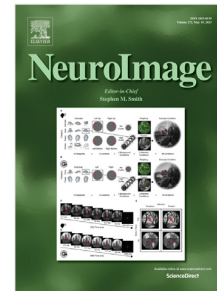


## Journal Pre-proof

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4. Highlights (for review)

- Spatial-temporal decompositions are pivotal in interpretation of EEG or MEG data
- RSA links brain-imaging modalities and models using second order similarity metrics
- RSA requires source activation time series and uses exhaustive source space search
- ReDisCA decomposes EEG\MEG into representationally relevant space-time components
- ReDisCA boosts detectability and localization of representationally relevant sources

Journal Pre-proof

# 1 Representational dissimilarity component analysis (ReDisCA)

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## 9 Abstract

10 The principle of Representational Similarity Analysis (RSA) posits that neural repre-  
11 sentations reflect the structure of encoded information, allowing exploration of spatial and  
12 temporal organization of brain information processing. Traditional RSA when applied to  
13 EEG or MEG data faces challenges in accessing activation time series at the brain source  
14 level due to modeling complexities and insufficient geometric/anatomical data.

15 To address this, we introduce Representational Dissimilarity Component Analysis (Re-  
16 DisCA), a method for estimating spatial-temporal components in EEG or MEG responses  
17 aligned with a target representational dissimilarity matrix (RDM). ReDisCA yields informa-  
18 tive spatial filters and associated topographies, offering insights into the location of "repre-  
19 sentationally relevant" sources. Applied to evoked response time series, ReDisCA produces  
20 temporal source activation profiles with the desired RDM. Importantly, while ReDisCA does  
21 not require inverse modeling its output is consistent with EEG and MEG observation equa-  
22 tion and can be used as an input to rigorous source localization procedures.

23 Demonstrating ReDisCA's efficacy through simulations and comparison with conventional  
24 methods, we show superior source localization accuracy and apply the method to real EEG  
25 and MEG datasets, revealing physiologically plausible representational structures without  
26 inverse modeling. ReDisCA adds to the family of inverse modeling free methods such as  
27 independent component analysis [34], Spatial spectral decomposition [41], and Source power  
28 comodulation [9] designed for extraction sources with desired properties from EEG or MEG  
29 data. Extending its utility beyond EEG and MEG analysis, ReDisCA is likely to find ap-  
30 plication in fMRI data analysis and exploration of representational structures emerging in  
31 multilayered artificial neural networks.

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32 **Keywords**— EEG and MEG, spatial-temporal decomposition, representational similarity anal-  
33 ysis, source localization.

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## 34 1. Introduction

35 Representational Similarity Analysis (RSA) now stands as a pivotal technique within  
36 cognitive neuroscience, offering a profound lens into the organization and representation of  
37 information in the human brain. This method has revolutionized our capacity to comprehend  
38 neural bases of cognitive processes by elucidating relationships between neural representations  
39 of stimuli or concepts and relating them to behavioral variables and computational model-  
40 ing [12, 30]. The largely philosophical concept of representational similarity later received  
41 its practical implementations in the field of both invasive electrophysiological [42, 19, 56]  
42 and non-invasive functional magnetic resonance imaging (fMRI) based neuroimaging [5, 8]  
43 followed by explicitly matching similarity patterns of neural activity to the theoretically pre-  
44 supposed representational structure [1] including the attempts to match the representational  
45 structure of neural activity across species [31]. Capitalizing on the success of the early appli-  
46 cation of the RSA principle, a seminal paper by Kriegeskorte et al. [30] provided a step-by-step  
47 guide for the use of RSA to link the three whales of modern neuroscience: neuronal activity,  
48 behavior, and computational models. Since then a number of informative studies emerged  
49 that utilize the notion of representation [54] and employ RSA as an instrument to explore  
50 informational structure embodied in the neural substrate [29].

51 RSA was extended to merge fMRI and magnetoencephalography (MEG) non-invasive  
52 functional neuroimaging modalities [6]. This approach aimed to leverage the typically ac-  
53 knowledged high spatial resolution of fMRI alongside the high temporal resolution of MEG.  
54 MEG channels were used as features for constructing a classifier to yield the representational  
55 dissimilarity matrices (RDMs) corresponding to specific time intervals. These RDMs were  
56 then matched against those computed from spatial region of interest (ROI) activity patterns  
57 as measured by fMRI. This study revealed intriguing patterns of temporally persistent and  
58 recurrent representations [26] across the visual processing stream reflecting both bottom-up  
59 and top-down informational flows highlighting the concept of predictive coding implemented  
60 in our brains.

61 Several years later, MEG alone combined with cortical ROI multivariate pattern analysis  
62 and powered by the RSA framework [27] managed to provide both temporally and spatially  
63 informative maps highlighting the ventral vs. dorsal bifurcation of the visual pathway related  
64 to processing images of faces and tools contrasted against meaningless textures. Methodolog-  
65 ically, this paper is significant as to the best of our knowledge that was the first attempt to  
66 apply RSA to MEG data in the source space. To this end, the authors first computed a  
67 fine-grained distributed inverse solution using the sLORETA technique [47]. Applying it  
68 to each time slice in the MEG sensor data they obtained cortical distribution of activity  
69 for each vertex on the cortical mesh model. Then, they combined vertices into spatially  
70 extended coarse ROIs and retained only three principal components of activities in each  
71 cortical ROI. Then, a series of region and time-window specific linear discriminant analysis  
72 (LDA) classifiers were trained to distinguish between stimulus classes and to form regional  
73 RDMs. These regional RDMs were then employed within the standard RSA framework and  
74 compared against theoretical RDMs.

75 It is important to realize that in the case of fMRI, the source space signals are readily  
76 available after the application of a more or less standard collection of analysis steps including  
77 data preprocessing and calculation of the appropriate contrasts. Things are significantly

78 less transparent and standardized in the EEG or MEG cases [39, 10]. Here, to obtain the  
79 individual voxel or ROI activity profiles, the inverse modeling approaches are used to convert  
80 sensor signals into the source space activation time series. This is typically done by applying  
81 an inverse operator matrix to EEG / MEG sensor measurements. The inverse operator  
82 directly depends on the forward model. The latter approximates the way the source activity is  
83 mapped to the sensors and is computed by solving Maxwell equations within the head volume  
84 which typically requires approximating the head with a set of nested surfaces bounding the  
85 regions of constant conductivity. The accuracy of the forward model depends on the extent  
86 to which the geometry as well as conductivity and permeability properties of the model  
87 align with their real counterparts. Generally unknown conductivity profiles of the tissues  
88 comprising the head, the associated anisotropy of the conductivity tensor, and the limited  
89 coregistration accuracy of the sensor array to the volume conductor model are the sources  
90 of the forward model inaccuracies especially pronounced when dealing with EEG data. The  
91 precision of modeling magnetic fields from neuronal sources tends to yield accurate MEG  
92 forward models, showcasing an impressive fidelity with an estimated error rate of around  
93 10% [38]. Yet, despite this advantage, MEG systems are notably less accessible compared to  
94 their EEG counterparts. Even if the forward model is accurate enough the task of estimating  
95 neuronal sources from non-invasively collected EEG or MEG data is inherently ill-posed.  
96 Fundamentally, for a given set of measurements, there exist an infinite number of cortical  
97 source distributions that perfectly fit the measurements. This problem is resolved and a  
98 unique solution is guaranteed by regularization which makes the results depend heavily on  
99 the *a priori* assumptions about source distributions. Taken together, all this limits RSA  
100 applications in the realm of time-resolved neuroimaging furnished by the EEG and MEG,  
101 the techniques that offer a unique time-resolved window into the rapid neuronal processes.

102 To address this problem and broaden the potential applications of the powerful RSA  
103 principle here we propose novel representational dissimilarity component analysis (ReDisCA)  
104 - an inverse modeling free method designed to estimate the spatial-temporal components in  
105 evoked responses that adhere to a specific target (or theoretical) representational dissimilarity  
106 matrix (RDM). The output of this method is a set of spatial filters and the associated  
107 topographies (or patterns) that appear informative of the location of "representationally  
108 relevant" sources whose activity exhibits the sought representational profiles. Application of  
109 the discovered spatial filters to the evoked response time series matrix yields temporal source  
110 activation profiles with the desired RDM over the selected time window. It is worth noting  
111 that ReDisCA belongs to the class of spatial decomposition methods that resolve the inherent  
112 uncertainty of the inverse problem by adding the specific assumptions and looking for the  
113 number of sources or components whose count does not exceed the rank of the data matrix.  
114 Thus, ReDisCA looks for components (or sources) with specific representational dissimilarity  
115 profiles.

