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Multiway Canonical Correlation Analysis of Brain Signals

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Abstract

Brain signals recorded with electroencephalography (EEG), magnetoencephalog-2 raphy (MEG) and related techniques often have poor signal-to-noise ratio due to 3 the presence of multiple competing sources and artifacts. A common remedy is 4 to average over repeats of the same stimulus, but this is not applicable for tempo-5 rally extended stimuli that are presented only once (speech, music, movies, natu-6 ral sound). An alternative is to average responses over multiple subjects that were 7 presented with the same identical stimuli, but differences in geometry of brain 8 sources and sensors reduce the effectiveness of this solution. Multiway canonical 9 correlation analysis (MCCA) brings a solution to this problem by allowing data 10 from multiple subjects to be fused in such a way as to extract components common 11 to all. This paper reviews the method, offers application examples that illustrate 12 its effectiveness, and outlines the caveats and risks entailed by the method. 13

14 **1** Introduction

Stimulus-driven signals recorded with electroencephalography (EEG), magne-15 tencephalography (MEG) and related techniques compete with much stronger 16 sources within the brain, the body, and the environment. The signal of interest 17 usually represents only a fraction of the signal power at the electrode or sensor. 18 To overcome the noise and artifacts, a common practice is to present the same 19 stimulus multiple times and average the responses over repeated presentations. 20 Supposing that the response is the same for all presentations, and the noise is un-21 correlated between presentations, the signal-to-noise power ratio (SNR) improves 22 with the number of repeats. SNR can be further improved by combining sig-23 nals across sensors, i.e. spatial filtering. Spatial filters can be optimized based 24 on assumptions about signal and noise (de Cheveigné and Parra, 2014), and this 25

²⁶ combination of temporal averaging and spatial filtering can greatly improve the
²⁷ SNR. However, averaging and optimization are not applicable if the stimulus is
²⁸ presented only once, for example because it is too long to be repeated (e.g. a long
²⁹ sample of speech or music), or because one wishes to probe a phenomenon likely
³⁰ to fade with repetitions (e.g. surprise).

Instead of presenting the same stimulus multiple times to one subject, one 31 can also present the same stimulus to multiple subjects just once. To the extent 32 that different subjects' brains are functionally similar, we expect similar responses 33 (Hasson et al., 2004; Dmochowski et al., 2012; Lankinen et al., 2014). Unfortu-34 nately, the position or orientation of neural sources relative to sensors or electrodes 35 is likely to differ across subjects, so averaging over subjects in sensor space is sub-36 optimal. In order to compare between subjects, or average over subjects, we first 37 need some way to transform the data of each to a common representation that is 38 comparable across subjects. This can be accomplished with spatial filters that are 39 tuned to each individual subject (e.g. Haxby et al., 2011; Lankinen et al., 2014). 40

Canonical Correlation Analysis (CCA) is a powerful technique to find lin-41 ear components that are correlated between two data matrices (Hotelling, 1936). 42 Given two matrices X_1 and X_2 of size $T \times d_1$ and $T \times d_2$, CCA produces trans-43 form matrices V_1 and V_2 of sizes $d_1 \times d_0$ and $d_2 \times d_0$, where d_0 is at most equal 44 to the smaller of d_1 and d_2 . The columns of $\mathbf{Y}_1 = \mathbf{X}_1 \mathbf{V}_1$ are of norm 1 and mutu-45 ally uncorrelated between each other, as are the columns of $\mathbf{Y}_2 = \mathbf{X}_2 \mathbf{V}_2$, while, 46 more importantly, corresponding columns from each ("canonical correlate pairs") 47 are maximally correlated. The first pair of canonical correlates (CC) defines the 48 linear combinations of each data matrix with the highest possible correlation be-49 tween them. The next pair of CCs defines the most highly correlated combination 50 that is uncorrelated from the first pair, and so-on. Applied to data from two sub-51 jects, CCA can find spatial filters that maximize the brain activity common to 52

⁵³ both, transforming both subject's data so that they can more easily be compared
⁵⁴ or averaged. However, CCA does not address the issue of comparing or merging
⁵⁵ responses across more than two subjects.

Extensions to connect multiple data matrices have been proposed under names 56 such as multiple CCA (Gross and Tibshirani, 2015; Witten and Tibshirani, 2009), 57 multiway CCA (Sturm, 2016; Zhang et al., 2011), multiset CCA (Takane et al., 58 2008; Correa et al., 2010b,a; Hwang et al., 2012; Lankinen et al., 2014; Zhang 59 et al., 2017; Via, Javier, Ignacio Santamaria and Pérez, 2005; Li et al., 2009), or 60 generalized CCA (Kiers et al., 1994; Afshin-Pour et al., 2012; Melzer et al., 2001; 61 Tenenhaus, 2011; Tenenhaus et al., 2015; Velden, 2011; Fu et al., 2017). This 62 diversity in names covers a diversity of formulations (Kettenring, 1971) that all 63 share the aim of finding components that are similar across data matrices. Recent 64 progress addresses regularization (Tenenhaus, 2011), sparsity (Fu et al., 2017; 65 Tenenhaus et al., 2015), missing data (van de Velden and Takane, 2012), nonlin-66 earity (Melzer et al., 2001), or deep learning (Benton et al., 2017). Using similar 67 techniques, independent Component Analysis (ICA) has been generalized under 68 the name of group ICA (GICA) (Eichele et al., 2011; Calhoun and Adali, 2012; 69 Huster et al., 2015; Huster and Raud, 2018). 70

CCA has been used extensively for brain data analysis and modality fusion 71 (Sui et al., 2012; Dähne et al., 2015; Dmochowski et al., 2017), and several studies 72 have applied multiway CCA (MCCA) and variants thereof to merge data across 73 subjects (Correa et al., 2010b; Afshin-Pour et al., 2012, 2014; Lankinen et al., 74 2014; Zhang et al., 2017; Li et al., 2009; Hwang et al., 2012; Karhunen et al., 75 2013; Haxby et al., 2011; Lankinen et al., 2014; Sturm, 2016; Zhang et al., 2017; 76 Lankinen et al., 2018). This paper builds on those studies with the aim to better 77 understand the range of applicability of the tool, what is achieved, and what are 78 the caveats. We describe a simple formulation of MCCA that is easy to understand 79

⁸⁰ and explain.

We show that MCCA can be applied effectively to multi-subject datasets of 81 EEG or fMRI, both to *denoise* the data prior to further analyses, and to *summarize* 82 the data and reveal traits common across the population of subjects. MCCA-83 based denoising yields significantly better scores in an auditory stimulus-response 84 classification task, and MCCA-based joint analysis of fMRI data reveals detailed 85 subject-specific activation topographies. The aims of this paper are (a) to provide 86 an intuitive understanding of MCCA, (b) investigate ways in which it can be put 87 to use, and (c) demonstrate its effectiveness for a range of common tasks in the 88 analysis of brain data. 89

90 2 Methods

In this section we describe a simple formulation of MCCA, show how it can be applied to a variety of tasks, and give details of the real and synthetic data sets used by the examples reported in the Results.

