q_k$  in spite of the noise.

Roemer’s physical model has received most attention in the context of MR imaging. However, MR spectroscopy differs in several respects: spectroscopy is performed at lower resolution, but each voxel comprises complex data points with an additional chemical shift dimension; and importantly, spectra contain pure noise at extremes of chemical shift.

### Existing approaches to receive array MR spectroscopy

In his seminal paper, Roemer showed how to combine signals from an array with “maximum SNR” (2). His algorithms requires calibration experiments or detailed calculations (3,4) to determine the noise statistics and to determine the sensitivity and phase shift for each voxel and array element. In practice, this approach has not been widely used because the coil sensitivity and phase maps vary significantly with positioning and composition of the subject (3), especially with flexible array coils (4). Thus, field maps must be estimated for every subject, *e.g.* by comparing low resolution images from the array and a body coil (4). In practice, it is preferable to infer coil sensitivity maps from the data itself, much like the popular sum-of-squares method for array image combination which estimates them directly from the images (2).

The simplest ad hoc approach is to phase the spectra in each voxel manually and add them to give the combined spectrum for that voxel (5). This can be automated by fitting or integrating over a reference peak, using this to phase the spectra (3). The reference peak amplitudes can then be used to disregard

low SNR array elements (6). Better results are obtained by weighting the spectra according to the reference peak amplitudes (3) or SNRs (7) which approximate a matched filter. When performing  $^1\text{H}$  spectroscopy *in vivo*, particularly reliable reference peak data is obtained by repeating the experiment without water suppression since tissue contains water at  $\sim 40\text{M}$  concentration (8-11). Alternatively, one can use the whole chemical shift range of the spectra. Brown suggested scaling and phasing each spectrum by the first point in its FID (8), *i.e.* by the mean value of the spectrum. The singular value decomposition (SVD) also uses the whole spectra for combination (12). Yet notably, only Roemer's "maximum SNR" method deals properly with the fact that the noise in array spectra is correlated. Table 1 summarises these algorithms and defines short names that we use hereafter. Further details and references are found in reviews (13,14).

In the following pages, we formulate the combination problem afresh, employing Bayesian probability theory to dealing explicitly with the correlated noise that occurs experimentally. We introduce a simple and efficient "pre-whitened singular value decomposition" (WSVD) algorithm that finds the optimal (maximum likelihood) combined spectrum that is consistent with these data. We demonstrate the power of the WSVD approach using Monte Carlo simulations and experimental data from a phantom and from the human brain ( $^1\text{H}$ ), liver ( $^1\text{H}$ ) and heart ( $^1\text{H}$  and  $^{31}\text{P}$ ) at 1.5T and 3T.

## Theory

### Pre-Whitening (or "Noise standardisation")

According to Fig. 1 and Eq. [2], array spectra are not only scaled and phased but also contaminated with noise. In magnetic fields  $\geq 1\text{T}$  and with receive coils of diameter  $\geq 1\text{cm}$ , this is white Gaussian noise that arises predominantly from thermal fluctuations within the subject. All receive arrays exhibit correlation between the noise from different elements. Hence, the noise follows a multivariate normal distribution with zero mean and covariance matrix  $\Sigma$  (15-17). The WSVD algorithm begins by characterising the noise present in the data. For example, the covariance of noise samples from a region of the spectrum (or FID) that is devoid of signal approximates  $\Sigma$ .

To simplify the following analysis, we make a linear transformation of the received signals that removes the noise correlation and standardises the noise level. We calculate the Eigen decomposition of the noise covariance matrix

$$\Sigma = XDX^\dagger \quad [3]$$

where  $X$  is a unitary matrix of noise covariance eigenvectors,  $D$  is a diagonal matrix of eigenvectors and the dagger  $\dagger$  denotes the conjugate transpose. The scaling matrix

$$W = X(2D)^{-1/2} \quad [4]$$

standardises the noise correlations. Applying this transformation to the acquired spectra (or “element signals”)  $\bar{s}$  and to the as-yet-unknown element sensitivities  $\bar{\alpha}$  gives linear combinations, which we refer to as “channel signals”  $s$  and “channel sensitivities”  $\alpha$  :

$$s_{i,k} = \sum_j W_{ij} \bar{s}_{j,k} \quad \text{and} \quad \alpha_i = \sum_j W_{ij} \bar{\alpha}_j. \quad [5]$$

The inverse transformation, which recovers the individual element amplitudes from those for the channels, is

$$\bar{\alpha}_i = \sum_j (W^{-1})_{ij} \alpha_j = \sum_j \left( (2D)^{1/2} X^\dagger \right)_{ij} \alpha_j. \quad [6]$$

Applying the forward transformation to the noise covariance matrix

$$W^\dagger \Sigma W = (2D)^{-1/2} X^\dagger \Sigma X (2D)^{-1/2} = (2D)^{-1} D = I / 2 \quad [7]$$

yields a transformed noise correlation matrix that is diagonal ( $I$  is the identity matrix). Thus the “channels” are analogous to the elements of a hypothetical array, except that the noise in each channel is no longer correlated and is of identical amplitude. We rewrite Eq. [2] more simply in terms of channels as

$$S_{i,k} = \alpha_i Q_k + \text{uncorrelated noise with standard deviation } \sqrt{1/2} \quad [8]$$

and equivalently for Eq. [1] and proceed to analyse the data in terms of the channels ( $S_{i,k}$  or  $s_{i,k}$ ).