116 While ReDisCA does not necessitate an inverse modeling, its foundation lies in the classical  
117 linear EEG/MEG observation equation. It exercises the concept of spatial filtering, akin  
118 to already established techniques like Independent Component Analysis (ICA) [34], Spatial-  
119 Spectral Decomposition (SSD) [41], or Source Power Co-modulation (SPoC) [9]. This ensures  
120 that the discovered spatial patterns are suitable for implementing a rigorous source localization  
121 procedure based on the notion of signal subspace [40] as described for example in [44]  
122 in application to ICA.

123 This compatibility with the linear model positively distinguishes ReDisCA from the purely  
 124 sensor space applications of RSA to EEG or MEG data. For example, [37] used high-density  
 125 EEG and highlighted the detailed spatial and temporal patterns of responses underlying var-  
 126 ious aspects of meaningfulness in the presented visual stimuli. They achieved this by using  
 127 newly proposed differentiation analysis (DA) and computed temporal and spatial profiles of  
 128 the category differentiation index (CDI) that can be used to make judgments about time  
 129 windows and approximate spatial locations of the pivotal sources. However, due to their  
 130 empirical nature, the obtained spatial CDI maps can not be rigorously fitted with the elec-  
 131 tromagnetic model of the head and therefore are only tangentially related to the underlying  
 132 distribution of cortical sources with target representational properties. Therefore, the ap-  
 133 proach proposed here can be considered as a link between the existing purely sensor-space  
 134 applications of RSA to EEG and MEG data and the fully-fledged inverse modeling-based  
 135 technique described in [27].

136 In what follows we first describe a classical RSA formulation and then proceed to the  
 137 presentation of ReDisCA. As it will become clear, ReDisCA utilizes formally the same opti-  
 138 mization strategy as that used in SPoC, a well-established technique for extracting spatial-  
 139 temporal components corresponding to neuronal sources of rhythmic activity whose power  
 140 is co-modulated with the user-supplied behavioral variable. To illustrate this connection we  
 141 provide a table of explicit correspondence between the quantities defined in this paper and  
 142 those used in SPoC and then describe the optimization strategy based on solving the gener-  
 143 alized eigenvalue problem with appropriately formed matrices. Next, we evaluate ReDisCA's  
 144 performance and compare it against several versions of the source space RSA implementa-  
 145 tions in the two simulated scenarios, with either a single source or with four simultaneously  
 146 active sources each with its own RDM. Finally, we apply ReDisCA to the analysis of a real  
 147 EEG dataset that lacks the information necessary for source localization, a prerequisite for  
 148 the source space RSA analysis. We show how the new method can be used to discover rep-  
 149 resentationally relevant structure in the EEG and MEG evoked responses without the use  
 150 of inverse modeling. We conclude with a discussion of ReDisCA's strengths and weaknesses  
 151 and relate it to the existing modifications of RSA including accommodation of advanced  
 152 dissimilarity measures [58] and the data-driven estimation of the theoretical RDM [25, 21].

## 153 2. Methods

### 154 2.1. Problem statement

155 Consider a collection of data matrices denoted as  $\mathbf{X}_i^c$ , each with dimensions  $N \times T$ .  
 156 These matrices represent recordings of brain activity, specifically EEG, MEG, or potentially  
 157 ECoG or sEEG, performed with  $N$  channels over  $T$  time stamps. The length of the time  
 158 segment of interest in the entire response is  $T$  samples, corresponding to the number of  
 159 columns in  $\mathbf{X}_i^c$ . These recordings are obtained during the  $i$ -th trial out of a total of  $I_c$  trials,  
 160 corresponding to the experimental condition  $c = 1, \dots, C$ .

161 Averaged evoked response is one of the informative features extracted from electrophysi-  
 162 ological recordings obtained in the event-related paradigms. It can be calculated simply by  
 163 averaging  $\mathbf{X}_i^c$  over  $I_c$  trials to get  $\mathbf{X}^c = \frac{1}{I_c} \sum_{i=1}^{I_c} \mathbf{X}_i^c$ .  $\mathbf{X}^c$  emphasizes phasic components of the  
 164 response, i.e. those whose activity phase is consistent with the stimulus onset.

165 Our objective is to use a set of  $\mathbf{X}^c$  observed over  $C$  conditions and to identify spatial  
 166 and temporal components or subsequently brain regions whose temporal activity profiles  
 167 exhibit the target differences among the  $C$  experimental conditions. The target differences  
 168 in our case are defined by a predefined theoretical or model-based  $C \times C$  representational  
 169 dissimilarity matrix (RDM)  $\mathbb{D}$ .

## 170 2.2. Source space representational similarity analysis (RSA)

171 For EEG and MEG scenarios, we can achieve this by the two-step spot-light procedure  
 172 similar to that used in [27]. First we use an  $M \times N$  inverse operator denoted as  $\mathbf{W}_M$  whose  
 173  $m$ -th row is denoted as  $\mathbf{w}_m^\top$ ,  $m \in 1, \dots, M$ , and acts as a spatial filter tuned to the  $m$ -th  
 174 voxel or cortical vertex.

175 This precomputed spatial filter aids in estimating the  $1 \times T$  vector of the  $m$ -th voxel  
 176 activity during condition  $c$  as  $\mathbf{s}_m^{c\top} = \mathbf{w}_m^\top \mathbf{X}^c$ , allowing us to derive the time series corresponding  
 177 to every voxel in the predefined volumetric grid based on the sensor-space averaged evoked  
 178 response measurements  $\mathbf{X}^c$  defined above. Note that here and in the subsequent expressions  
 179 horizontally oriented vectors are marked with transpose superscript, i.e.  $\mathbf{s}_m^{c\top} = (\mathbf{s}_m^c)^\top$ .

180 Next, once having obtained regional time series vectors  $\mathbf{s}_m^{c\top}$  we can evaluate the dissimi-  
 181 larity measure of choice to obtain the  $m$ -th region-specific dissimilarity matrix  $\mathbf{D}_m = \{d_m^{ij}\}$ ,  
 182  $m = 1, \dots, M$ . In what follows we will stick to the square of the Euclidean distance as a  
 183 measure of response dissimilarity that can be readily extended to Mahalanobis distance once  
 184 the covariance matrix describing the dependencies between the time samples of the regional  
 185 response is available. Thus

$$\mathbf{D}_m = \{d_m^{ij}\} = \|\mathbf{s}_m^{ciT} - \mathbf{s}_m^{cjT}\|^2, \quad i, j = 1, \dots, C. \quad (1)$$

186 Once the regional RDMs are prepared, following the standard RSA procedure, we will  
 187 employ the correlation coefficient  $\rho_m$  to assess the similarity between regional RDMs ( $\mathbf{D}_m$ )  
 188 indexed by  $m$  and the theoretical RDM  $\mathbb{D} = \{d^{ij}\}$  typically supplied by the user.

$$\rho_m^{RSA} = \text{corr}(d^{ij}, d_m^{ij}) = \frac{2}{C(C-1)} \sum_{i=1}^C \sum_{j=i+1}^C \tilde{d}^{ij} \tilde{d}_m^{ij} \quad (2)$$

189 where the tilde represents standardized upper triangular elements of the respective RDM  
 190 matrices. The standardization operation applied to a vector lies in subtracting its mean and  
 191 dividing by the standard deviation.

192 The scores  $\rho_m^{RSA}$  reflect the similarity between the theoretical and regional RDMs. They  
 193 can be visually represented on the cortical surface or within the brain volume by interpolating  
 194 the scores associated with each of the  $M$  voxels or cortical mesh nodes. Then, to identify the  
 195 spots of significant similarity, a statistical testing procedure is applied. This procedure should  
 196 consider the limited spatial resolution inherent in EEG and MEG-based inverse mapping, and  
 197 correction should be made for the effective number of multiple comparisons. This may be  
 198 accomplished using, for example, the cluster-based permutation testing procedure [36] where  
 199 the surrogate data are obtained by permuting the labels of  $C$  conditions which essentially  
 200 corresponds to computing  $\rho_m^{RSA}$  but for a randomly reshuffled upper triangle of the theoretical  
 201 RDM.