94 2.1 Data analysis

Signal model. Assume a data set consisting of N data matrices, each comprised 95 of a time series matrix \mathbf{X}_n of dimensions T (time) $\times d_n$ (channels). These could 96 represent EEG, MEG or fMRI data recorded from N different subjects in response 97 to the same stimulus. They could also be data from multiple imaging modalities 98 gathered from the same subject. Each matrix X_n consists of linear combinations 99 of a set of sources S common to all data matrices, to which is added a "noise" ma-100 trix N_n of sources uncorrelated with S, and uncorrelated with the noise matrices 101 $N_{n'\neq n}$ added to the other data matrices: 102

$$\mathbf{X}_n = \mathbf{A}_n \mathbf{S} + \mathbf{N}_n,\tag{1}$$

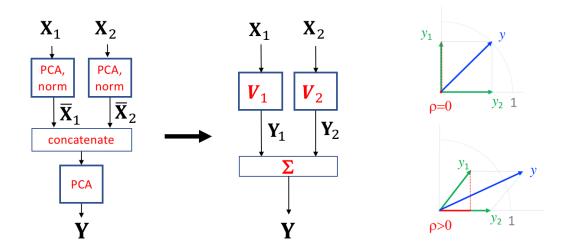


Figure 1: Block diagram of the simple CCA formulation. Left: each data matrix is whitened by PCA followed by normalization. Normalized PCs from both data matrices are concatenated side by side and submitted to a final PCA. Center: the matrix \mathbf{Y} of summary components (SC) can be expressed as the sum of individual transforms $\mathbf{Y}_1 = \mathbf{X}_1 \mathbf{V}_1$ and $\mathbf{Y}_2 = \mathbf{X}_2 \mathbf{V}_2$ (canonical correlates, CC). The transforms \mathbf{V}_1 and \mathbf{V}_2 combine the whitening and PCA matrices. Right: rotating vectors y_1 and y_2 to maximize the norm of their sum is equivalent to maximizing their correlation coefficient ρ symbolized by the projection of y1 on y2 (red line).

where A_n is a mixing matrix specific to subject *n*. The sources S might represent brain sources or networks driven by the same stimulus similarly across different subjects. We are interested in finding these "shared sources" and suppressing the noise. Note that this model assumes that responses of different subjects share the same source *time course*, but not necessarily the same spatial pattern over channels. The assumption of uncorrelated noise is usually only approximately met, due to spurious correlations.

A simple CCA formulation. Consider two data matrices, X_1 and X_2 of size $T \times d$ where T is time and d the number of channels. All data are assumed to have

¹¹² zero mean. Each matrix is spatially whitened by applying principal component ¹¹³ analysis (PCA) and scaling each principal component (PC) to unit norm to obtain ¹¹⁴ whitened matrices $\bar{\mathbf{X}}_1$ and $\bar{\mathbf{X}}_2$. Whitened data are then concatenated and submit-¹¹⁵ ted to a new PCA to obtain a matrix $\mathbf{Y} = [\mathbf{X}_1, \mathbf{X}_2]\mathbf{V}$ of size $T \times 2d$, where \mathbf{V} ¹¹⁶ combines the whitening and second PCA matrices (Fig. 1 left). The submatrices ¹¹⁷ \mathbf{V}_1 and \mathbf{V}_2 formed of the first and last d rows of \mathbf{V} define transforms applicable ¹¹⁸ to each data matrix:

$$\mathbf{Y}_1 = \mathbf{X}_1 \mathbf{V}_1, \tag{2}$$
$$\mathbf{Y}_2 = \mathbf{X}_2 \mathbf{V}_2,$$

with $\mathbf{Y} = \mathbf{Y}_1 + \mathbf{Y}_2$ (Fig. 1 center).

The outcome of this analysis is equivalent to standard CCA, as explained in the Discussion, the first *d* columns of \mathbf{Y}_1 and \mathbf{Y}_2 forming canonical pairs (within a scaling factor). Indeed, rotating $\bar{\mathbf{X}}_1$ and $\bar{\mathbf{X}}_2$ to maximize the correlation of the resulting \mathbf{Y}_1 and \mathbf{Y}_2 , as required by the CCA objective, is equivalent to rotating with the goal of maximizing the norm of their sum, $\mathbf{Y}_1 + \mathbf{Y}_2$, as achieved by the second PCA (Fig. 1 right). The appeal of this formulation is that it is easily extendable to multiple data matrices.

A simple MCCA formulation. Consider N data matrices \mathbf{X}_n each of size $T \times d$ 127 with zero mean. Each data matrix is spatially whitened by applying PCA and 128 scaling all PCs to unit norm to obtain whitehed matrices $\bar{\mathbf{X}}_n$. Whitehed data are 129 then concatenated along the component dimension and submitted to a second PCA 130 to obtain a matrix $\mathbf{Y} = [\mathbf{X}_1 \dots \mathbf{X}_N] \mathbf{V}$ of size $T \times D$, D = Nd, where \mathbf{V} combines 131 the whitening and second PCA matrices (Fig. 2 left). The submatrices V_n of V of 132 size $d \times D$ formed by extracting successive d-row blocks of V define transforms 133 applicable to each data matrix: 134

$$\mathbf{Y}_n = \mathbf{X}_n \mathbf{V}_n,\tag{3}$$

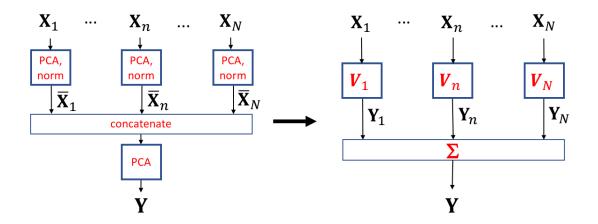


Figure 2: Block diagram of the simple MCCA formulation. Left: each data matrix \mathbf{X}_n is whitened by PCA followed by normalization. Normalized PCs from all data matrices are concatenated side by side and submitted to a final PCA. Right: the matrix \mathbf{Y} of summary components (SC) can be expressed as the sum of individual transforms $\mathbf{Y}_n = \mathbf{X}_n \mathbf{V}_n$ (canonical correlates, CC).

with $\mathbf{Y} = \sum_{n} \mathbf{Y}_{n}$ (Fig. 2, right). If data matrices have different numbers of chan-135 nels d_n , then \mathbf{V}_n has size $d_n \times D$ where $D = \sum_n d_n$. We call the columns of \mathbf{Y}_n 136 canonical correlates (CCs) by analogy with CCA, and those of Y summary com-137 ponents (SC). Each SC is a sum of CCs over data sets. Columns of Y are mutually 138 orthogonal by virtue of the final PCA, but the same is not usually true of \mathbf{Y}_n . With 139 D > d columns, \mathbf{Y}_n forms an *overcomplete basis* of the patterns spanned by \mathbf{X}_n . 140 This formulation of MCCA is equivalent to the SUMCORR formulation of Ket-141 tenring (1971) as explained in the Discussion (Parra, 2018). The appeal of this 142 formulation is that it is conceptually and computationally straightforward. PCs 143 can be discarded from the initial PCAs, so as to control dimensionality and limit 144 overfitting effects (next section). 145

The variances of the summary components (the columns of **Y**) reflect the degree to which temporal patterns are shared between data matrices (Fig. 3) – the variance of each SC corresponding to the degree of correlation of each shared

dimension found in the data. If the data matrices X_n share no components, the variances of all SCs are one (Fig. 3 a). If a component is shared by all N data matrices, the norm of the first SC is N (Fig. 3 d). For data matrices with a small number of samples, spurious correlations may cause the variance profile to be skewed (Fig. 3 b). In real data, shared activity often shows up as components with variance elevated relative to this background (Fig. 3 c).

Reduced-rank MCCA. It is often convenient to reduce the rank of each data 155 matrix $ilde{\mathbf{X}}_n$ to $\mathring{d} < d$ by discarding PCs with smallest variance after the initial 156 PCA. The MCCA transform matrices \mathbf{V}_n are then of size $d \times \mathring{D}$, $\mathring{D} = N\mathring{d}$, and 157 the CC and SC matrices of size $T \times \mathring{D}$. This serves as a form of regulariza-158 tion that avoids computational issues with rank-deficient data, reduces the risk of 159 overfitting, and limits computation and memory requirements. Importantly, this 160 approach preserves the constraint that the resulting SCs are uncorrelated (Parra et 161 al., 2018). 162

Dealing with data matrices with more channels than samples. CCA fails if the data matrices have fewer samples than channels $(T \le d)$, as is typically the case for fMRI or calcium imaging data for which there are many more voxels or pixels than observation samples (Asendorf, 2015). A simple solution is to replace each data matrix \mathbf{X}_n (size $T \times d$) by a matrix \mathbf{X}_n of size $T \times \mathbf{T}$ with $\mathbf{T} < T$ columns that capture the principal temporal patterns spanned by \mathbf{X}_n . This can be done by applying singular value decomposition (SVD) to express the data as

$$\mathbf{X}_n = \mathbf{U}\mathbf{S}^{\mathsf{t}}\mathbf{V} \tag{4}$$

and setting $\mathring{\mathbf{X}}_n = \mathring{\mathbf{U}}$ where $\mathring{\mathbf{U}}$ consists of the first \mathring{T} columns of \mathbf{U} . Since the $\mathring{\mathbf{X}}_n$ have more samples than channels there is no obstacle to applying MCCA to them. This sequence of operations can be represented by a set of transform matrices