### Bayesian approach

Applying Bayes’ theorem (18,19) to the reconstruction problem, we write

$$P(\{\alpha_i\}, \{Q_k\} | \{S_{i,k}\}) = \frac{P(\{S_{i,k}\} | \{Q_k\}, \{\alpha_i\}) \times P(\{Q_k\}, \{\alpha_i\})}{P(\{S_{i,k}\})} \quad [9]$$

which is the probability of the channel sensitivities equalling  $\alpha_i$  and spectral points  $Q_k$  given the observed channel spectra  $S_{i,k}$ . The quantities in Eq. [9] are called

$$\text{posterior} = \frac{\text{likelihood} \times \text{prior}}{\text{evidence}} \quad [10]$$

According to Eq. [8], when written in terms of the real and imaginary parts of the spectra from each channel, the likelihood is

$$\begin{aligned} L &= P(\{S_{i,k}\} | \{Q_k\}, \{\alpha_i\}) \\ &= \prod_{i,k} \frac{\exp(-\Re(S_{i,k} - \alpha_i Q_k)^2)}{\sqrt{\pi}} \times \frac{\exp(-\Im(S_{i,k} - \alpha_i Q_k)^2)}{\sqrt{\pi}} \\ &= \prod_{i,k} \frac{\exp(-|S_{i,k} - \alpha_i Q_k|^2)}{\pi} \end{aligned} \quad [11]$$

We wish to solve Eq. [9] for the true spectrum  $Q_k$ . The channel amplitudes  $\alpha_i$  are therefore “nuisance parameters” which should be eliminated by integration to give the marginal posterior probability of the true spectrum given the channel data

$$\text{MPP} = P(\{Q_k\} | \{S_{i,k}\}) = \iint P(\{\alpha_i\}, \{Q_k\} | \{S_{i,k}\}) d\alpha_i^{\text{Re}} d\alpha_i^{\text{Im}} \quad [12]$$

in which  $\alpha_i = \alpha_i^{\text{Re}} + i\alpha_i^{\text{Im}}$ . For a particular guess at the spectrum  $Q_k$ , Eq. [12] gives the probability that this is consistent with the data recorded from the array.

### Singular value decomposition

If we are interested only in the maximum likelihood solution to Eq. [12], rather than the full distribution, we can proceed as follows. Since the exponential function increases monotonically, Eq. [11] implies that the maximum likelihood occurs at the minimum value of

$$\xi = \sum_{i,k} |S_{i,k} - \alpha_i Q_k|^2 \quad [13]$$

The optimal  $\alpha_i$  and  $Q_k$  may be found using the singular value decomposition (SVD) (20,21).

To see why, consider the numbers  $S_{i,k}$  as elements of an  $N_i \times N_k$  ( $N_i \leq N_k$ ) complex matrix  $\mathbf{S}$  which may be decomposed using the “economy size” SVD (22) thus

$$\mathbf{S} = \mathbf{U}\mathbf{\Psi}\mathbf{V}^\dagger \quad [14]$$

where  $\mathbf{U}$  is an  $N_i \times N_i$  matrix whose orthonormal columns are the left singular vectors of  $\mathbf{S}$ ,  $\mathbf{\Psi}$  is a diagonal matrix whose  $N_i$  elements, arranged in non-increasing order, are the singular values of  $\mathbf{S}$  and  $\mathbf{V}$  is an  $N_k \times N_i$  orthogonal matrix whose columns are the right singular vectors of  $\mathbf{S}$ .

The SVD decomposes a matrix,  $\mathbf{S}$  here, into a series of contributions of increasing rank with maximum power at each step (20, Theorem 5.9).

$$\mathbf{S} = \sum_j \psi_{j,j} \begin{pmatrix} u_{1,j} \\ \vdots \\ u_{N_i,j} \end{pmatrix} \begin{pmatrix} v_{1,j}^* & \cdots & v_{N_k,j}^* \end{pmatrix} \quad [15]$$

In this case, we wish to find the best rank-1 (vector) decomposition of  $\mathbf{S}$  in terms of two vectors: a column vector  $\mathbf{a}$  comprising the channel amplitudes  $\alpha_i$ ; and a row vector  $\mathbf{Q}^T$  containing the optimal spectrum  $Q_k$ . Taking only the first singular value gives the maximum likelihood solution to Eq. [12]:

$$\alpha_i = u_{i,1} / \phi \text{ and } Q_k = v_{k,1}^* \psi_{1,1} \times \phi \quad [16]$$

where  $\phi$  is an arbitrary complex scaling that reflects the fact that the overall phase of the sample magnetisation is not determined by the array data alone. To obtain the array *element* amplitudes and to produce combined maximum likelihood spectra, we use Eq. [6]:

$$\bar{\alpha}_i = \sum_j (W^{-1})_{i,j} u_{j,1} / \phi \text{ and } Q_k = \sum_j (W^{-1})_{k,j} v_{j,1}^* \psi_{1,1} \times \phi. \quad [17]$$

For a uniquely defined solution, we (arbitrarily) constrain the amplitude vector to have unit norm

$|\bar{\mathbf{a}}|^2 = 1$  so that the array has unit gain, and set the phase of the combined spectrum to match that of

the array element with the highest SNR, which we label “max”, by letting  $\phi = |\bar{\alpha}| \times \bar{\alpha}_{\max} / |\bar{\alpha}_{\max}|$  so that

$\bar{\alpha}_{\max} \geq 0$  and  $\bar{\alpha}_{\max} \in \mathbb{R}$ .

A useful measure of consistency (quality) of this combination is

$$\Gamma = \left( \frac{\|\mathbf{a}\mathbf{q}^T\|_F}{\|\mathbf{S}\|_F} \sqrt{N_i} - 1 \right) / (\sqrt{N_i} - 1) = \left( \frac{\psi_{1,1}}{\sqrt{\sum \psi_{i,i}^2}} \sqrt{N_i} - 1 \right) / (\sqrt{N_i} - 1) \quad [18]$$

$$1 \geq \Gamma \geq 0$$

The bounds arise because the singular values are by definition non-negative and in non-increasing order (20,21). Hence, for a perfect reconstruction,  $\psi_{i,i} = 0 \forall i > 1$ , and  $\Gamma$  tends to 1; in the worst case when the data are pure noise,  $\psi_{i,i} = \psi_{1,1}$  and hence  $\Gamma$  tends to 0.