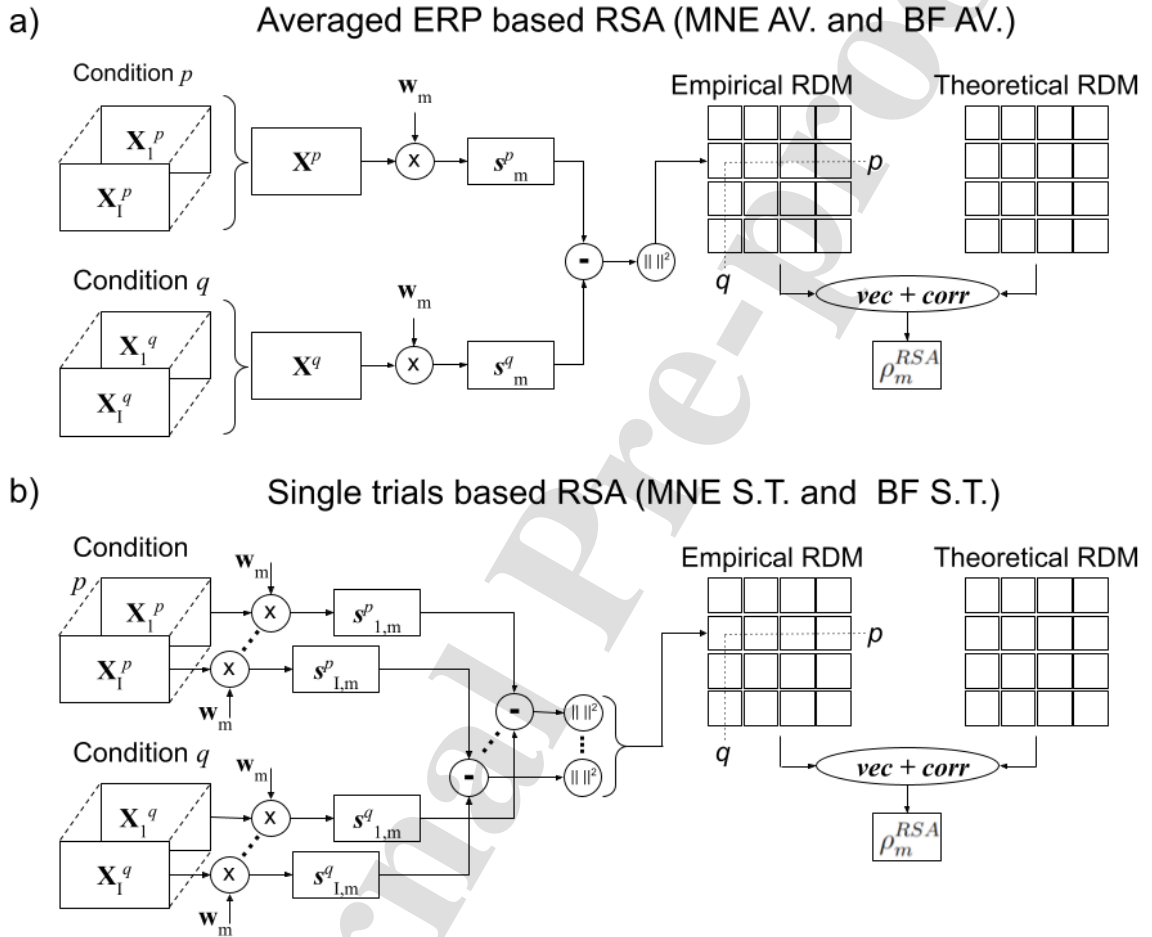


Figure 1: Source space RSA diagrams. a) RSA applied to the averaged evoked response (AV). The inverse operator is applied to already averaged evoked response data  $\mathbf{X}^p$  observed during condition  $p$ ,  $p = 1, \dots, C$ , then the empirical RDM entry is calculated as the quadratic difference between the evoked source time series in conditions  $c_i = p$  and  $c_j = q$ . b) RSA applied to single trials (S.T.). The inverse operator is applied to every single  $l$ -th trial in the data, followed by computing the quadratic difference that gets then averaged over trials within each condition. In both cases, different inverse operators ( $\mathbf{W}_M = \{\mathbf{w}_m^T\}$ ) can be used. We experimented with two inverse solvers - MNE and LCMV BF.



202 The diagrams in Figure 1 schematically show the described process. In the first case illus-  
 203 trated in panel Figure 1.a an inverse operator is applied to already averaged evoked response  
 204 data  $\mathbf{X}^p$  observed during condition  $p$ ,  $p = 1, \dots, C$ , and then the empirical RDM entry is  
 205 calculated as the quadratic difference between the evoked source time series in condition  $p$   
 206 and  $q$ . In Figure 1.b we show an alternative approach where the inverse operator is applied  
 207 to the single ( $l$ -th) trial data, followed by computing the quadratic difference that then gets  
 208 averaged over trials within each condition. In our experiments with source space RSA, we will  
 209 also distinguish between the use of two different inverse solvers - Minimum norm estimator  
 210 (MNE) and Linearly constrained minimum variance beamformer (LCMV BF). This gives us  
 211 in total four versions of the source space RSA that we will compare our new approach with.

### 2.3. Representational dissimilarity component analysis (ReDisCA)

213 Here we propose an alternative method for identifying brain activity components with  
 214 the desired representational dissimilarity. Instead of using the pre-computed inverse operator  
 215  $\mathbf{W}_M = \{\mathbf{w}_m^\top\}$ ,  $m = 1, \dots, M$  whose  $m$ -th row serves the  $m$ -th cortical vertex and conducting  
 216 an exhaustive search over all  $M$  cortical vertices (or voxels) as in the spotlight source space  
 217 RSA illustrated in Figure 1, we analytically seek a vector of coefficients  $\mathbf{w}$  such that the  
 218 empirical RDM of spatially filtered data  $\mathbf{s}_w^{cT} = \mathbf{w}^\top \mathbf{X}^c$ ,  $c \in 1, \dots, C$ , closely approximates the  
 219 target RDM  $\mathbb{D}$ . Note that this analytically found spatial filter weights vector  $\mathbf{w}$  conceptually  
 220 plays the same role as the rows  $\mathbf{w}_m$  of the inverse operator in the source space RSA.

221 To implement this we posit and solve the following optimization problem

$$\mathbf{w} = \operatorname{argmax} \operatorname{corr} (d_w^{ij}, d^{ij}) = \operatorname{argmax} \operatorname{corr} (\|\mathbf{s}_w^{c_i T} - \mathbf{s}_w^{c_j T}\|^2, d^{ij}), \quad (3)$$

222 where following (1) to gauge similarity between the empirical RDM  $\mathbf{D}_w = \{d_w^{ij}\}$  of the spa-  
 223 tially filtered data  $\mathbf{s}_w^{cT} = \mathbf{w}^\top \mathbf{X}^c$  and the target RDM matrix  $\mathbb{D}$  we use the Pearson correlation  
 224 coefficient between the two RDMs upper triangular elements indexed by  $(i, j)$ . Also, as a  
 225 representational dissimilarity measure we employ the squared Euclidean distance between  
 226 condition-specific spatially filtered temporal activation profiles. However, in this case, the  
 227 spatial filter  $\mathbf{w}$  is unknown and needs to be found by solving this optimization problem. Once  
 228 the weights are found they can be turned into source topographies. The relation between  
 229 spatial filter weights and the associated source topographies has been described in [17] and  
 230 will also be addressed below. The obtained topographies of sources with desired RDM profiles  
 231 can then be used for inverse modeling and localization of the underlying neuronal sources.  
 232 Note that we used subscript  $w$  to denote the elements of the empirical RDM corresponding  
 233 to the spatial filter  $\mathbf{w}$  that we are about to identify, see (2) for comparison.

234 To solve the optimization problem (3) we use the fact that  $\mathbf{s}_w^{c_i T} = \mathbf{w}^\top \mathbf{X}^{c_i}$  and rewrite (3)  
 235 as an explicit function of  $\mathbf{w}$ :

$$\mathbf{w} = \operatorname{argmax} \operatorname{corr} \left( \mathbf{w}^\top (\mathbf{X}^{c_i} - \mathbf{X}^{c_j}) (\mathbf{X}^{c_i} - \mathbf{X}^{c_j})^\top \mathbf{w}, d^{ij} \right). \quad (4)$$

236 For compactness, we denote  $\mathbf{R}^{ij} = (\mathbf{X}^{c_i} - \mathbf{X}^{c_j}) (\mathbf{X}^{c_i} - \mathbf{X}^{c_j})^\top$  to obtain the following opti-  
 237 mization problem

$$\mathbf{w}_{max} = \operatorname{argmax} \operatorname{corr} (\mathbf{w}^\top \mathbf{R}^{ij} \mathbf{w}, d^{ij}), \quad i = 1, \dots, C, \quad j = 1, \dots, C. \quad (5)$$

238 In Equation (5),  $N \times N$  matrix  $\mathbf{R}^{ij}$  represents the unscaled correlation matrix of the sensor-  
 239 space time series differences recorded between condition  $i$  and condition  $j$ . This expression  
 240 formally exactly matches the optimization problem solved in SPoC [9] where the role of  $\mathbf{R}^{ij}$   
 241 is played by the time-segment specific sensor data correlation matrix.