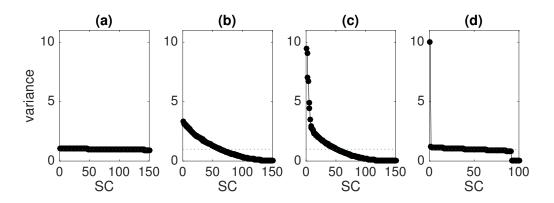


Figure 3: Behavior of the SC variance as a function of order for MCCA analyses applied to 4 different types of dataset, each involving 10 data matrices. (a) Each data matrix consisted of an independent 10000×15 matrix of Gaussian white noise. In this case the SC variance profile is flat since there is no (or little) correlation between data matrices. (b) Each data matrix consisted of a 165×15 matrix of independent and uncorrelated Gaussian noise. In this case the SC variance profile is skewed, reflecting spurious numerical correlations between the statistically independent columns. (c) Each data matrix consisted of a 165×15 matrix of values derived from fMRI responses of 10 subjects in response to 165 sounds. Prior to MCCA the 6309 voxels were reduced to 15 channels using SVD (see description of Example 6 in the Methods). (d) Each data matrix consisted of a 10000×10 matrix of Gaussian white noise with an embedded sinusoid (Example 1, Fig. 4) that was the same in all data matrices. In the last two examples, only a small subset of the MCCA components reflect shared activity as evident by the low SC variance at higher MCCA orders.

¹⁷³ \mathbf{V}_n of size $d \times N\mathring{T}$. Applying them to the data yields canonical correlate and ¹⁷⁴ summary matrices of size $T \times N\mathring{T}$. Using this approach, it is straightforward to ¹⁷⁵ apply MCCA to datasets with a large number of "channels" such as data from ¹⁷⁶ calcium imaging or fMRI. An alternative to SVD is to apply PCA to ^t \mathbf{X}_n and use ¹⁷⁷ a subset of the matrix of projection vectors to form $\mathring{\mathbf{X}}_n$, a useful option if \mathbf{X}_n is ¹⁷⁸ too large to fit in memory (the required covariance matrix can be calculated in ¹⁷⁹ chunks).

180 2.2 Applications of MCCA

Quantifying correlation between N data matrices. The variance of each column of Y indicates the degree to which a component is shared across data matrices. The value is 1 if the data matrices are perfectly uncorrelated, and N if all data matrices include that component (Fig. 3). The profile of variances over SCs thus offers a measure of "sharedness" between data matrices (but see Caveats).

Summarizing a set of data matrices. The first few columns of $\mathbf{Y} = \sum_{n} \mathbf{Y}_{n}$ represent temporal patterns that capture most of the correlation across data matrices \mathbf{X}_{n} . They form a basis of the signal subspace that contains those shared patterns.

Denoising. Each data matrix \mathbf{X}_n may be denoised by projecting it to the overcomplete basis of CCs, selecting the first $\mathring{D} < D$ components, and projecting back. We refer to this procedure as "denoising", as it can be used to attenuate components that are least shared across subjects. This can be summarized by a denoising matrix \mathbf{D}_n product of the first \mathring{D} columns of \mathbf{V}_n by the first \mathring{D} rows of its pseudoinverse. The denoised data are obtained as $\tilde{\mathbf{X}}_n = \mathbf{X}_n \mathbf{D}_n$.

Dimensionality reduction. Dimensionality reduction is often performed by applying PCA to a data matrix and truncating the PC series (Cunningham and Yu,
2014). However, this equates relevance to variance, which may not be appropriate
because noise sources can have high variance and useful targets small variance.
MCCA can be used to weight dimensions according to their *consistency across data matrices*, which may be a better criterion than variance.

Outlier detection. Temporally-local glitches and artifacts may interfere with data interpretation and analysis. Analysis algorithms based on least-squares are particularly sensitive to high-amplitude artifacts. MCCA can be used to derive a cross-subject 'consensus' response, so that individual subject's data points that deviate greatly from the consensus can be flagged as outliers and excluded from analysis.

208 2.3 Details of the evaluation examples

The methods are evaluated using six datasets, including synthetic data, EEG, and fMRI.

Example 1 - sinusoidal target in separable noise. Synthetic data for this ex-211 ample consisted of 10 data matrices, each of dimensions 10000 samples \times 10 212 channels. Each was obtained by multiplying 9 Gaussian noise signals (indepen-213 dent and uncorrelated) by a 9×10 mixing matrix with random coefficients. To 214 this background of noise was added a "target" consisting of a sinusoidal time se-215 ries (Fig. 4, left) multiplied by a 1×10 mixing matrix with random coefficients. 216 The target was the same for all data matrices, but the mixing matrices differed, as 217 did the noise sources. The SNR was set to 10^{-20} , i.e. a very unfavorable SNR, 218 but because the noise is not of full rank the target and background are in principle 219

²²⁰ linearly separable.

Example 2 - sinusoidal target in non-separable noise. Synthetic data for this example consisted of 10 matrices of dimensions 10000 samples \times 10 channels, each obtained by multiplying 10 Gaussian noise sources (independent and uncorrelated) by a 10 \times 10 mixing matrix with random coefficients. To this background was added a sinusoidal target as in the previous example, with SNR varied as a parameter. The noise here is full rank so the target and background are not linearly separable.

Example 3 - sinusoidal target in EEG noise. Data for this example used EEG 228 to simulate realistic neural activity as background noise. EEG data were recorded 229 during approximately 20 minutes from one subject in the absence of any task, 230 from 40 electrodes (32 standard positions plus additional electrodes on forehead 231 and temple) at 2048 Hz sampling rate with a BioSemi system. A robust polyno-232 mial detrending routine (de Cheveigné and Arzounian, 2018) was used to remove 233 slow drifts. Ten "data matrices" were produced by selecting three-second inter-234 vals of EEG data with random offsets, removing their means, and adding a target 235 consisting of 4 cycles of a 4 Hz sinusoid multiplied by a 1×40 mixing matrix 236 with random coefficients, renewed for each data matrix. The SNR of the target 237 was varied as a parameter. 238

Example 4 - EEG response to tones. Data for this example were borrowed from a study on auditory attention (Southwell et al., 2017). EEG data were recorded using a 64-channel EEG system in response to 120 repetitions of a 1 kHz tone pip with interstimulus interval (ISI) randomized between 750 and 1550 ms (recorded for the purpose of locating electrodes responsive to sound). Data from a subset of 10 subjects were detrended using a robust detrending routine,

bad channels were interpolated using spherical interpolation (EEGLAB), and the 245 data were filtered between 2-45 Hz. A peristimulus epoch of duration 1.2 s (start-246 ing 0.2 s prestimulus) was defined for each trial, and the corresponding data were 247 extracted as a 3D matrix of dimensions time \times channel \times trial. For each channel, 248 the 0.2 s prestimulus waveform was averaged over trials and subtracted from that 249 channel's waveform ("baseline correction"). After applying the first PCA (of the 250 two-step MCCA) to each subject, the first 30 PCs were retained and the remainder 251 discarded. 252

Two analyses were performed on these data to try to extract the cortical re-253 sponse to the 1 kHz tone from the background EEG noise. In the first, repetition 254 over trials was exploited to design a spatial filter for each subject using the joint 255 diagonalization algorithm (JD) that maximizes the ratio of trial-averaged variance 256 to total variance (de Cheveigné and Simon, 2008; de Cheveigné and Parra, 2014). 257 This resulted in a set of 10 analysis matrices of size 64×30 , one for each subject. 258 In the second analysis, MCCA was applied, using 30 PCs from each subject in the 259 first PCA, resulting in 10 subject-specific analysis matrices of size 64×300 . 260

For each subject, the first column of the JD analysis matrix defines the best linear combination of channels to maximize repeat-reliability across trials, while the first column of the MCCA analysis matrix defines the best linear combination of channels to maximize correlation with the other subjects.