### Multiple acquisitions

MR spectroscopy often requires signal averaging to obtain acceptable SNR, in which case two simple extensions of the WSVD algorithm are possible. Extending Eq. [1], the matrix of raw spectra from the  $j^{\text{th}}$  acquisition may be written  $\bar{\mathbf{S}}^{(j)}$  where  $j = 1 \dots N_{\text{rep}}$ .

When there is good stability in the frequency and phase of the spectra from each acquisition, it is simplest to average the results for each array element individually:

$$\bar{\mathbf{S}} = \sum_j \bar{\mathbf{S}}^{(j)} \quad [19]$$

before applying the WSVD algorithm.

If the relative phases of data from the different array elements are the same during each acquisition even though the overall amplitude, phase, and centre frequency may vary, one can perform the process over the entire data set by setting

$$\bar{\mathbf{S}} = \begin{pmatrix} \bar{\mathbf{S}}^{(1)} & \bar{\mathbf{S}}^{(2)} & \dots & \bar{\mathbf{S}}^{(N_{\text{rep}})} \end{pmatrix} \quad [20]$$

to give an  $N_i \times N_k N_{\text{rep}}$  matrix of data. The WSVD algorithm then calculates a  $1 \times N_k N_{\text{rep}}$  complex vector comprising the optimal combined spectra for each acquisition joined end-to-end. This procedure reduces the number of free parameters, giving combined spectra for each acquisition which are of higher SNR and therefore more amenable to accurate frequency correction before being averaged.

## Methods

### Simulations

Simulations comparing the WSVD algorithm with existing combination methods, excluding those requiring manual intervention or knowledge of  $B_1$  profiles (see Table 1), were performed as follows. The FID for a model spectrum comprising three Lorentzian peaks was calculated:

$$s(t) = \sum_{p=1}^3 a_p \exp(-d_p t + i2\pi\delta_p \nu_0 t). \quad [21]$$

Next, synthetic data modelling an 8-element array were generated by scaling and phasing by  $\alpha_i$  for each element before adding realistic correlated noise according to Eq. [1]. The synthetic data were input into the array combination algorithm under test, forming a single combined spectrum. This was processed with AMARES non-linear routines, from the MRUI software package (23-25), to yield fitted amplitudes for the three peaks, which could be compared against the true amplitudes  $a_p$ .

Further Monte Carlo simulations appraised the importance of accurate noise whitening as a function of SNR and arrays size. Inspired by measurements from an 8-element array, random noise covariance matrices  $\Sigma$  were generated as follows: diagonal elements were set to 38; the real and imaginary parts of elements above the diagonal were chosen from a normal distribution with zero mean and standard deviation  $3/\sqrt{2}$ ; corresponding elements below the diagonal were set to preserve Hermiticity; and correlations between array elements more than 16 places apart were set to zero. Noise covariance matrices are symmetric positive definite, so this procedure was repeated until such a matrix was produced. Combinations were made using the SVD alone, using the noise covariance matrix estimated from a region of the spectra between 15 and 35ppm containing 251 noise samples, and with the exact noise covariance matrix as would be determined by prior acquisition of noise samples. The three peaks in the combined spectrum were fitted by least squares.

### Experimental

The performance of different combination algorithms as a function of SNR was assessed using a phantom at 3T (Siemens Trio) using an 8-element  $^{31}\text{P}$  array (Rapid Biomedical) comprising anterior (4 elements + 1  $\times$   $^{31}\text{P}$  transmit) and posterior (4 elements) pieces. The phantom consisted of three loading phantoms (Siemens) and a vial containing sodium tripolyphosphate (STPP) dissolved in 17mL ultrapure water (0.4M solution) doped with  $\text{GdCl}_3$  (160 $\mu\text{M}$ ,  $T_1 = 300\text{ms}$ ). Data were first recorded overnight such

that 180 averages gave a good quality spectrum, whilst each acquisition gave  $\text{SNR} < 1$ . Averages were selected at random and combined according to Eq. [19] to produce data with intermediate SNR. For example, there are more than  $10^{31}$  combinations of 25 acquisitions, each producing 5x the SNR. To test performance at a particular SNR, 100 random combinations were chosen and processed using the WSVD and Brown's algorithms. To extend the SNR range, the experiment was repeated with 50x larger flip angle.

To demonstrate the WSVD algorithm in vivo, volunteers were recruited and scanned at 3T (Siemens Trio) or at 1.5T (Siemens Avanto) in accordance with UK law and the requirements of the University of Oxford. Point resolved spectroscopy (PRESS) (26,27), stimulated echo acquisition mode (STEAM) (26,28) and ultrashort echo time CSI (29) were used for localization. The WSVD algorithm was implemented in C++, using the LAPACK (30) and Boost (31) libraries in the Siemens Image Calculation Environment (ICE), and ran on the scanner. A Matlab reference implementation was used for simulations and off-line processing. The average processing time for 32 array elements with 2048 complex points is 16ms per spectrum in Matlab on a 3.16 GHz dual core system, and is faster on the scanner. Spectral fitting used AMARES (23-25).

## Results

### Simulations

Figs. 2 and 3 assess the quality of array combinations produced from synthetic data by four algorithms. Fig. 2 uses a single model spectrum to generate synthetic data which is supplied to the combination algorithms. The combined spectra formed from one set of synthetic data by the WSVD and Brown's algorithms are contrasted with the model spectrum in Figs. 2A and B. Neither algorithm completely eliminates the noise added during simulation. However, the baseline standard deviation is 2.44 for Brown's algorithm and only 2.02 for the WSVD algorithm.