242 SPoC deals with a collection of time segments (or epochs) indexed by  $e$  in the original  
 243 paper, and aims to find a spatial filter for isolating a source whose power follows the desired  
 244 temporal profile  $z(e)$ . In our approach, we work with a collection of condition pairs  $(i, j)$   
 245 and seek a source whose RDM  $\mathbf{D}_w = \{d_w^{ij}\}$  matches the target RDM  $\mathbb{D} = \{d^{ij}\}$ . While SPoC  
 246 computes correlation matrices  $\mathbf{C}(e)$  specific to the  $e$ -th epoch of EEG(MEG) data, in our  
 247 approach we calculate correlation matrices  $\mathbf{R}^{ij}$  of the difference of EEG (MEG) time series  
 248 observed during the pairs of conditions indexed by  $(i, j)$ . The role of index  $e$  in the original  
 249 SPoC is played by the pair of indices  $(i, j)$  whose combinations enumerate the collection of  
 250 the upper triangular elements of the RDM. One may also express this correspondence as  
 251  $e = (i - 1)C + j$ ,  $i > j$ ,  $i = 1, \dots, C$ ,  $j = 1, \dots, C$ . Essentially, the  $e$ -th segment time series  
 252 in SPoC is replaced by the time series of the difference between condition pair  $(i, j)$ . The  
 253 role of the desired power profile  $z(e)$  from the original SPoC is played by the elements  $d^{ij}$   
 254 of the theoretical RDM  $\mathbb{D}$  driving the proposed here representational dissimilarity components  
 analysis (ReDisCA). This correspondence is summarized in Table 1 below.

Var. SPoC	Var. ReDisCA	Role in SPoC	Role in ReDisCA
$e$	$(i, j)$	time window index	conditions pair index
$\mathbf{C}(e)$	$\mathbf{R}^{ij}$	data correlation matrix	data diff. corr. matrix
$z(e)$	$d^{ij}$	desired response pattern	desired RDM pattern

Table 1: Correspondence between main SPoC variables as defined in [9] and the variables used to define ReDisCA in this manuscript.

255 There are two ways to solve the optimization problem (5). The first one is to use the gra-  
 256 dient descent and to identify  $\mathbf{w}$  as the solution for (5) to maximize the correlation coefficient  
 257 between the empirical and the desired theoretical RDM profiles. While this is entirely possi-  
 258 ble, the SPoC paper describes a more attractive alternative to approximate the correlation  
 259 coefficient with covariance which allows for a closed-form solution.  
 260

261 To ensure that optimization of covariance (the non-normalized version of the correlation  
 262 coefficient) is a good approximator of the correlation coefficient optimization we

- 263 • use standardized elements of the RDM  $\tilde{d}^{ij}$
- 264 • use the constraint  $\mathbf{w}^\top \bar{\mathbf{R}} \mathbf{w}^\top = 1$  where

$$\bar{\mathbf{R}} = \frac{2}{C(C-1)} \sum_{i=1}^C \sum_{j=i+1}^C \mathbf{R}^{ij} \quad (6)$$

265 is the average correlation matrix.

266 For compactness we also denote the weighted average correlation matrix

$$\bar{\mathbf{R}}^d = \sum_{i=1}^C \sum_{j=i+1}^C \tilde{d}^{ij} (\mathbf{R}^{ij} - \bar{\mathbf{R}}) \quad (7)$$

267 The resulting optimization problem can then be written as

$$\mathbf{w} = \operatorname{argmax} (\mathbf{w}^\top \bar{\mathbf{R}}^d \mathbf{w}), \text{ s.t. } \mathbf{w}^\top \bar{\mathbf{R}} \mathbf{w} = 1 \quad (8)$$

268 and can be analytically solved using the method of Lagrange multipliers.

269 The problems formally identical to (8) often arise in the domain of multivariate signal  
 270 processing, see beamforming [57], common spatial patterns [49], spatial spectral decompo-  
 271 sition (SSD) [41] and SPoC [9] as EEG (MEG) specific examples. The optimal  $\mathbf{w}$  is found  
 272 as the solution to the following generalized eigenvalue problem corresponding to the largest  
 273 eigenvalue

$$\bar{\mathbf{R}}^d \mathbf{w} = \lambda \bar{\mathbf{R}} \mathbf{w} \quad (9)$$

274 When solving this problem for an  $N$ -channel data we will arrive at an  $N \times N$  matrix  $\mathbf{W}$   
 275 whose columns are the eigenvectors of matrix pair  $(\bar{\mathbf{R}}^d, \bar{\mathbf{R}})$  or in other words

$$\bar{\mathbf{R}}^d \mathbf{W} = \mathbf{\Lambda} \bar{\mathbf{R}} \mathbf{W}, \quad (10)$$

276 where  $\mathbf{\Lambda} = \{\lambda_n\}$ ,  $n = 1, \dots, N$  is the diagonal matrix of generalized eigenvalues. The above  
 277 procedure is referred to as the maximization of covariance option in the original SPoC paper  
 278 [9]. In this case, matrix  $\mathbf{W}$  resulting from solving the generalized eigenvalue problem (10) is  
 279 square and also full rank as we assume that both  $\bar{\mathbf{R}}^d$  and  $\bar{\mathbf{R}}$  are invertible. Then,  $\mathbf{W}$  can be  
 280 simply inverted to obtain a matrix  $\mathbf{A} = \{\mathbf{a}_n^\top\} = \mathbf{W}^{-1}$  whose rows  $\mathbf{a}_n^\top$  are the topographies  
 281 of sources with the desired representational properties. In the case when the generalized  
 282 eigenvalue problem (10) is not full rank the described procedure can be performed in the  
 283 lower dimensional principal space and the obtained topographies can be transformed back to  
 284 the original sensor space.

285 Note, that by solving (10) instead of (9) we obtain  $N$  spatial filters  $\mathbf{w}_n$  and source to-  
 286 pographies  $\mathbf{a}_n^\top$ ,  $n = 1, \dots, N$ . The  $n$ -th generalized eigenvalue  $\lambda_n$ ,  $n = 1, \dots, N$  reflects the  
 287 extent to which the empirical RDM corresponding to the time series extracted using spatial  
 288 filter  $\mathbf{w}_n$  is similar to the desired theoretical RDM  $\mathbb{D}$ .

289 We call the topographies  $\mathbf{a}_n^\top$  combined with the corresponding data derived RDM profiles  
 290  $\hat{\mathbf{D}}_n = \{\hat{d}_n^{ij}\} = \{\mathbf{w}_n^\top \mathbf{R}^{ij} \mathbf{w}_n\}$  the *representational dissimilarity components* and the described  
 291 process of obtaining them the *REpresentational DISsimilarity Component Analysis* or Re-  
 292 DisCA.

293 The significance of the similarity between the component-specific data-derived RDMs  
 294  $\hat{\mathbf{D}}_n$ ,  $n = 1, \dots, N$  and the theoretical RDM  $\mathbb{D}$  can be established by the permutation test-  
 295 ing procedure suggested in SPoC. The idea of this approach is to solve a large number of  
 296 surrogate problems of the form (10) but based on the matrices created from the data with  
 297 permuted condition labels. The mutual correspondence between the set of difference corre-  
 298 lation matrices  $\mathbf{R}^{ij}$  and the condition pair labels  $(i, j)$  is destroyed and the corresponding  
 299 asymptotic  $p$ -values are calculated as a fraction of cases when the surrogate generalized  
 300 eigenvalue exceeds that obtained on the original data.

301 The collection of  $K$  topographies  $\mathbf{A}_K = [\mathbf{a}_1, \dots, \mathbf{a}_K]$  corresponding to the components  
 302 with significantly high similarity between the data-derived and the theoretical RDM spans  
 303 *representational dissimilarity subspace*, *ReDisS*. These topographies together with the corre-  
 304 sponding spatially filtered ERP time series furnish the decomposition of the evoked response

305 potential (ERP) data into a set of *relevant* constituents with respect to the used theoretical  
 306 RDM.

307 Technically this completes ReDisCA's description whose result is a set of spatial com-  
 308 ponent topographies  $\mathbf{a}_k$  and the corresponding spatial filters  $\mathbf{w}_k$  that can be used to obtain  
 309 component-specific response time series vectors  $\mathbf{u}_k^{cT}$  in the  $c$ -th condition as  $\mathbf{u}_k^{cT} = \mathbf{w}_k^\top \mathbf{X}^c$ .  
 310 More generally, one can write this in a matrix form as

$$\mathbf{U}^{cT} = \mathbf{W}^\top \mathbf{X}^c. \quad (11)$$

311 From the above and given that the matrix of spatial filters  $\mathbf{W}^\top$  is invertible we can write

$$\mathbf{X}^c = \mathbf{W}^{-1} \mathbf{U}^{cT} = \mathbf{A} \mathbf{U}^{cT} = \sum_{k=1}^N \mathbf{a}_k \mathbf{u}_k^{cT}, \quad (12)$$

312 which shows that after obtaining ReDisCA components the sensor data in the  $c$ -th condition  
 313 can be reconstructed as a superposition of rank-1 contributions  $\mathbf{a}_k \mathbf{u}_k^{cT}$  of ReDisCA compo-  
 314 nents.