Example 5 - EEG response to speech. Data for this example were taken from a study on auditory cortical responses to natural speech (Di Liberto et al., 2015). The same data were also used in a recent study on the application of CCA to speech/EEG decoding (de Cheveigné et al., 2018). We borrowed the data from the first study, and the decoding methods and evaluation metrics from the second, with the purpose of evaluating the benefit of introducing a denoising stage based

²⁷¹ on MCCA before the speech/EEG decoding stage.

In brief, EEG data were recorded from 8 subjects using a 128-channel BioSemi 272 system with standard electrode layout, at 512 Hz sampling rate. Each subject lis-273 tened to 32 speech excerpts, each of duration 155 s, from an audio book, presented 274 diotically via headphones, for a total of approximately 1.4 hours. The database in-275 cluded both the audio stimuli and the EEG responses. Further details about the 276 stimulus and recording are available in Di Liberto et al. (2015). The EEG were 277 preprocessed (downsampling to 64 Hz, detrending, artifact removal), and the stim-278 ulus temporal envelope calculated as described in de Cheveigné et al. (2018). 279

A decoding model (de Cheveigné et al., 2018; Dmochowski et al., 2017) was evaluated according to several metrics: correlation, d-prime, and percent-correct classification scores for a match vs mismatch classification task. The classification task consisted in deciding whether a segment of EEG matched the segment of stimulus of same duration that produced it (match) or some unrelated segment (mismatch). The duration of the segment was varied as a parameter from 1 to 64 S.

This task is related to that of determining which of two concurrent voices is 287 the focus of a listener's attention (cocktail party phenomenon) (Ding and Simon, 288 2012; Fuglsang et al., 2017; Lalor et al., 2009; Khalighinejad et al., 2017; Koski-289 nen and Seppä, 2014; Martin et al., 2014; Mesgarani and Chang, 2012; Mirkovic 290 et al., 2015; O'Sullivan et al., 2014; Tiitinen et al., 2012; Zion Golumbic et al., 29 2013), of potential use for the "cognitive control" of an external device such as 292 a hearing aid. The decoding model used CCA to relate the stimulus to the EEG 293 response, producing multiple stimulus-response CC pairs that were used for dis-294 crimination. Further details of the decoding model, classification task, and metrics 295 can be found in de Cheveigné et al. (2018). Here, we are only interested in know-296 ing if scores for single-source decoding are improved by introducing a stage of 297

EEG denoising based on MCCA.

For this denoising, the EEG data of each subject were submitted to MCCA, keeping 40 PCs in the first PCA, resulting in a 128×320 analysis matrix for each subject. The first 110 columns of this matrix were multiplied by the first 110 rows of its pseudoinverse to yield a 128×128 subject-specific denoising matrix. This has the effect of attenuating activity that is *least* correlated with the other subjects.

Example 6 - fMRI response to natural sounds. Data for this example were 304 taken from a study that measured fMRI responses to natural sounds (Norman-305 Haignere et al., 2015). Responses were gathered from 10 subjects to each of 165 306 sounds belonging to 11 categories including speech, music, animal vocalizations, 307 and others. For each subject, the recording session was repeated either twice or 308 3 times. See Norman-Haignere et al. (2015) for further details. For the present 309 analysis, data for each subject were averaged over repeats and organized as a 310 matrix \mathbf{X}_n of 165 sounds \times 6309 voxels (voxels from both hemispheres were 311 used, and voxels outside a subject-specific region of interest that included primary 312 and secondary auditory cortex were set to zero). In this analysis we are interested 313 in finding particular profiles of response over sounds (for example speech vs non-314 speech, or music vs non-music) and also the brain areas associated with such 315 profiles in each subject. 316

As there are more "channels" (voxels) than samples (T < d), an SVD was used as described in the Methods and the first 10 dimensions were used for MCCA. The columns of \mathring{X}_n are white so the first PCA can be dispensed of. Matrices \mathring{X}_n were concatenated and subjected to the second-step PCA of the MCCA algorithm, and the 15 first columns (arbitrary number) of the SC matrix were selected as a basis spanning the profiles over sounds that were most similar across subjects.

To find profiles specific to particular sound categories (e.g. speech, music,

etc.), Joint Decorrelation (de Cheveigné and Parra, 2014) was used to find a linear transform applicable to the 15-column basis to maximize the variance over the selected category, relative to the other categories. This can be seen as a rotation of the basis so as to isolate activity specific to processing of that sound category. This 165×1 activation profile was then cross-correlated with the 165×6309 matrix of fMRI response data of each subject to find the topography specific to that subject (Haufe et al., 2014).

331 3 Results

The MCCA method is evaluated first with synthetic data to get an understanding of its basic properties and capabilities, and then with real EEG and MEG data to see whether these extend to situations of practical use.

335 3.1 Synthetic data

Example 1 - sinusoidal target in separable noise. The data consist of 10 ma-336 trices made up of a sinusoidal target (Fig. 4, left) common to all data matrices, 337 with added noise distinct across matrices (see Methods). At the unfavorable SNR 338 of 10^{-20} the target is not visible in the raw signal of any of the data matrices 339 (Fig. 4 center), and it cannot be extracted by averaging because of the extremely 340 low SNR and the fact that the mixing coefficients are of random sign. Since the 341 data are separable (the rank of the noise is only 9), the target can be recovered by 342 applying the appropriate demixing matrix (inverse of the mixing matrix), however 343 that matrix is unknown. 344

MCCA applied to the dataset produced projection matrices V_n that recover the target from X_n (Fig. 4 right). This benefit is similar to that of methods that leverage multiple repetitions to blindly discover spatial filters to improve SNR

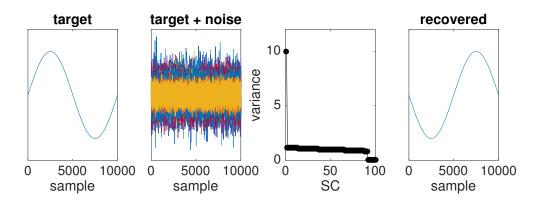


Figure 4: Simulation with separable noise. Left: target signal. Next to left: target in noise at $SNR=10^{-20}$. Next to right: variance of SCs as a function of order. The variance of the first SC is equal to 10 as target is perfectly shared across subjects and mixed in separable noise. Right: target recovered by MCCA (with arbitrary sign).

(de Cheveigné and Simon, 2008; de Cheveigné and Parra, 2014), but instead of
repetitions, MCCA leverages the fact that the same target is mixed into multiple
data matrices. To summarize, MCCA can reveal a target common across data
matrices despite an extremely unfavorable SNR.

Example 2 - sinusoidal target in non-separable noise. Data are the same as in 352 the previous example, except that the noise is full rank (10 independent sources 353 mixed in 10 channels) so the target is no longer linearly separable, and one cannot 354 expect to recover the target perfectly, especially at extremely low SNRs. Nonethe-355 less, at a moderately unfavorable SNR (10^{-2} in power) MCCA can recover an 356 estimate of the target that is noisy (Fig. 5 center) but much cleaner than the raw 357 data (not shown). Figure 5 (right) shows the proportion of residual noise in the 358 signal recovered by MCCA as a function of SNR, together with the same pro-359 portion for the best raw channel. MCCA provides a clear benefit over a range 360 of SNRs. Two factors can contribute to failure: non-separability per se, and the 36 fact that the algorithm fails to find the ideal demixing matrix. Figure 5 (right) also 362

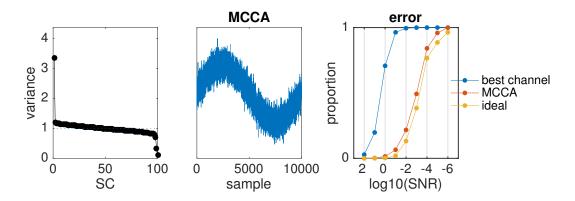


Figure 5: Simulation with inseparable noise. Left: variance of SCs as a function of their order at $SNR=10^{-2}$. Center: target signal recovered from mixture at $SNR=10^{-2}$. Right: proportion of residual noise power as a function of SNR for the raw data (blue), first SC (red) or ideal demixing matrix (yellow).

shows the proportion of residual noise for the ideal demixing matrix (yellow). The
 MCCA-derived matrix performs only slightly less well than the ideal matrix. To
 summarize, MCCA is of use even if the data are not separable.