Figs. 2C-F develop this comparison by repeating with 13600 different sets of synthetic data, fitting the combined spectra with AMARES (23-25) and plotting histograms of the fitted amplitudes of peak 3 (peaks 1 and 2 behave identically). The WSVD and unsuppressed water algorithms have the lowest standard deviation of fitted amplitude, *i.e.* they give the most consistent combined spectra. A red vertical line shows the true peak amplitude and a grey line shows the mean of the fitted amplitudes. The position of these lines differs least in the unsuppressed water algorithm, followed by the WSVD algorithm, indicating that these are the least biased.

Equivalent calculations were performed with the same noise covariance but different peak amplitudes to investigate the effect of SNR on the performance of the combination algorithms. Fig. 3 summarises the resulting distributions of fitted amplitudes of peaks 1 and 2 (peaks 2 and 3 behave identically). Figs. 3A1 and A2 plot the relative error in the mean of this distribution (a measure of bias) and Figs. 3B1 and B2 show the relative standard deviation (a measure of consistency) as a function of the model peak amplitudes  $a_1$  ("reference") on the x-axis and  $a_2 = a_3$  ("metabolite") on the y-axis. The coordinate corresponding to Fig. 2 is marked in white. All algorithms perform well when all peaks of interest in the spectrum have high SNR and fail eventually for low SNR. The performance of the WSVD algorithm compares favourably with the others, as discussed in detail below.

Similar plots in Fig. 4 examine the influence of the noise pre-whitening step in the WSVD algorithm for arrays with different numbers of elements. These demonstrate the significant advantage offered by the WSVD algorithm (right) compared to combination using the SVD but ignoring noise correlation (left) (12). This advantage increases with the number of array elements, providing that the noise is properly characterised (centre).

### Phantom

Fig. 5 compares experimentally the performance of the WSVD and Brown's algorithm as a function of SNR. When the noise dominates totally (left, 1 acquisition), neither method can recover the true spectrum. Thereafter, the WSVD produces combined spectra with higher SNR until the SNR becomes very high (far right). Then, both algorithms give the same peak signal which may be assumed to be the true value. The WSVD algorithm remains closer to this value as the SNR decreases and is therefore shown to be less biased than Brown's algorithm. These results confirm the theoretically anticipated advantages of the WSVD algorithm.

### In vivo

Fig. 6 shows a  $^{31}\text{P}$  cardiac spectrum acquired at 3T from the interventricular septum of a normal volunteer using the same 8-element  $^{31}\text{P}$  receive array as in Fig. 5. Both WSVD and Brown's combined spectra are reasonable, showing the anticipated phosphocreatine and ATP resonances. Significantly, however, the ratio of maximum absolute signal to baseline standard deviation is 60% higher for WSVD combination.

Fig. 7 shows a  $^1\text{H}$  spectrum acquired at 3T from the occipital lobe of a normal volunteer using 12 receive elements. These spectra have high SNR and it is readily apparent that the different combination methods all perform well as expected.

Fig. 8 shows a  $^1\text{H}$  spectrum acquired at 3T from the liver of a normal volunteer using 12 receive elements with ECG gating and breath holds. The WSVD and unsuppressed water algorithms give slightly higher SNR, although all algorithms performed well, because of the strong residual water signal at 0ppm.

Cardiac  $^1\text{H}$  spectra (not shown) were also acquired in 7 acquisitions during each of 8 breath holds with ECG gating using similar parameters, with 15 receive array elements (6 “BodyMatrix” and 9 “SpineMatrix”) at 3T. Data from all acquisitions were averaged per Eq. [19] and combined. The WSVD algorithm gave spectra of comparable to the unsuppressed water method.

Fig. 9 shows liver  $^1\text{H}$  spectra acquired using a 32-element receive array at 1.5T. Breath holds were employed but not ECG gating. Hence, noticeable motion-induced frequency shifts occurred between acquisitions. In this situation, the WSVD algorithm is best applied before averaging separate acquisitions as described near Eq. [20]. Inspecting Fig. 9, it is apparent that this approach provides comparable results to using prescans without water suppression for frequency correction and array combination.

## Discussion

### Comparison of methods

The performance of the WSVD and other combination algorithms was assessed in detail in Fig. 3 using synthetic data with a range of SNRs. Before comparing these algorithms, we note that all algorithms show a region of overestimation for very low intensity peaks (at the left of Fig. 3A1 and the bottom of Fig. 3A2). The origin of this artefact is illustrated in Fig. 10 for a simple case of a two-element array with a single peak of amplitude  $a/\sqrt{2}$  and uncorrelated noise ( $\sigma = 1$  in real and imaginary parts). Adding the spectra from each element, and dividing by  $\sqrt{2}$  for normalisation as defined above near Eq. [17], gives a spectrum with a peak of amplitude 1 and  $\sigma = 1$  which is denoted by the green curves in Fig. 10 and is to be compared with using the WSVD (blue) or Brown’s algorithm (magenta). Figs. 10A and C compare the mean fitted vs true amplitudes. All methods overestimate at low SNR because the amplitude changes from a normal to Rayleigh distribution. Since the Rayleigh distribution has non-zero mean, the fitted amplitudes are overestimated as the signal approaches the noise level. The green curve

in Fig. 10B shows the same effect for the standard deviation, which is constant at high SNR, but becomes  $\sqrt{2/(4-\pi)}$  times smaller.

Between these limiting cases, Fig. 10C and the blue areas in Figs. 3A show that the WSVD and Brown's algorithm tend to underestimate the fitted peak amplitude slightly. This occurs because these algorithms must estimate the relative phase of the signals from the array elements. This is like placing several unit vectors end-to-end. If there is some scatter in their orientations, the resultant vector will always be shorter than if they were all precisely aligned. Hence, data-driven algorithms underestimate the fitted amplitude of peaks with low SNR, although the WSVD is the least susceptible (Fig. 3) and closest to the theoretical limit (Fig. 10).