### Representational dissimilarity component analysis (ReDisCA)

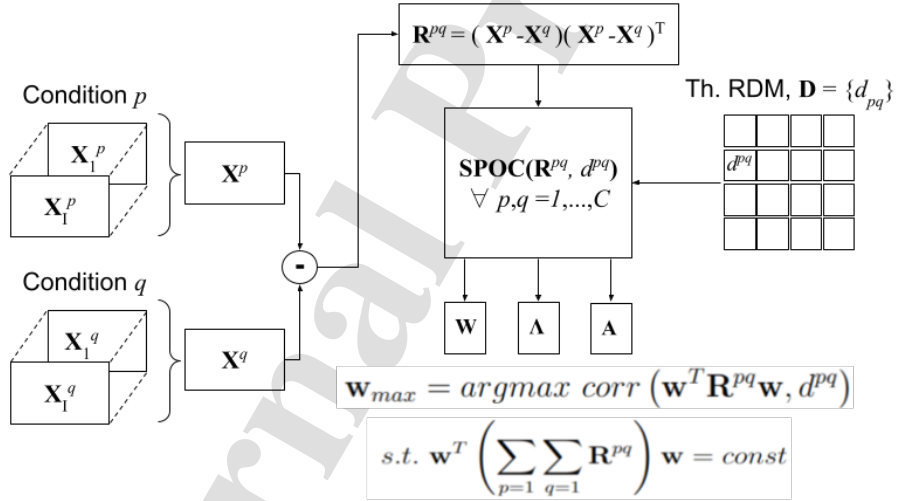


Figure 2: Representational dissimilarity component analysis (ReDisCA) diagram. The problem of finding the spatial components whose output ERP follow the desired RDM is reduced to SPoC covariance optimization. Instead of time-window covariance matrices  $\mathbf{C}(e)$  and the associated values of behavioral variable  $z(e)$  observed for a set of latency values  $e = 1, \dots, E$  ReDisCA uses activation difference covariance matrices  $\mathbf{R}^{pq}$  and the elements  $d^{pq}$  of the theoretical RDM correspondingly, see also Table 1.

315 Note that using ReDisCA does not require an explicit electromagnetically informed in-  
 316 verse modeling to identify the spatial components within multichannel EEG (MEG) data  
 317 that exhibit the desired representational properties aligned with the user-supplied theoreti-  
 318 cal RDM.

319 However, to compare ReDisCA’s results to those obtained with the more conventional  
 320 source space RSA approaches we can apply the electromagnetic inverse modeling to the  
 321 identified spatial topography vectors  $\mathbf{a}_k$ . This allows us to quantitatively assess the locations  
 322 of sources underlying each of the components. The simplest way to associate ReDisCA  
 323 results with neuronal sources is to compute the cosine similarity score between each forward  
 324 model-based topography vector  $\mathbf{g}_m$ ,  $m = 1, \dots, M$  corresponding to the  $m$ -th vertex of the  
 325 cortical mesh and the ReDisCA derived pattern  $\mathbf{a}_1$  corresponding to the largest generalized  
 326 eigenvalue  $\lambda_1$ , i.e.

$$\rho_m^{CS} = \frac{\mathbf{g}_m^\top \mathbf{a}_1}{\|\mathbf{g}_m\| \|\mathbf{a}_1\|}. \quad (13)$$

327 This procedure can be applied to each statistically significant topography.

328 Alternatively, to localize sources corresponding to the entire  $K$ -dimensional represen-  
 329 tational dissimilarity subspace spanned by the topographies of statistically significant com-  
 330 ponents stored in  $\mathbf{A}_K$  we can perform a simple multiple signal classification (MUSIC) scan  
 331 using subspace correlation metric as

$$\rho_m^{MUSIC} = \text{subcorr}(\mathbf{g}_m^\top, \mathbf{A}_K) \quad (14)$$

332 Similarly to  $\rho_m$  used in the classical RSA setting, the scores  $\rho_m^{MUSIC}$  and  $\rho_m^{CS}$  can be visually  
 333 represented on the cortical surface or within the brain volume by interpolating the scores  
 334 associated with each of the  $M$  voxels or cortical mesh nodes. Note also that  $\rho_m^{MUSIC}$  is a  
 335 more general measure of similarity between the subspaces of the arbitrary dimensions and  
 336 reduces to  $\rho_m^{CS}$  for  $K = 1$ .

#### 337 2.4. Simulations setting

338 To validate the proposed ReDisCA approach, we conducted two sets of simulations. The  
 339 best way to ensure that ReDisCA derived components are informative with respect to the  
 340 underlying sources is to actually find these sources given the components estimated by Re-  
 341 DisCA. Therefore in both simulations we mapped the obtained topographies to the source  
 342 space using (14) and assessed the location of the MUSIC scan’s peak with respect to the  
 343 simulated source location(s).

##### 344 2.4.1. Generation of source activation time series with desired representational structure

345 In both simulations we used the following strategy to generate the source activation time  
 346 series for each of the  $C$  conditions and associate them with the representational structure  
 347 across  $C$  conditions.

- 348 • For each source generate a random mixing matrix  $\mathbf{M}$  by sampling its elements from  
 349 zero mean and unit variance Gaussian distribution  $\mathcal{N}(0, 1)$
- 350 • Generate  $C \times T$  matrix  $\mathbf{S}$  of condition-specific source evoked response potentials as  
 351  $\mathbf{S} = \mathbf{MZ}$  where  $\mathbf{Z}$  is a  $C \times T$  matrix of Gaussian random variables whose rows are  
 352 low-pass filtered by the 6-th order Butterworth filter with a cut-off frequency of 2 Hz.  
 353 We will refer to the  $c$ -th row of this matrix as  $\mathbf{s}^{c\top}$  for  $c = 1, \dots, C$ .

- Compute the resultant dissimilarity profile matrix  $\mathbb{D}^0$  from the obtained condition-specific time series vectors  $\mathbf{S}$  according to equation (1).

As described later the noisy version of  $\mathbb{D}^0$  will be supplied to the tested here RSA approaches as a theoretical RDM. For each Monte-Carlo iteration we generated a new matrix  $\mathbf{Z}$ , and thus a new set of condition-specific source time series  $\mathbf{S}$ . In the first set of simulations where we generated only one active source we kept the mixing matrix  $M$  constant over all Monte-Carlo iterations. In the second set of simulations with  $P = 4$  sources, we used four mixing matrices  $\mathbf{M}_p$ , one for each source, that remained unchanged throughout Monte-Carlo trials.

#### 2.4.2. ReDisCA vs. source space RSA

Within the first set of simulations we compared ReDisCA against the source space RSA using a single source scenario. In this comparison, to generate the observed EEG (MEG) data we placed a single source iteratively in a node of the cortical mesh whose index was randomly generated and activated the source with the condition-specific time series. Here we used  $C = 5$  conditions and generated condition-specific ERP time series. For each source position (iteration) the time series were randomly regenerated from a newly sampled matrix of random variables according to the procedure described above.

At each Monte-Carlo iteration corresponding to a specific source location in the  $m_0$ -th node of the cortical mesh we obtained condition-specific source time series observed in the  $l$ -th trial as

$$\mathbf{X}_l^c = (\mathbf{g}_{m_0} + \boldsymbol{\delta}) \mathbf{s}^{c\top} + \gamma \boldsymbol{\Upsilon}_l^x. \quad (15)$$

In (15)  $\mathbf{g}_{m_0}$  is the  $N \times 1$  forward model vector (or topography) corresponding to the source located in the  $m_0$ -th vertex of the cortical mesh with coordinate  $\mathbf{r}_{m_0}$ . In order to account for inevitable forward modeling errors we used normally distributed  $N \times 1$  source model noise vector  $\boldsymbol{\delta}$  with covariance matrix  $\mathbf{C}_\delta = \sigma_\delta^2 \mathbf{I}$  and  $\sigma_\delta = 0.15 \|\mathbf{g}_{m_0}\|$ . Row vector  $\mathbf{s}^{c\top}$  is the  $c$ -th row of  $\mathbf{S}$  and  $\boldsymbol{\Upsilon}_l^x$  is a  $N \times T$  realistic brain noise matrix generated by 1000 randomly seeded cortical sources activated with  $1/f$  noise, similar to the way it was done in [43] with factor  $\gamma$  controlling the signal-to-noise ratio in the simulated data. Note that each trial had a different realization of the spatially correlated noise  $\boldsymbol{\Upsilon}_l^x$  and new  $\boldsymbol{\delta}$  was generated for each Monte-Carlo iteration.

We then use the simulated noisy sensor data  $\mathbf{X}_l^c$  for  $l = 1, \dots, I_c$  and  $c = 1, \dots, C$  and we aim to use the approximate RDM of a specific source to find spatial component(s) whose time series, see (11), exhibits the desired representational structure defined by the approximate RDM. The approximate RDM is used to simulate the real-world scenario where we naturally lack precise knowledge of the dissimilarity profile. To this end, we incorporate a random  $C \times C$  noise matrix  $\boldsymbol{\Upsilon}^d$  at each Monte-Carlo iteration. This addition modifies the theoretical RDM  $\mathbb{D}^0$  to  $\mathbb{D} = \mathbb{D}^0 + \boldsymbol{\Upsilon}^d$ .