Example 3 - sinusoidal target in real EEG noise. EEG background noise dif-366 fers from the white Gaussian noise that was used in the previous simulations in 367 several ways: it usually has full rank (in particular because of electrode-specific 368 noise), but the variance is unequally distributed across dimensions. It is also 369 temporally structured, with strong temporal correlation and an overall low-pass 370 spectrum. The first component recovered by MCCA is plotted in Fig. 6 (right) 37 for several values of SNR. For SNRs of 0.1 or better the target is almost per-372 fectly recovered. At SNR=0.03 the recovered waveform is somewhat noisy, and 373 at SNR=0.01 or below the target is lost. For comparison Fig. 6 (left) shows the 374 time course of a raw data channel (the channel that showed the largest correlation 375 with the target). For SNR=10 the target waveform is obvious in the raw data, but 376 for smaller values of SNR it is lost in the EEG noise. Comparing Fig. 6 left and 377

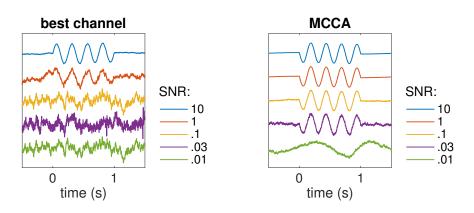


Figure 6: Simulation with EEG noise. Left: time course of the best raw data channel for several values of SNR. Right: time course of the first MCCA component for several values of SNR.

right, there is a range of SNRs (roughly 0.03 to 1) for which MCCA provides a
clear benefit. Below SNR=0.03 the algorithm switched to some other component
within the data (Fig. 6 right, lowest trace) that happened to be similar across data
matrices because of random correlations.

To summarize, MCCA is effective at extracting a weak target from within real EEG noise.

384 3.2 Real data.

Example 4 - EEG response to tones. In this example, contrary to the previous 385 one, the target is not known. However, since the data were collected in response 386 to multiple repeats and for multiple subjects, we can apply two different methods 387 (JD and MCCA) to isolate stimulus-evoked activity common to all subjects and 388 compare the results. JD finds a linear transform that optimizes signal to noise 389 ratio assuming that the signal repeats over trials. Figure 7 (top) shows the result 390 of applying the JD analysis to the data of one subject. In the plot on the top left, 391 the blue line shows the mean over repeats of the first component, and the gray 392 band shows ± 2 SD of a bootstrap resampling of this mean. On the top right is 393

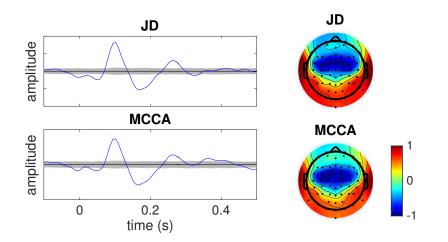


Figure 7: Comparison between JD solution (within-subject repeat-reliability) and MCCA solution (between-subject similarity) for one subject among ten. Data were in response to repeated tones. Left: average over trials (blue) and ± 2 SD of a bootstrap resampling (gray) of the first JD component, which maximizes reliability across trials (top), or first subject-specific CC (bottom). Right: associated topographies (correlation between trial-averaged component and trial-averaged electrode waveforms).

the topography associated with this component (computed as the map of cross-394 correlation coefficients between the component and each channel (Haufe et al., 395 2014)). MCCA can similarly be used to design a subject-specific spatial filter that 396 improves SNR. The plots on the bottom of Figure 7 show the result of applying 397 the subject-specific matrix derived from the MCCA analysis for the same subject. 398 Despite the different criteria used by the two analyses (consistency over trials for 399 JD, consistency between subjects for MCCA) the patterns are remarkably similar. 400 To summarize, it appears that MCCA can exploit between-subject consistency to 401 find a spatial filter that is as effective as that found by JD that exploits between-402 trial consistency. This is useful for data that do not involve repeated trials. 403

The subject-specific MCCA analysis matrices (\mathbf{V}_n) transform each subject's data (\mathbf{X}_n) into CCs (\mathbf{Y}_n) that are well correlated across subjects so that it makes

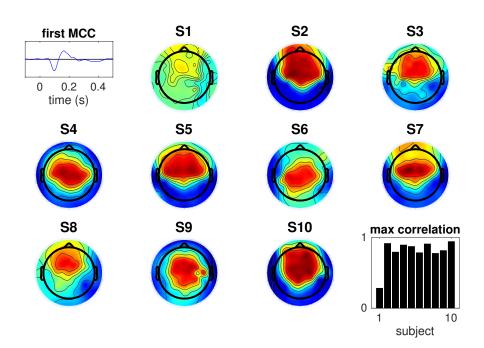


Figure 8: MCCA analysis of tone response, summary over 10 subjects. Top left: trial-averaged time course of the first SC. Bottom right: maximum absolute value of correlation between that component and each electrode, for each subject. Other panels: topography of correlation values (of the SC with each electrode) for each subject (the color code is the same as in Fig. 7, bottom).

sense to average them across subjects and interpret the SCs (Y) as reflecting 406 shared activity. Figure 8 top left shows the trial- and subject-averaged time course 407 of the first SC, which can be interpreted as our best estimate of stimulus-evoked 408 activity common to all subjects. It benefits from several stages of enhancement: 409 (a) spatial filtering within each subject, (b) averaging over trials, (c) averaging 410 across subjects. Also shown in Fig. 8 are the ten subject-specific topographies 411 associated with this component. Despite some differences, topographies are quite 412 similar across most subjects except S1. The bottom left plot shows the maxi-413 mum over electrodes of the correlation coefficient between the first SC and each 414 electrode (trial-averaged). Correlation coefficients are relatively high except for 415 Subject 1 for whom the EEG response did not match the other subjects. 416

Example 5 - EEG response to speech. For stimuli presented once only, one 417 cannot use repetition to distinguish the brain response from the noise. Instead, 418 systems identification techniques (Lalor et al., 2009; Holdgraf et al., 2017; Crosse 419 et al., 2016) are used to fit an encoding model to estimate the part of brain response 420 that is driven by the stimulus, using some representation of the stimulus (e.g. 421 envelope or spectrogram) that can be linearly related to the brain signals. The part 422 of the response that fits the model can be taken as the "true" response, and the 423 rest discarded as noise. However, this partition is contingent on the validity of 424 the stimulus representation and the quality of the model. With MCCA, a "ground 425 truth" response can instead be estimated based on similarity of brain responses 426 across subjects. 427

EEG were recorded in response to continuous speech (see Methods), and a 428 model was fit to stimulus and response to capture their correlation (de Cheveigné 429 et al., 2018; Dmochowski et al., 2017). The model used CCA to form pairs of 430 maximally-correlated linear transforms of the audio stimulus features and of the 431 EEG respectively (audio-EEG CCs). Note that this usage of CCA is unrelated 432 to our usage of MCCA to merge data across subjects. The quality of that model 433 was evaluated using a match vs mismatch classification task (see Methods). We 434 compute *correlation*, *d-prime* and *percent correct* classification scores to evaluate 435 the benefit of inserting a stage of MCCA-based denoising within the EEG prepro-436 cessing pipeline. 437

Figure 9 (a) shows the correlation between the first audio-EEG CC pair (thick blue line) and subsequent pairs (thin lines), with and without MCCA-based denoising, for one subject. To the extent that correlation is limited in part by EEG noise, the higher scores on the right suggest that denoising was effective. The d-prime metric measures the degree of separation between distributions of correlation scores for matched and mismatched segments. Figure 9 (b) shows the

d-prime metric for the first pair (thick blue) and subsequent pairs (thin lines), 444 with and without MCCA-based denoising for segments of duration 64 s. The dot-445 ted line shows the d-prime metric for the multivariate distributions of audio-EEG 446 CC pairs. The larger d-prime scores with MCCA-based denoising suggest that it 447 can effectively contribute to improved discrimination. Figure 9 (c) shows classi-448 fication scores as a function of segment duration with (red) and without (black) 449 MCCA-based denoising. The higher scores with MCCA-based denoising show its 450 benefit for this task. Figure 9 (d) shows that a similar benefit is found in all sub-451 jects. The thick lines are scores for a duration of 16 s, whereas the thin lines are 452 for segments of 2 s (lowest lines) or 64 s (highest lines). To summarize, MCCA is 453 of benefit as a denoising tool for EEG responses to speech. 454