Fig. 3 also shows that combination with coil amplitudes from prescans with "unsuppressed water" is the least biased algorithm (A) and that it retains good precision in low SNR spectra (B). The simulation assumed that unsuppressed water peaks have sufficient SNR to determine the coil amplitudes exactly. The limits of this approach are seen in the "residual water" plots, which show significant bias and imprecision unless the reference peak (peak 1) is strong.

### Noise whitening

Initial noise whitening allows the maximum likelihood combined spectrum to be calculated efficiently from the SVD. With different reasoning, others have suggested using the SVD to combine images (32,33) and spectra (12) from receive arrays without accounting for noise correlations. Fig. 4 demonstrates the importance of noise whitening: with the exact noise covariance matrix, the WSVD algorithm is significantly less biased at all amplitudes and for all sizes of receive array than the SVD alone. Noise whitening also improves the precision at intermediate SNR. Noise whitening becomes progressively more beneficial in larger arrays, which suggests that its importance will grow in years to come.

Nevertheless, the WSVD algorithm does require a reliable estimate of the noise covariance matrix in order to realise these advantages. In Fig. 4 (centre), with only 251 noise samples, the WSVD algorithm remained effective for small arrays but with more elements, the bias and relative standard deviation increased even for relatively high SNR signals. These failings occur if the noise covariance matrix is poorly estimated. The accuracy of estimating covariance matrices is a well known problem, which could be tackled analytically in terms of Wishart distributions (34,35). Alternatively, numerical tests in Fig. 11 show a simple relationship between the number of array elements and the number of noise samples that are required to estimate the noise covariance matrix to a given precision in its eigenvalues. For

arrays containing up to 128 elements, convergence to 1% requires  $10^5$  noise samples. For example, for a 16x8x8 CSI experiment, the thermal noise is identical in every voxel and it suffices to take 100 noise samples from the spectrum in each voxel ( $16 \times 8 \times 8 \times 100 > 10^5$ ). These may be obtained by increasing the acquisition bandwidth without altering the length of acquisition.

When signal averaging is employed, noise samples should be accumulated separately from every average rather than processing only the averaged spectrum. For  $N$  noise samples  $n_{ki}$ , where  $k$  labels the spectral point and  $i$  the array element, accumulating the quantities  $\sum_k (n_{ki})^* n_{kj}$  and  $\sum_k n_{ki}$  allows the noise covariance matrix

$$(\Sigma)_{ij} = \frac{1}{N-1} \left( \sum_k (n_{ki})^* n_{kj} - \frac{(\sum_k n_{ki})(\sum_k n_{ki})}{N} \right) \quad [22]$$

to be calculated in a fixed amount of RAM.

It is important that the region where noise is sampled is not contaminated with signal. Although the derivation of the WSVD algorithm applies equally well to spectra and to FIDs, it is usually easier to obtain high quality noise samples in the frequency domain because in the time domain, it is necessary to sample for much longer than the longest  $T_2^*$  in the sample. Pulse sequences that implement phase cycling can sum the data separately to obtain signal and noise with high quality, minimising these difficulties.

Finally, it is easy to obtain noise samples by adding an additional acquisition before the first RF pulse in the pulse sequence. In long experiments, the time used would merely be part of the TR delay whilst waiting for recovery of longitudinal magnetization ready for the next repetition.

### Experimental demonstration

The  $^{31}\text{P}$  phantom experiments in Fig. 5 confirm experimentally the theoretical predictions from Figs. 3 and 10. In particular, when all the data is noise limited, neither the WSVD nor Brown's algorithm can form a sensible combined spectrum. At the other extreme, both algorithms produce essentially identical combined spectra with very high SNR data. In between, the WSVD algorithm gives higher SNR and less bias than Brown's algorithm.

Figs. 6-9 presented *in vivo* experiments performed in the human brain, heart and liver at 1.5T and 3T, on  $^1\text{H}$  and  $^{31}\text{P}$  nuclei and employing PRESS, STEAM and CSI localisation. In each case, spectra from the WSVD algorithm are credible, and have equal or higher ratio of peak amplitude to baseline standard deviation than those from other algorithms. Results for  $^1\text{H}$  spectra using unsuppressed water prescans were found not to be biased (Fig. 3). Thus the WSVD algorithm, which gives very similar results, is also not biased *in vivo*. This was confirmed by comparing a spectrum made with a single average with the full result from Fig. 7.

### Practical considerations

Methods that require manual intervention for array combination are undesirable because they introduce operator variability and quickly become intractable e.g. for CSI. Algorithms that require fitting to individual spectra suffer similar difficulties because they require prior information about the peaks to be fitted from the operator. Methods that require calibration experiments, such as Roemer's "maximum SNR" algorithm, are also undesirable in a clinical setting. The enduring popularity of the simple sum-of-squares algorithm (2) in MR imaging bears witness to this.

### Heteronuclear spectroscopy

Heteronuclear spectroscopy presents special challenges for array combination because there is no equivalent to the strong unsuppressed water reference peak. Combination using other reference peaks was seen in Fig. 3 to produce biased results unless the reference peak is strong. Baseline artefacts or small peaks overlapping the reference peak might cause similar difficulties. Strategies that employ  $B_1$  maps are also not feasible for many heteronuclear applications because there is normally no heteronuclear body coil, because heteronuclear imaging is slow, and because the  $T_1$  and  $T_2$  values for heteronuclear metabolites are not always well known. These make the data-driven WSVD algorithm particularly well-suited to heteronuclear spectroscopy.

### Multiple measurements

Spectra are often acquired using multiple measurements which immediately improves estimation of the noise covariance matrix via Eq. [22]. Furthermore, in Fig. 9 experimental results at 1.5T from the liver demonstrate that the WSVD algorithm gives opportunity for effective automated correction of motion-induced frequency shift artefacts through Eq. [20].