To verify the result we then apply the source localization procedure to the discovered component(s) to determine the location  $\hat{\mathbf{r}}$  of a source (or its index, denoted as  $\hat{m}$ ) the discovered spatial component pertains to and whose activity exhibits the intended theoretical similarity profile. We then use the obtained location to calculate the performance metrics as described in Section 3.1. When source space RSA is applied to this simulated data our goal

394 is to directly identify the cortical source of interest using the procedures outlined in Figure  
395 1.

396 In our simulations we have chosen  $T = 200$  ms as the length of the window to which RSA  
397 is applied. The spectral profiles of the source evoked activity occupied the frequency range  
398 below 2 Hz to impose the smoothness characteristic of the real evoked responses. As we will  
399 show in the example of applying ReDisCA to real EEG data the method can be applied in  
400 a sliding window mode and remains operable at  $T = 150$  ms. The constraint on the length  
401 of the time interval is dictated primarily by the condition number of the resultant correlation  
402 matrices (4) and can be further reduced with proper regularization and/or dimension  
403 reduction procedures. Alternatively, ReDisCA can be applied to the entire evoked response  
404 time interval and then a statistical testing procedure can be used to determine the intervals  
405 of significant difference, see Section 4.2.2.

406 To evaluate the performance of ReDisCA in comparison to the four versions of the source  
407 space RSA, we employed the Receiver Operating Characteristic (ROC) curve. This measure,  
408 devoid of specific thresholds, gauges the overall informational capacity in the output of these  
409 approaches concerning the detection task. For a detailed explanation of how the ROC curve  
410 is calculated, please refer to Section 3.1.

#### 411 2.4.3. Realistic simulations with multiple sources

412 Another simulation scenario reproduces the situation when the observed evoked responses  
413 are generated by a superposition of several sources each with its own representational dis-  
414 similarity matrix. To this end we experimented with  $P = 4$  sources and their corresponding  
415 dissimilarity matrices  $\mathbb{D}^{0p}$  and their noisy versions  $\mathbb{D}^p$ ,  $p = 1, \dots, P$ . The ideal RDMs  $\mathbb{D}^{0p}$ ,  
416  $p = 1, \dots, P$  of the evoked responses for each of  $P = 4$  sources among  $C = 6$  conditions  
417 are shown in Figure 3. To evaluate the RSA's robustness we have also experimented with a  
418 subset of  $C = 3, 4, 5$  conditions.

419 At each Monte-Carlo iteration we have randomly seeded four sources over the cortical  
420 mantle with the restriction of no source being closer than  $\delta_{min} = 2$  cm to any of the other  
421 sources. This gave us  $P = 4$  true source location vectors  $\mathbf{r}_p^{true}$  and true source topography  
422 vectors  $\mathbf{g}_p^{true}$ ,  $p = 1, \dots, P$ . We have then added noise to these true source topographies,  
423 projected source activation time series to the sensors and added realistic  $1/f$  brain noise  
424 similarly to (15) as

$$425 \mathbf{X}^c = \sum_{p=1}^P (\mathbf{g}_p^{true} + \delta_p) \mathbf{s}_p^{c\top} + \gamma \mathbf{\Upsilon}^x, \quad (16)$$

426 Overall the approach to constructing the simulated data in this second experiment matched  
427 that of the first one with the exception that in the current experiment the simulated data  
428 contained the superposition of activity of  $P = 4$  simultaneously active task-related sources  
each with its own RDM.

### 429 3. Performance metrics

430 As we described in Section 2 ReDisCA itself does not require the electromagnetic inverse  
431 modeling, see also Figure 2. At the same time the source space RSA applied to EEG(MEG)

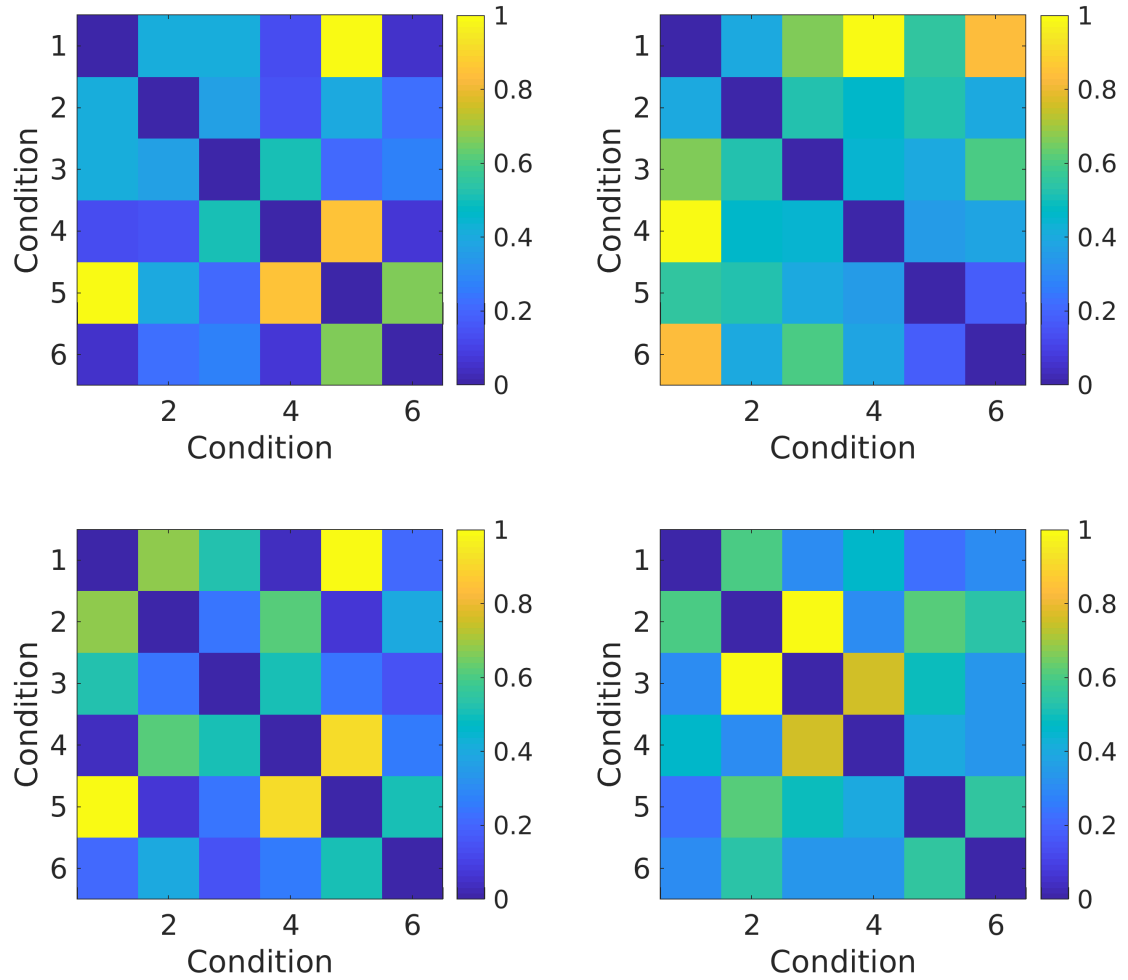


Figure 3: Theoretical RDM matrices for each of the four simulated sources generated within an exemplar Monte-Carlo trial.



432 data explicitly uses inverse modeling as highlighted by the diagrams shown in Figure 1.  
 433 Therefore, to evaluate ReDisCA's performance and match it against the source space RSA  
 434 we use components discovered by ReDisCA and fit them with the electromagnetic model as  
 435 described in Section 2 and equations (13, 14).

### 436 3.1. ROC curves

437 Within the first set of simulations we evaluated the methods' performance using area  
 438 under ROC curve (ROC AUC) metrics. To compute the ROC curves we first determine the  
 439 counts of true positives (TP), false positives (FP), true negatives (TN), and false negatives  
 440 (FN).

441 To this end as described in Section 2.4 at each  $k$ -th Monte-Carlo iteration corresponding to  
 442 a neuronal source placed at a randomly chosen location  $\mathbf{r}_k$  we use the scans  $\rho_m$ ,  $m = 1, \dots, M$   
 443 described in Section 2 and for each threshold value  $\theta$  we find a set of indices  $\mathcal{M}_>$  of cortical  
 444 vertices  $m$  for which  $\rho_m \geq \theta$ . Then, we count the number of vertices in  $\mathcal{M}_>$  that fall within  
 445 a sphere with  $r_{max} = 0.01$  m centered around the true source location  $\mathbf{r}_k$  simulated during  
 446 the  $k$ -th Monte-Carlo iteration and save it to the corresponding true positives count array  
 447  $TP_k(\theta)$ . The count of vertices from  $\mathcal{M}_>$  that fall outside the sphere with radius  $r_{max}$  is added  
 448 to the false-positives count array  $FP_k(\theta)$ .