Example 6 - fMRI responses to natural sounds Data were taken from a study 455 that investigated fMRI responses to natural sounds (Norman-Haignere et al., 2015), 456 in which 10 subjects listened to a set of 165 sounds belonging to 11 different 457 classes. MCCA was applied to find patterns of selectivity to sound that were com-458 mon across subjects as explained in the Methods. In brief, the 165×6309 matrix 459 of voxel activations for each subject was reduced to a 165×12 matrix using SVD, 460 the reduced matrices concatenated, and submitted to PCA to obtain a 165×120 461 matrix of SCs. Their variances are plotted in Fig. 10 (top left). The first 10 SCs 462 were subjected to a JD analysis to enhance the contrast between musical sounds 463 (classes 'Music' + 'VocalMusic') and other sounds as explained in the Methods. 464

The profile of activation over sounds of the first JD component is plotted in Fig. 10 (top right), with sounds ordered by class and coded as different colors. Activations of the first two classes ('Music' + 'VocalMusic') are clearly distinct from that of the other classes. The corresponding topography of activation over voxels for each subject can be calculated by cross-correlating this component with

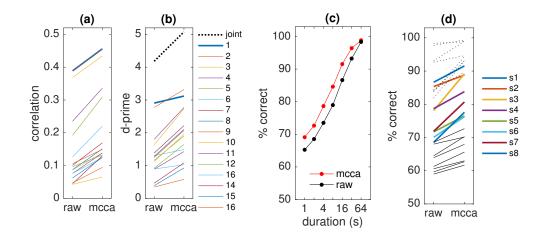


Figure 9: Speech-EEG decoding. (a) Correlation coefficient for the audio-EEG first CC pair (thick blue line) and subsequent pairs (thin lines) for a CCA model, with and without MCCA-based denoising. (b) d-prime metric for a classification task for the first audio-EEG CC pair (thick blue line) and subsequent pairs (thin lines), with and without MCCA-based denoising. The dotted line is for multivariate classification based on all CC pairs. (c) Percentage correct classification as a function of interval duration, with and without MCCA-based denoising. (d) Percentage correct for intervals of duration of 16s (thick lines) for 8 subjects, with and without MCCA-based denoising. Thin lines are scores for 64 s (uppermost) or 2 s (lowermost).

the profile of activation over sounds of each voxel. Topographies for the left hemi-470 sphere for all subjects are plotted in Fig. 10 (bottom). To a first approximation, to-47 pographies are consistent in that a dorso-frontal concentration of activity is found 472 in most subjects. To a second approximation, each topography includes additional 473 regions, suggesting a wider network of activation that is more subject-specific. 474 Such subject-specific details would be smoothed out by averaging over subjects. 475 A similar JD analysis to enhance speech-specific activation revealed patterns with 476 more ventral topographies (not shown). The outcome of this analysis is consis-477 tent with that reported by Norman-Haignere et al. (2015) using an ICA-related 478 technique. 479

The benefit of MCCA here can be interpreted in terms of dimensionality re-480 duction, based here on consistency across subjects rather than variance as with 481 PCA. Dimensionality reduction allowed the final JD analysis to be performed on 482 a matrix of size $165 \times 12 \times 10$ rather than $165 \times 6309 \times 10$, making it more 483 effective by reducing overfitting. If PCA had been used instead of MCCA, the 484 12 selected dimensions might well have been dominated by noise. Using MCCA 485 ensures that they are instead dominated by activity similar across subjects, which 486 is likely to be relevant because all subjects heard the same stimuli. 487

This example demonstrates that MCCA can be applied also to data with more channels (pixels or voxels) than data points. MCCA offers a powerful, alternative, way of summarizing the high-dimensional data without having to explicitly model what parts of the brain response are driven by the stimulus features.

492 **4 Discussion**

⁴⁹³ MCCA finds a linear transform applicable to each data matrix within a data set ⁴⁹⁴ to align them to common coordinates and reveal shared patterns. It can be used

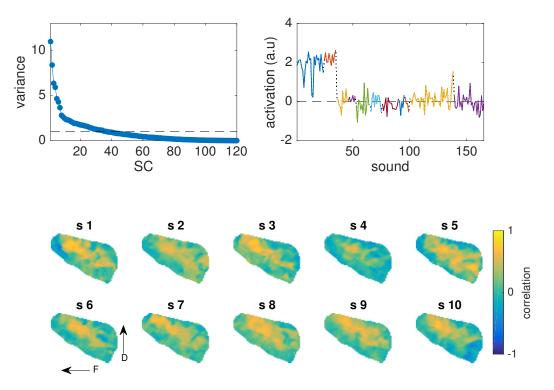


Figure 10: MCCA of fMRI responses to natural sounds. Top left: SC variance as a function of order. Top right: activation as a function of sound of a component selective for music obtained by applying JD to the first 15 SCs (see text). Each color represents a different sound category; the first two categories are 'music' and 'vocal music'. Bottom: topographies of correlation between the music-selective JD component and the profile of response over sound of each voxel of the right hemisphere, for each subject.

in several ways: as a *denoising* tool applicable to an individual data matrix, as a tool for *dimensionality reduction*, as a tool to *align* data matrices within a common space to allow comparisons, or as a tool to *summarize* data and reveal patterns that are general across data matrices. As formulated here, MCCA is easy to understand, straightforward to apply, and computationally cheap. Care is nonetheless required when applying it, in particular to avoid phenomena such as overfitting.

As reviewed in the Introduction, several versions of MCCA have What is new? 50[.] been proposed in the literature and applied to the analysis of brain data. The 502 contributions of this paper are the following. First, the formulation as a cascade 503 of PCA, normalization, concatenation, and PCA offers an intuitive explanation 504 that may help practitioners gain insight into this method. Past formulations may 505 be hard to follow for the non-mathematically inclined, and their sheer number is 506 bewildering. We used a similar 2-step formulation in a recent tutorial on joint 507 decorrelation (de Cheveigné and Parra, 2014), and we hope that the present paper 508 too will have tutorial value. Second, our usage of MCCA as a denoising tool, 509 to attenuate noise within individual subjects based on across-subject consistency 510 by projection on the overcomplete basis of its SCs, seems to be new. Third, we 511 provide tutorial examples that may encourage researchers to put MCCA to work 512 for a wider range of tasks, including denoising, outlier detection, summarization, 513 and cross-subject statistics. 514

How does it work? The effect of the processing steps is schematized in Fig. 11. Multiple data matrices contain the same source component S, illustrated as a color gradient, mixed here into two 2-dimensional data matrices (Fig. 11 a). Each point represents a sample in time (row of the data matrix) and the two axes represent two channels (columns of the data matrix). The color could represent a hidden sensory response that is similar across two subjects. The initial PCAs sphere each

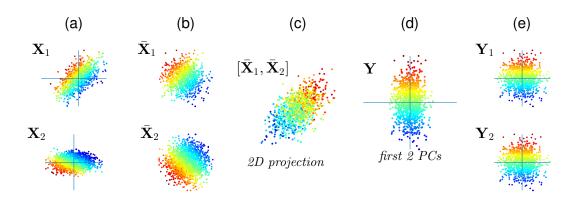


Figure 11: Principle of MCCA. (a) Several data matrices share a common component (coded as color) but its orientation and nature are unknown. (b) Whitening makes the data matrices free to rotate. (c) Concatenation creates a cloud in 4D space (projected here to 2D) with a direction of greater correlation/variance due to the shared component. (d) The second PCA aligns this direction with the axes. (e) In the process, the whitened data matrices are rotated such that shared dimensions are maximally aligned.

data matrix (b), so that the cloud of points is free to rotate in any direction. However, concatenating the sphered data matrices creates a cloud (in a 4-dimensional space) that is not spherical because of the shared component correlation along some direction in 4-D space (projected to 2D in panel (c)). The second PCA finds this direction of correlation between the data matrices and aligns it with the first axis (d), in the process transforming each data matrix so that it is optimally aligned with the other (e).