### Generalizations

The WSVD algorithm uses the simplest possible form of the likelihood, which means that the maximum likelihood combined spectrum can be determined using the SVD. This analysis can, in principle, be extended to admit more sophisticated models, containing prior knowledge about the spectra or element amplitudes.

### Procedure

In summary, we recommend the following procedure for receive array MR spectroscopy:

- (1) Increase acquisition bandwidth so that sufficient noise samples will be obtained.
- (2) Acquire spectra.
- (3) Accumulate noise samples from every repetition.
- (4) Check whether multiple repetitions have consistent phases and reference frequency.
- (5) If so, use Eq. [19] and apply the WSVD algorithm to give the combined spectra.
- (6) Otherwise, use Eq. [20] and apply the WSVD algorithm on all data; correct the phase and frequency of the combined spectra at each repetition; and average.

### Conclusions

The WSVD algorithm presented here combines spectra from receive array coils robustly, precisely and with minimal bias. It makes maximum use of the available data, handles correlations in the noise properly and is computationally efficient and stable for data of any quality. When there are strong “reference” peaks in the spectrum, the WSVD algorithm automatically uses them to determine the contributions from different elements, giving results as good as the best previously published approach. Yet, in the limit of very low SNR and without any strong spectral peaks, the WSVD algorithm remains especially effective. The WSVD algorithm is applicable to proton and heteronuclear spectroscopy.

We have characterized the WSVD algorithm by simulation, validated it through experiments on phantoms and demonstrated that it works in practice with in vivo experiments on the brain, heart and liver of normal volunteers at field strengths of 1.5T and 3T with a range of acquisition methods (CSI, STEAM, PRESS), coils containing up to 32 elements, and for  $^1\text{H}$  and  $^{31}\text{P}$  nuclei.

Since clinical MR now uses receive arrays routinely, we believe that a reliable, accurate and high SNR method of array combination is essential if spectroscopic acquisitions are to be integrated into clinical

practice. The WSVD approach provides the required functionality and should be adopted as the standard coil combination method for MR spectroscopy.

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## References

- Hyde JS, Jesmanowicz A, Froncisz W, Kneeland JB, Grist TM, Campagna NF. Parallel Image Acquisition from Noninteracting Local Coils. *J Magn Reson* 1986;70(3):512-517.
- Roemer PB, Edelstein WA, Hayes CE, Souza SP, Mueller OM. The NMR Phased Array. *Magn Reson Med* 1990;16(2):192-225.
- Hardy CJ, Bottomley PA, Rohling KW, Roemer PB. An Nmr Phased-Array for Human Cardiac P-31 Spectroscopy. *Magn Reson Med* 1992;28(1):54-64.
- Schaffter T, Bornert P, Leussler C, Carlsen IC, Leibfritz D. Fast H-1 spectroscopic imaging using a multi-element head-coil array. *Magn Reson Med* 1998;40(2):185-193.
- Maril N, Lenkinski RE. An automated algorithm for combining multivoxel MRS data acquired with phased-array coils. *J Magn Reson Imaging* 2005;21(3):317-322.
- Prock T, Collins DJ, Dzik-Jurasz ASK, Leach MO. An algorithm for the optimum combination of data from arbitrary magnetic resonance phased array probes. *Phys Med Biol* 2002;47(2):N39-N46.
- Wald LL, Moyher SE, Day MR, Nelson SJ, Vigneron DB. Proton Spectroscopic Imaging of the Human Brain Using Phased-Array Detectors. *Magn Reson Med* 1995;34(3):440-445.
- Brown MA. Time-domain combination of MR spectroscopy data acquired using phased-array coils. *Magn Reson Med* 2004;52(5):1207-1213.
- Dong ZC, Peterson B. The rapid and automatic combination of proton MRSI data using multi-channel coils without water suppression. *Magn Reson Imaging* 2007;25(8):1148-1154.
- Natt O, Bezkorovayny V, Michaelis T, Frahm J. Use of phased array coils for a determination of absolute metabolite concentrations. *Magn Reson Med* 2005;53(1):3-8.
- Barker PB, Soher BJ, Blackband SJ, Chatham JC, Mathews VP, Bryan RN. Quantitation of Proton NMR-Spectra of the Human Brain Using Tissue Water as an Internal Concentration Reference. *NMR Biomed* 1993;6(1):89-94.
- Sandgren N, Stoica P, Frigo FJ, Selen Y. Spectral analysis of multichannel MRS data. *J Magn Reson* 2005;175(1):79-91.
- Wright SM, Wald LL. Theory and application of array coils in MR spectroscopy. *NMR Biomed* 1997;10(8):394-410.
- Bydder M, Hamilton G, Yokoo T, Sirlin CB. Optimal phased-array combination for spectroscopy. *Magn Reson Imaging* 2008;26(6):847-850.
- Brown R, Wang Y, Spincemaille P, Lee RF. On the noise correlation matrix for multiple radio frequency coils. *Magn Reson Med* 2007;58(2):218-224.
- Hayes CE, Roemer PB. Noise Correlations in Data Simultaneously Acquired from Multiple Surface Coil Arrays. *Magn Reson Med* 1990;16(2):181-191.
- Redpath TW. Noise Correlation in Multicoil Receiver Systems. *Magn Reson Med* 1992;24(1):85-89.
- Brooks SP. Bayesian computation: a statistical revolution. *Philosophical Transactions of the Royal Society of London Series a-Mathematical Physical and Engineering Sciences* 2003;361(1813):2681-2697.
- MacKay DJC. Information theory, inference and learning algorithms. Cambridge: Cambridge University Press; 2005. xii, 628 p. p.