449 Next we find a complementary set  $\mathcal{M}_<$  of cortical vertex indices  $m$  such that  $\rho_m < \theta$ . We  
 450 then count the number of vertices from  $\mathcal{M}_<$  that appear within the sphere with  $r_{max} = 0.01$   
 451 m centered around the true source location  $\mathbf{r}_k$  and save it to the corresponding false negatives  
 452 count array  $FN_k(\theta)$ . The count of vertices from  $\mathcal{M}_<$  outside the sphere with radius  $r_{max}$  is  
 453 saved to the true-negatives count array  $TN_k(\theta)$ .

454 Then, for each threshold value  $\theta$  we compute the average true positive rate ( $TPR(\theta)$ ) or  
 455 sensitivity and the average false positive rate  $FPR(\theta)$  equal to  $1 - specificity$  as

$$456 \quad TPR(\theta) = \frac{\sum_{k=1}^{N_{mc}} TP_k(\theta)}{\sum_{k=1}^{N_{mc}} TP_k(\theta) + FN_k(\theta)} \quad (17)$$

$$457 \quad FPR(\theta) = \frac{\sum_{k=1}^{N_{mc}} FP_k(\theta)}{\sum_{k=1}^{N_{mc}} FP_k(\theta) + TN_k(\theta)} \quad (18)$$

456 The pair  $(FPR(\theta), TPR(\theta))$  parameterized by  $\theta$  forms the ROC curve that we use to compare  
 457 between different RSA approaches studied in this paper.

### 458 3.2. Performance gauges for realistic simulations

459 In the realistic simulations with multiple sources described in Section 2.4.3 we created  
 460  $P = 4$  simultaneously active sources placed randomly on the cortex during each Monte-Carlo  
 461 iteration, each with the specific theoretical RDM  $\mathbb{D}^p$ . In this case, we gauged the performance  
 462 based on the distance between the simulated source locations and those that were estimated  
 463 using ReDisCA and the two source space RSA implementations that performed best during  
 464 the first set of simulations with a single source, see Section 2.4.2.

465 To compute this metric at each Monte-Carlo iteration we used the scans  $\rho_m^p$ ,  $m =$   
 466  $1, \dots, M$ ,  $p = 1, \dots, P$  corresponding to the  $p$ -th source RDM  $\mathbb{D}^p$  and identified the cortical  
 467 vertex index  $m^*$  corresponding to the maximum of  $\rho_m^p$  as  $m^* = \operatorname{argmax}(\rho_m^p)$ . We then used

468 the coordinates vector  $\mathbf{r}^*$  of the  $m^*$  vertex and computed the distance between it and the  
 469 true location of the  $p$ -th source  $\mathbf{r}_p^{true}$ , see Section 2.4.3 as  $\delta\mathbf{r}_p = \|\mathbf{r}_p^{true} - \mathbf{r}^*\|$ . We then plotted  
 470 the histograms  $\delta\mathbf{r}_p$  observed in the Monte-Carlo trials for each of the compared methods.

471 At each Monte-Carlo iteration we have also computed the correlation coefficients between  
 472 spatial topography vector  $\mathbf{a}_1^p$  of the first ReDisCA component and the corresponding true  
 473 source topography vectors  $\mathbf{g}_{true}^p$ ,  $p = 1, \dots, P$ . Having performed a set of Monte-Carlo trials  
 474 we summarized the observed correlation coefficient distributions in the form of histograms.

475 Finally, we have compared the target RDMs  $\mathbb{D}^p = \{d_{ij}^p\}$  from the  $p$ -th source to the  
 476 empirical RDMs  $\hat{\mathbf{D}}^p$ . These empirical RDMs can be obtained from spatially filtered data  
 477 using ReDisCA-derived filters  $\mathbf{w}^p$  as  $\hat{\mathbf{D}}^p = \{\hat{d}_{ij}^p\} = \{\mathbf{w}_p^T \mathbf{R}^{ij} \mathbf{w}_p\}$ , where  $\mathbf{R}_{ij}$  is the  $i$ -th and  
 478  $j$ -th condition difference time series covariance matrix as described in section 2.3. Then, we  
 479 measured the correlation coefficients between the vectors derived from the upper triangular  
 480 elements of  $\mathbb{D}^p$  and  $\hat{\mathbf{D}}^p$  for each  $p$ -th source,  $p = 1, \dots, P$ . Using multiple Monte-Carlo  
 481 trials, we summarized the distributions of these correlation coefficients in histograms.

## 482 4. Results

### 483 4.1. Simulations

484 In Figure 4, we illustrate the outcomes of the first set of our simulations where we com-  
 485 pared ReDisCA with four versions of the source space RSA, see Figure 1 for their detailed  
 486 diagram. As described before, the aim here was to detect a single neuronal source using  
 487 a noisy version of its specific RDM. In Figure 4.a, the blue curve represents ReDisCA's  
 488 performance in the detection of the representational dissimilarity subspace using the aver-  
 489 aged evoked response data. This method significantly outperforms four different versions  
 490 of the source space RSA that employ two different inverse operators: the minimum norm  
 491 estimator and the LCMV beamformer. Out of the four source space RSA approaches LCMV  
 492 beamformer based on single trials (BF S.T.) approach appears to perform best. Impor-  
 493 tantly, ReDisCA yields better ROC AUC values in detecting spatial component linked to  
 494 the targeted neuronal source without relying on electromagnetic inverse modeling and with  
 495 significantly fewer computations as compared to the source space RSA. To make this con-  
 496 clusion and enable the comparison we employed the electromagnetic inverse modeling to  
 497 align ReDisCA's results with those of conventional RSAs that operate explicitly in the space  
 498 of neuronal sources, see expressions (13) and (14). Figure 4.b illustrates noisy (blue) and  
 499 noise-free (red) averaged ERP time series and the theoretical dissimilarity matrix used in  
 500 simulations is shown at the bottom. Figures 4.c and 4.d show similar results but for SNR  
 501  $= 0.1$ . As we can see, in this atypically low SNR case ReDisCA's performance only slightly  
 502 deteriorates and remains superior to that of the other methods. ReDisCA appears capable of  
 503 accurately locating the target source in nearly 85% of cases at almost zero false alarms rate.  
 504 Comparing the curves of classical RSA approaches (MNE AV RSA, MNE S.T. RSA, BF AV  
 505 RSA, BF S.T. RSA) across two SNR values (panels a) and c) in Figure 4), an interesting  
 506 finding emerges. We notice an improvement in the performance of the source space RSA  
 507 methods under low SNR conditions compared to higher SNR scenarios in this single-source  
 508 simulation. Our analysis reveals that this seeming paradox arises due to a decrease in false  
 509 positives in the traditional RSA outputs as SNR decreases. Despite the use of a realistic  
 510 brain noise model with spatial correlations, the resulting data matrix appears 'empty'. This

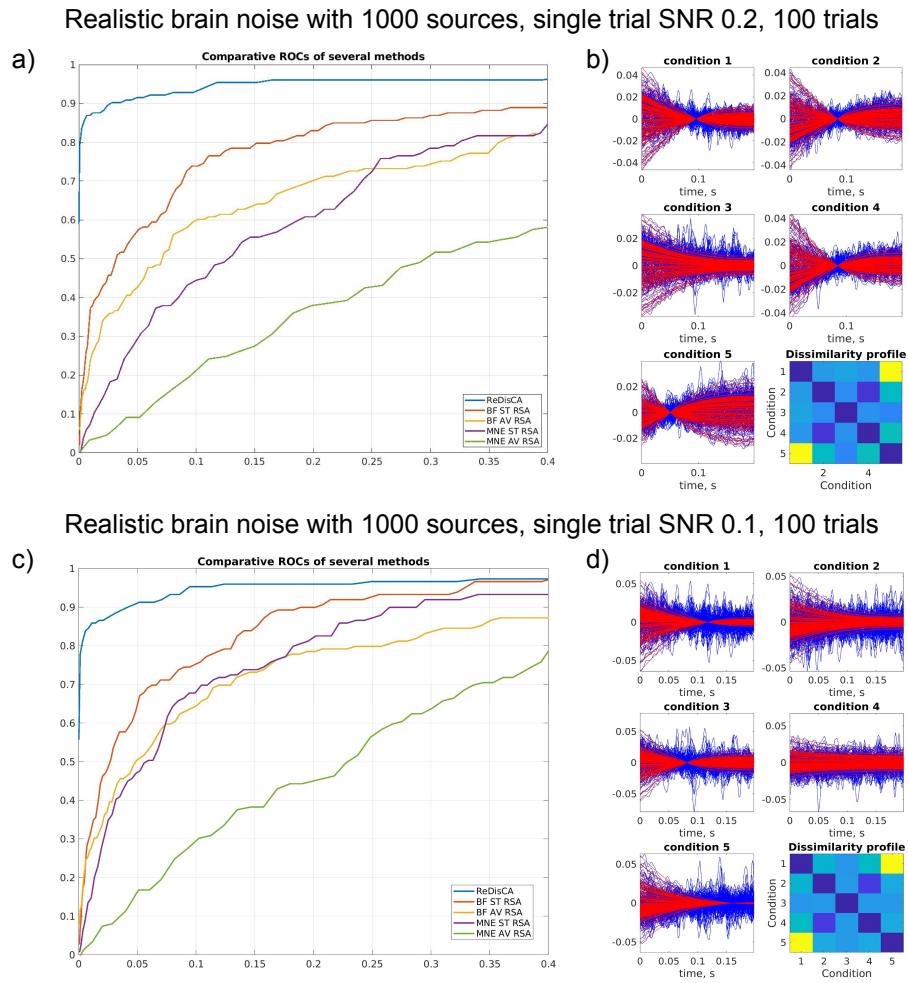


Figure 4: Results of 100 MC trials of simulations in single source detection scenario. a) and c) the ROC curves for ReDisCA and four source space RSA versions, see Section 2 for two different SNR levels. b) and d) - noisy (blue) and noise-free (red) averaged ERP time series for the two SNR values and the theoretical dissimilarity matrix used in the simulations.