Relation with other formulations of CCA and MCCA As explained by Parra (2018), the aim of MCCA is to find projection vectors \mathbf{v}_n applicable to \mathbf{X}_n that maximize the ratio of between-set to within-set covariance:

$$\rho = \frac{1}{N-1} \frac{r_B}{r_W} \tag{5}$$

531 with:

$$r_B = \sum_{n} \sum_{n' \neq n} {}^{\mathrm{t}} \mathbf{v}_n \mathbf{R}_{nn'} \mathbf{v}_n$$
$$r_W = \sum_{n} {}^{\mathrm{t}} \mathbf{v}_n \mathbf{R}_{nn} \mathbf{v}_n.$$

where $\mathbf{R}_{nn} = {}^{t}\mathbf{X}_{n}\mathbf{X}_{n}$ and $\mathbf{R}_{nn'} = {}^{t}\mathbf{X}_{n}\mathbf{X}_{n'}$ are covariance and cross-covariance matrices of the data. The divisor 1 - N ensures that ρ scales between 0 and 1. Setting to zero the derivative of ρ with respect to \mathbf{v}_{n} , the solution is obtained by solving the equation

$$\mathbf{R}\mathbf{v} = \mathbf{D}\mathbf{v}\lambda,\tag{6}$$

536 with

$$\mathbf{R} = \begin{bmatrix} \mathbf{R}_{11} & \mathbf{R}_{12} & \cdots & \mathbf{R}_{1N} \\ \mathbf{R}_{21} & \mathbf{R}_{22} & \cdots & \mathbf{R}_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{R}_{N1} & \mathbf{R}_{N2} & \cdots & \mathbf{R}_{NN} \end{bmatrix}, \mathbf{D} = \begin{bmatrix} \mathbf{R}_{11} & 0 & \cdots & 0 \\ 0 & \mathbf{R}_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_{NN} \end{bmatrix},$$
(7)

where $\lambda = \rho/(N-1) + 1$. Now, first decompose $\mathbf{D} = \mathbf{U} \mathbf{\Lambda}^{t} \mathbf{U}$. Because \mathbf{D} is the block-diagonal matrix of the covariances in each data set, this decomposition implies doing PCA on each data set separately, i.e whitening each data set. With this decomposition Eq. 6 can be rewritten as:

$$\mathbf{R}\mathbf{v} = \mathbf{U}\mathbf{\Lambda}^{\mathsf{t}}\mathbf{U}\mathbf{v}\lambda$$
$$\mathbf{\Lambda}^{-1/2 \mathsf{t}}\mathbf{U}\mathbf{R}\mathbf{v} = \mathbf{\Lambda}^{1/2 \mathsf{t}}\mathbf{U}\mathbf{v}\lambda$$
$$[\mathbf{\Lambda}^{-1/2} \mathsf{t}\mathbf{U}\mathbf{R}\mathbf{U}\mathbf{\Lambda}^{-1/2}][\mathbf{\Lambda}^{1/2 \mathsf{t}}\mathbf{U}\mathbf{v}] = [\mathbf{\Lambda}^{1/2 \mathsf{t}}\mathbf{U}\mathbf{v}]\lambda$$
$$\tilde{\mathbf{R}}\tilde{\mathbf{v}} = \tilde{\mathbf{v}}\lambda \qquad (8)$$

where $\tilde{\mathbf{R}} = \mathbf{\Lambda}^{-1/2} {}^{\mathrm{t}} \mathbf{U} \mathbf{R} \mathbf{U} \mathbf{\Lambda}^{-1/2}$ is the covariance of the whitened concatenated data. Equation 8 thus corresponds to performing PCA on the concatenated whitened

data. In summary, the two-step PCA describe in the Methods ('simple MCCA
formulation') maximizes correlation between data sets. This corresponds to the
standard SUMCORR formulation of MCCA described by Kettenring (1971) (see
Parra, 2018). The relations between this and other MCCA formulations are described in (Asendorf, 2015).

MCCA vs CCA MCCA is understood as a generalization of CCA but some dif-548 ferences are worth noting. For CCA the focus is usually on the CCs \mathbf{Y}_n (n = 1, 2), 549 whereas for MCCA it may also be on the SCs Y. For standard CCA the projec-550 tion matrices are restricted to d (or $\min_n d_n$) columns for each data set, whereas 551 for MCCA it may be useful to consider more than d columns (as in Example 5). If 552 the objective were to capture sources common to all data matrices, d components 553 would suffice, but to capture also sources shared by several sources but not all, 554 more than d columns are required. For CCA the d columns of \mathbf{Y}_1 are mutually 555 uncorrelated as are those of \mathbf{Y}_2 , whereas for MCCA the *D* columns of \mathbf{Y}_n are mu-556 tually correlated in general. Columns of their sum Y are uncorrelated, however. 557

The large number (D > d) and non-orthogonality of the columns of \mathbf{Y}_n might 558 be disconcerting for the researcher familiar with CCA. The method may be modi-559 fied such that \mathbf{Y}_n is instead constituted of d orthogonal columns. For this, MCCA 560 is applied as above, for each n the first column of \mathbf{Y}_n is projected out of \mathbf{X}_n , 561 and MCCA applied again. This deflationary procedure terminates after d steps 562 because the dimensionality of each data matrix is then exhausted. Smaller ma-563 trices with orthogonal columns might be convenient in certain situations, but as 564 pointed out they might not capture all shared sources. The procedure described in 565 the Methods is better in this respect. 566

⁵⁶⁷ **Group analysis of multi-subject data.** Gathering data from multiple subjects ⁵⁶⁸ in response to the same stimulus serves several purposes. First, to counteract

variability by increasing the number of observations, analogous to recording from repeated trials. Second, to make inferences at the population level via group-level statistical analysis. Third, to allow data-dependent analysis to improve SNR based on similarity between subjects, analogous to methods that improve SNR based on similarity between trials (de Cheveigné and Parra, 2014).

The conventional strategy of calculating a "grand average", with correspond-574 ing channels or voxels of each subject being averaged together (Choi et al., 2013; 575 Luck, 2005), is hampered by inter-subject differences in source-to-sensor map-576 ping. The problem is mild for sources with broad topographies (as in Fig. 8), 577 but for sources with more local spatial characteristics a mismatch between sub-578 jects may result in destructive summation. A similar problem affects measures of 579 inter-subject correlation (ISC) applied directly to channels or voxels (Hasson et 580 al., 2004), or to linear combinations that assume the same mixing vectors for all 58 subjects (Dmochowski et al., 2012; Parra et al., 2018). 582

One simple expedient is to select, for each subject, a group of channels based 583 on responses to a "localizer" stimulus or task, calculate a root mean square av-584 erage waveform over these channels, and then average these over subjects (e.g. 585 Chait et al. (2010)). However, this packs the multidimensional cortical activity 586 into a single time course from which it may be hard to infer the richer dynam-587 ics of cortical activity. Another approach is to apply inverse modeling to map 588 the activity to a source space common across subjects (Litvak and Friston, 2008). 589 However, this requires accurate anatomical information for each subject and is 590 subject to the validity of the reconstruction models (Mahjoory et al., 2017), as 591 well as between-subject variability in source positions and orientations (Lio and 592 Boulinguez, 2016). 593