20. Trefethen LN, Bau D, III. Numerical Linear Algebra. 1997.
21. Golub GH, Van Loan CF. Matrix computations. Baltimore ; London: Johns Hopkins University Press; 1996. xxvii, 694 p. p.
22. Higham DJ, Higham NJ. MATLAB guide. Philadelphia: Society for Industrial and Applied Mathematics; 2005. xxiii, 382 p. p.
23. The MRUI Home Page.
24. Vanhamme L, van den Boogaart A, Van Huffel S. Improved method for accurate and efficient quantification of MRS data with use of prior knowledge. J Magn Reson 1997;129(1):35-43.
25. Naressi A, Couturier C, Castang I, de Beer R, Graveron-Demilly D. Java-based graphical user interface for MRUI, a software package for quantitation of in vivo/medical magnetic resonance spectroscopy signals. Comput Biol Med 2001;31(4):269-286.
26. De Graaf RA. In vivo NMR spectroscopy : principles and techniques. Chichester: John Wiley & Sons; 2007. xxi, 570 p., [578] p. of plates p.
27. Bottomley PA. Spatial Localization in NMR-Spectroscopy Invivo. Ann NY Acad Sci 1987;508:333-348.
28. Frahm J, Merboldt KD, Hancike W, Haase A. Stimulated Echo Imaging. J Magn Reson 1985;64(1):81-93.
29. Robson MD, Tyler DJ, Neubauer S. Ultrashort TE chemical shift imaging (UTE-CSI). Magn Reson Med 2005;53(2):267-274.
30. Anderson E. LAPACK users' guide. Philadelphia: Society for Industrial and Applied Mathematics; 1999. xxi, 407 p. p.
31. The Boost C++ Libraries. <http://www.boost.org/>.
32. Erdogmus D, Larsson EG, Yan R, Principe JC, Fitzsimmons JR. Asymptotic SNR-performance of some image combination techniques for phased-array MRI. Signal Processing 2004;84(6):997-1003.
33. Erdogmus D, Yan R, Larsson EG, Principe JC, Fitzsimmons JR. Image construction methods for phased array magnetic resonance imaging. J Magn Reson Imaging 2004;20(2):306-314.
34. Anderson TW. Asymptotic Theory for Principal Component Analysis. The Annals of Mathematical Statistics 1963;34(1):122-148.
35. Fey A, Van der Hofstad R, Klok MJ. Large Deviations for Eigenvalues of Sample Covariance Matrices, with Applications to Mobile Communication Systems. Advances in Applied Probability 2008;40(4):1048-1071.



## Figures and Tables

Short name	Source of amplitudes and phases	Prescan required	References
Maximum SNR	Calculated from predetermined coil $B_1^{Tx}$ and $B_1^{Rx}$ field maps, the measured noise resistance matrix and knowledge of the spatial location of the voxel of interest.	Yes, demanding prescan or calculation to measure field map.	Original (2), derivation via reciprocity theorem (13). Using noise resistance matrix and coil field maps (2,3). Estimate by comparing image from array and body coil (4).
Unsupp. water	Prescan for unsuppressed water peak ("1")	Yes, spectrum without water suppression. Only for $^1H$ .	(8,9)
Ref. Amplitude	Use amplitude of ever-present reference peak ("1") e.g. residual water for $^1H$ or PCr for $^{31}P$	No	(5) or PCr (3)
Ref. SNR	Use SNR of ever-present reference peak ("1")	No	(7)
Brown's	From first point in FID = mean of entire spectrum	No	(8) (15) or with absolute calibration using body coil (10).
Cut-off	Phase from strong peak ("1"). $ \bar{\alpha}_i  = 1$ unless below SNR limit.	No	(6)
SVD	Determined from whole spectrum. Strong peaks ("1", "2", and "3") all contribute.	No	(12,14,33)
WSVD	Determined from whole spectrum. Strong peaks ("1", "2", and "3") and noise all contribute.	No	This manuscript.

**Table 1: Summary of array combination algorithms for spectroscopy data. Peak numbering refers to the model spectrum in Fig. 2A. See text for further details.**

**Fig. 1: Roemer's model of a receive array. Each element in the array receives signals from the voxel indicated, but with different magnitudes and phases because of the differing  $B_1$  sensitivity patterns of the coils comprising the receive array. Raw cardiac  $^{31}\text{P}$  spectra are drawn for each array element along with the WSVD combination (see Fig. 6 for details).**

**Fig. 2: Preliminary Monte Carlo comparison of WSVD and three previous array combination algorithms (defined in Table 1). A and B: Model spectra (smooth line) were calculated according to Eq. [21], with damping  $d_p = 50\text{Hz}$ , reference frequency  $\eta_0 = 49\text{MHz}$  (i.e. approximate  $^{31}\text{P}$  frequency at 3T), 1024 time points with 4kHz bandwidth, chemical shifts  $d_p = 0, -6$ , and  $-9\text{ppm}$  and amplitudes  $a_1 = a_2 = a_3 = 10^{1.1} \gg 12.6$ . The noise covariance matrix  $\Sigma$  was taken from a preliminary 3D UTE-CSI  $^{31}\text{P}$  cardiac experiment analogous to Fig. 6. Noisy lines: combined spectra. D-F: Calculations were repeated 13600 times at the Oxford Supercomputing Centre to obtain smooth distributions of fitted peak amplitudes.**

**Fig. 3: Monte Carlo comparison of the effect of SNR on array combination algorithms. For each pixel, simulations were as Fig. 2, but used a model spectrum whose peak amplitudes are indicated on the x- and y-axes. A1: Colours show the relative error in the fitted amplitude of peak 1, A2 shows peak 2, which was essentially identical to peak 3 (not shown). B1 and B2 show corresponding relative standard deviations in the fitted amplitudes. Calculations were repeated 102 times for each pixel at the Oxford Supercomputing Centre.**