⁵⁹⁴ Data-driven methods such as MCCA are attractive in that they find a map-⁵⁹⁵ ping between subjects based only on shared temporal aspects of the data, without

requiring external information. MCCA and related methods have been widely 596 used for fMRI data (Li et al., 2009; Correa et al., 2010b; Hwang et al., 2012; 597 Afshin-Pour et al., 2012; Karhunen et al., 2013; Haxby et al., 2011; Afshin-Pour 598 et al., 2014) and EEG/MEG (Lankinen et al., 2014; Sturm, 2016; Zhang et al., 599 2017). In contrast to MCCA, which finds variance dimensions that are similar 600 across subjects with no attempt to ensure that they correspond to sources within 601 the brain, ICA-based approaches attempt to to isolate sources common across 602 subjects based on criteria of statistical independence (Calhoun and Adali, 2012; 603 Eichele et al., 2011; Huster et al., 2015; Chen et al., 2016; Madsen et al.; Huster 604 and Raud, 2018). Group ICA (GICA) as formulated by Eichele et al. (2011) can 605 be seen as a concatenation of MCCA (as described here) with ICA. Isolating the 606 MCCA step, as we do here, is useful conceptually and avoids the computational 607 cost and assumptions associated with ICA. Hyperalignment, as used by Haxby et 608 al. (2011), is conceptually the same as MCCA but restricting the transformations 609 to rotations, i.e. Procrustes analysis (Xu et al., 2012). Hyperalignment has the 610 advantage to maintain metric distance of patterns in the original and transformed 611 space, but the disadvantage that it cannot favor channels with higher inter-subject 612 correlation. 613

The focus here is on *temporal patterns* common to all subjects and thus in the MCCA procedure the data are concatenated along the spatial dimension (channels). It is also possible to extract *spatial patterns* common across subjects by concatenating data along the temporal dimension. Methods for group analysis of data from multiple subjects are reviewed by Correa et al. (2010a,b); Calhoun and Adali (2012); Sui et al. (2012); Afshin-Pour et al. (2014); Dähne et al. (2015); Chen et al. (2016); Huster and Raud (2018).

Denoising and dimensionality reduction. As described in the Methods and il-621 lustrated in the Results, data from single subjects can be denoised by projecting on 622 the overcomplete basis of D CCs, truncating, and projecting back. Data dimen-623 sions that are not shared with other subjects are *downweighted* but not removed, 624 so in general the rank of the data remains the same. Setting the cutoff D < D to 625 a relatively high order suppresses only those components that are very different 626 from those found in other subjects, most likely to be noise. In Example 5, the set 627 of 40 PCs that represented each subject were transformed into 320 CCs, of which 628 110 were selected before being projected back to obtain "denoised" data, yielding 629 the benefit shown in Fig. 9. The CCs that were rejected absorbed some of the 630 subject-specific patterns of noise, improving the outcome. 631

It is often useful to reduce the dimensionality of the data for computational 632 reasons (to reduce memory or computation time), or to avoid overfitting. The 633 standard procedure of applying PCA and truncating the series of PCs implicitly 634 equates variance to relevance, which may not be justified, as artifact sources may 635 have high variance, and useful sources may be weak. MCCA is of use in this 636 respect to replace the variance criterion by a criterion of consistency with other 637 data. This can be done conservatively by removing a small fraction of SCs that 638 represent the most atypical patterns within the data set. 639

As a tool to analyze or denoise the data of a single subject, MCCA is comparable to data-driven linear analysis techniques such as PCA, Independent Component Analysis (ICA), Joint Diagonalization, CCA and others. The fact that it uses a different criterion makes it *complementary* to those methods as a denoising or dimensionality reduction tool (e.g one can apply MCCA before or after ICA, JD, etc.).

35

A risk, common to other data-driven methods such as Caveats and cautions. 646 ICA or JD, is circularity of the analysis (Kriegeskorte et al., 2009). The method 647 is designed to optimize correlation between data matrices, and therefore the ob-648 servation that the components that it finds are correlated between data matrices 649 is of little weight, unless corroborated by careful cross-validation. Related to this 650 issue is overfitting: each SC depends on $D = \sum_n d_n$ parameters, a number that 651 can be large if there are many data matrices involved. Overfitting can be detected 652 using resampling and cross-validation methods, and the risk of overfitting can be 653 reduced by dimensionality reduction or other regularization techniques. 654

MCCA can easily latch on to artefacts and noise patterns shared across data 655 matrices. Uninteresting linear or polynomial trends (for example EEG drift po-656 tentials) may thus appear among the first MCCA components. More generally, 657 MCCA can be biased towards narrowband or low-frequency components com-658 mon across data matrices, even if their phase is not aligned, particularly if the 659 noise is spectrally-shaped or contains narrow-band components. This is illus-660 trated in Fig. 12 that shows the result of applying MCCA to ten "data matrices", 661 each of 12 s duration, extracted at random from the same 40-channel EEG data 662 that was used as background noise in Example 3. No known signal is common 663 across these data matrices, nonetheless the lowest-order SCs have narrow spectra 664 (Fig. 12 left) and quasi-sinusoidal waveforms (right) that might make them seem 665 significant. It is easy to understand why MCCA might take such components to 666 be shared: a sinusoid of arbitrary phase can be expressed as the weighted sum of 667 a sine and a cosine, and thus narrowband activity can be approximated as result-668 ing from two sinusoidal components in quadrature phase. As this is the case for 669 all datasets, MCCA will select the two-component sinusoidal basis as common. 670 Such spurious components compete with genuine shared activity, complicating 671 the analysis. 672

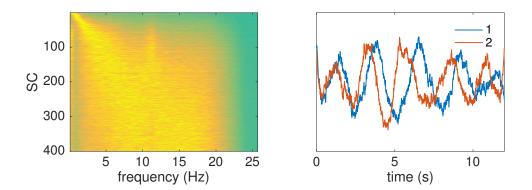


Figure 12: MCCA's bias towards narrowband and low-frequency activity. Left: power spectra of SCs derived from an MCCA analysis of 10 EEG "data matrices" of duration 12 s randomly sampled from 40-channel EEG data. Power is coded as color. Right: time course of the first two SCs.

MCCA assumes that temporal patterns are common across data matrices. A 673 difference in latency of a brain response between different subjects may reduce the 674 ability of MCCA to extract this activity. A common outcome in that case is two 675 components, one with a shape similar to the average pattern over subjects, and the 676 other similar to their difference (or derivative). MCCA can readily be extended to 677 include time-lags to account for differences in response latency between subjects, 678 although this comes at the expense of a greater number of parameters and a greater 679 risk of overfitting. MCCA is obviously of no benefit in the absence of synchronous 680 patterns, for example it is not well suited for analyzing resting-state data of a group 681 of subjects. 682

MCCA yields both CCs and SCs, either of which can be exploited. When reporting, it is important to specify which, to avoid confusion. As an example, the phrase 'MCCA was applied as a preprocessing step' is not sufficient to specify what was done.

Applicability to real-time processing. This work was motivated in part by the
 need to steer an auditory assistive device using brain signals. An obstacle to reli-

able decoding is the high-level of noise and artifacts in the EEG signals, and anal-689 ysis and denoising methods are essential for the success of this application. To be 690 useful, a method must be applicable to real-time processing, whereas MCCA as 691 described here works in batch mode. It may nonetheless be of use in the following 692 fashion. EEG data is recorded from a pool of subjects to a calibration sample of 693 speech, and MCCA is used to derive a "canonical" EEG response to that sam-694 ple. To adapt the system to a new user, EEG data are recorded in response to 695 the calibration sample, and a spatial filter is designed (for example using CCA) 696 to maximize similarity between the subject's and the canonical response. This 697 spatial filter is then used in the real-time processing pipeline. This suggests that 698 MCCA can also be put to use in a practical application such as cognitive control 699 of a hearing aid. 700

701 5 Conclusion

Multiway CCA is a powerful tool for analysis of multi-subject multivariate datasets. 702 It can be used both to design spatial filters to denoise data of each individual sub-703 ject, and to summarize data across subjects. Many related methods have been pro-704 posed in the literature, but the processing principles behind them, and the range of 705 tasks that they can be used for, are not widely appreciated. The use of MCCA (or 706 similar techniques) should be more prevalent given the ubiquitous need for merg-707 ing data across subjects. In this paper we presented a formulation of MCCA that 708 is relatively easy to understand, illustrated in detail how it works, and showed how 709 it can be put to use for a wide range of common tasks in multi-subject multivariate 710 data analysis. 711

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