**Fig. 4: Monte Carlo simulations demonstrating the importance of accounting for noise correlations in SVD-based array combination for the model peak amplitudes on the x-axis, and numbers of array elements on the y-axis. Noise covariance matrices  $\Sigma$  were generated as described in the methods. Coil amplitudes were  $\bar{a}_i = i^{-1} / \hat{a} \sum_{j=1}^{N_i} j^{-2}$ , modelling a typical array with a few well-positioned elements. A: relative error of the least-squares fitted amplitudes for peak 3, and B: corresponding relative standard deviations. Combinations were made ignoring noise correlation (left), estimating  $\Sigma$  from 251 baseline points (centre), and using the exact  $\Sigma$  (right). Calculations were repeated 8000 times at the Oxford Supercomputing Centre to obtain smooth distributions.**

**Fig. 5: Effect of data SNR on the performance of the WSVD and Brown's algorithms. Two sets of 2D CSI measurements were made on the  $^{31}\text{P}$  phantom for a grid of  $8 \times 8$  voxels with dimensions  $25 \times 25 \times 25\text{mm}$  with  $\text{TR}=1500\text{ms}$ ,  $\text{TE}=2.3\text{ms}$ , reference frequency mid-way between a strong  $^{31}\text{P}$  doublet, 2048 data points per FID and 8 kHz bandwidth. Left: 180 averages with tiny flip angle, Right: 192 averages with larger flip angle. Top: Mean and standard deviation of combined spectrum peak signal. Bottom: Corresponding measured SNR.**

**Fig. 6: Comparison of combination algorithms applied to a cardiac 3T  $^{31}\text{P}$  spectrum.** Spectra are normalised to the baseline standard deviation for clarity. Data were acquired using the 8-element array from Fig. 5 from a  $15 \times 15 \times 25\text{mm}$  voxel located in the interventricular septum (see inset) of a normal volunteer with a 3D UTE-CSI sequence (29), for  $16 \times 16 \times 8$  voxels, with  $\text{TR} \approx 900\text{ms}$  (i.e. 1 R-R interval), acquisition weighting with 10 averages at  $k=0$ , 4kHz bandwidth and 1024 points per FID. Total measurement time was 30min. Two saturations bands suppressed the anterior chest muscle signal. A spectrally narrow RF pulse was employed. Spectra are normalised to the baseline standard deviation for clarity.

**Fig. 7: Comparison of combination algorithms applied to  $^1\text{H}$  spectroscopy of the brain at 3T** using a 12-channel  $^1\text{H}$  “HeadMatrix” birdcage receive coil (Siemens) running in Triple mode and body coil transmit. Localisation was achieved with both point resolved spectroscopy (PRESS) (26,27) with  $\text{TE}=30\text{ms}$  and a voxel of size  $20 \times 20 \times 20\text{mm}$  in the occipital lobe of a normal volunteer and water suppression. Additional scans were made without water suppression for the “unsuppressed water” combination method. For the WSVD and Brown’s algorithm, the residual water peak was deleted from the spectrum before combination. Similar results (not shown) were obtained with STEAM localization ( $\text{TR}=2\text{s}$  and  $\text{TE}=20\text{ms}$ ). Spectra are normalised to the baseline standard deviation for clarity.

**Fig. 8: Comparison of combination algorithms for  $^1\text{H}$  single voxel spectroscopy of the liver.** Data were acquired at 3T using the body coil for transmit and 12 elements from the Siemens “BodyMatrix” (6) and “SpineMatrix” (6) receive array coils operating in Triple mode. Acquisition employed a water suppressed (STEAM) pulse sequence (26,28) with parameters:  $\text{TM}=7\text{ms}$ , 4 kHz bandwidth,  $\text{TR} \approx 2\text{s}$  (i.e. 2 R-R intervals),  $\text{TE} = 10\text{ms}$  and a voxel of size  $14 \times 20 \times 33\text{mm}$ . To minimise errors due to motion spectra were collected in 6 acquisitions during each of 10 breath holds. Spectra are normalised to the baseline standard deviation for clarity.

**Fig. 9: Single voxel  $^1\text{H}$  spectrum of the liver acquired at 1.5T (Siemens Avanto) using a 32-element cardiac receive array (Siemens, Germany) with STEAM localization,**  $\text{TR}=1500\text{ms}$ ,  $\text{TE}=20\text{ms}$ ,  $\text{TM}=10\text{ms}$ , 2 kHz bandwidth, 2048 points per FID, body coil transmit and voxel dimensions  $20 \times 20 \times 20\text{mm}$ . ECG gating was not used to test for robustness in the presence of motion-induced artefacts. WSVD combination followed Eq. [20] to give combined spectra for each acquisition which were automatically frequency and phase corrected using the data point with maximum absolute value. Unsuppressed water combination used a prescan without water suppression to determine the relative amplitude and phase for each array element, before combining the data for each acquisition. The residual water peak in each of these spectra was then fitted in order to correct for variations in phase and frequency between acquisitions before averaging. Spectra are normalised to the baseline standard deviation for clarity.

**Fig. 10: Comparison of coil combination algorithms for idealized model with a single Lorentzian peak and normally distributed noise ( $\sigma = 1$ ), or from two spectra with model peak amplitude  $1/\sqrt{2}$  in each and with independently normally distributed noise of standard deviation 1. The sum of the two spectra has the same distribution as the single spectrum. A: Mean least squares fitted amplitudes from single spectrum (green), or combining with WSVD or Brown's algorithm. B: Standard deviation of the fitted amplitudes. C: Relative error in the fitted amplitudes. D: Relative standard deviation in the fitted amplitudes. In all plots, the limiting Gaussian and Rayleigh distributions are shown with black and red dotted lines.**

**Fig. 11: Number of noise samples required for convergence of noise covariance matrix eigenvalues for arrays comprising 2-128 elements (see legend). A covariance matrix is drawn at random as for Fig. 4, samples of correlated noise are generated and then used to estimate the noise covariance matrix. Data points show the maximum absolute % error in the eigenvalues. Best fit lines are drawn to guide the eye.**