511 results in the situation where despite the inverse modeling the sole persistent component of  
 512 the single source remains spread across numerous cortical vertices in the source time series  
 513 estimates, which leads to a surplus of high correlations between the observed and theoretical  
 514 RDMs. The increased noise levels, however, rectify this issue, rendering RDM correlation  
 515 scans more specific which in turn improves the corresponding ROC curves.

516 This observation aligns with the lower ROC-AUC values observed in the source space  
 517 RSAs based on the averaged ERP data (BF AV and MNE AV) compared to their single-trial  
 518 counterparts (BF S.T. and MNE S.T.). In the latter case, dissimilarity scores are computed  
 519 on individual trials before averaging, while in the former the averaging precedes computation  
 520 of the vertex-specific between-condition dissimilarity scores based on the inverse modeling of  
 521 these averaged ERP data (refer to Figure 1). This paradoxical behavior, however, does not  
 522 manifest in more realistic simulations involving multiple cortical sources, as described next.

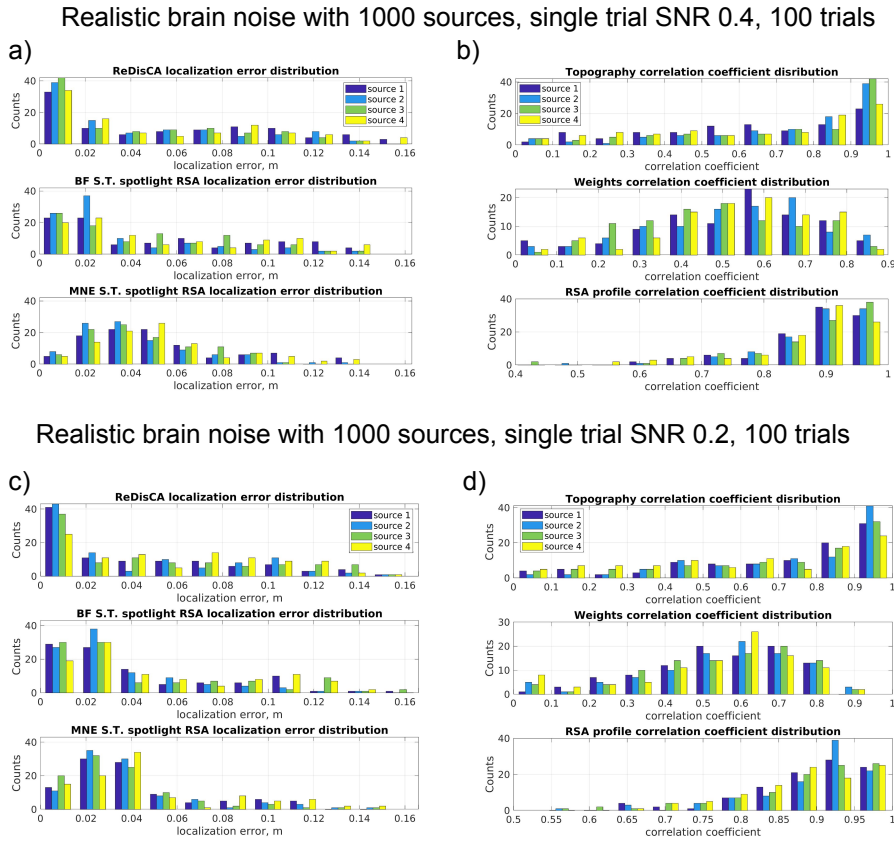


Figure 5: Results of 100 MC trials of realistic simulations with  $M = 4$  randomly seeded sources and  $C = 6$  conditions: a) Distribution of the true topography and ReDisCA derived pattern correlation coefficient, b) Distribution of the true topography and ReDisCA spatial filter weight vector correlation coefficient, c) Distribution of the correlation coefficient of true RDM and RDMs derived from the multichannel data with the first ReDisCA derived spatial filter, d) Distribution of ReDisCA source localization error, e) Distribution of the MNE spotlight RSA source localization error.

523 Next we describe the results of more realistic simulations where at each Monte Carlo trial  
 524 we randomly seeded  $M = 4$  sources each with its own RDM, see Section 2.4.3 for details.  
 525 The results from 100 Monte Carlo trials of these realistic simulations for  $C = 5$  conditions  
 526 are presented in Figure 5 for two SNR values.

527 In Figure 5.a we show the distribution of source localization errors for four sources (dif-  
 528 ferent colors) for the three methods: ReDisCA, BF S.T. RSA, and MNE S.T. RSA. Out  
 529 of compactness considerations we have chosen to present here the results of only two best-  
 530 performing source space RSA methods, BF S.T. and MNE S.T. As one can see ReDisCA's  
 531 distribution appears to have the largest proportion of cases where all four sources are local-  
 532 ized with errors below 1 cm. The distributions of source localization errors delivered by BF  
 533 S.T. and MNE S.T. are increasingly shifted to the right and result in greater median source  
 534 localization error as compared to ReDisCA.

535 Panel b) shows ReDisCA-specific metrics described in Section 3.2. From top to bottom we  
 536 show the distributions of 1) topography correlation coefficient between ReDisCA identified  
 537  $\mathbf{a}_1$  and the true simulated source topography  $\mathbf{g}_p^{true}$ , 2) ReDisCA weights  $\mathbf{w}_1$  and the true  
 538 topography  $\mathbf{g}_p^{true}$  correlation coefficient and finally 3) correlation coefficient between the target  
 539  $\mathbb{D}^p$  and observed RDMs  $\hat{\mathbf{D}}^p$  for  $p = 1, \dots, 4$ .

540 Since the spatial filters derived by ReDisCA get not only tuned to the target source but  
 541 also attempt to tune away from the interfering sources [17, 48] the true source topographies  
 542 appear to be much better aligned with ReDisCA derived topographies (patterns) than with  
 543 the corresponding weight vectors. As evident from the bottom plot in Figure 5.b the observed  
 544 RDMs appear to be well correlated with the target RDMs for all four sources. Panels c) and  
 545 d) of Figure 5 show similar plots but for the decreased Signal-to-Noise Ratio (SNR) equal  
 546 to 0.2, allowing us to observe that ReDisCA remains operable in these harsh conditions. It  
 547 is important to note that in simulations by combining noiseless sensor data with noise data  
 548 matrices, see equation (16), we effectively control the SNR based on the ratio of root mean  
 549 powers between these two matrices. Therefore, as the number of sources within the noiseless  
 550 data matrix increase, the SNR per individual source automatically decreases. Hence, in the  
 551 case of four sources, the SNR of 0.2 represents a notably more challenging task compared to  
 552 a single-source scenario with the SNR of 0.1.

553 Finally, we explore the dependence of localization error on the number of conditions  
 554 employed in RSA analysis. It is intuitive to expect that the increase in the number of  
 555 conditions should lead to improved source localization performance in the classical RSA  
 556 scenario and better identification of the representationally relevant components by ReDisCA.  
 557 As before, to align ReDisCA's results with those of source space RSA approaches we fitted  
 558 a dipole to ReDisCA-derived source topography vectors  $\mathbf{a}_1^p$ ,  $p = 1, \dots, 4$ . The results are  
 559 presented in Figure 6 in the form of three graphs corresponding to the average median  
 560 localization error achieved by the three techniques. As expected the increase in the number  
 561 of conditions leads to the decrease of source localization error. ReDisCA furnishes the best  
 562 performance for all  $C$ , the mean median error appears to be less than 2 cm for  $C = 6$   
 563 conditions.

#### 564 4.2. Real data analysis examples

565 In this section we demonstrated the use of ReDisCA for analysis of two real-life datasets.  
 566 The first dataset is a publicly available low-density EEG N170 dataset available at <https://osf.io/pfde9/>

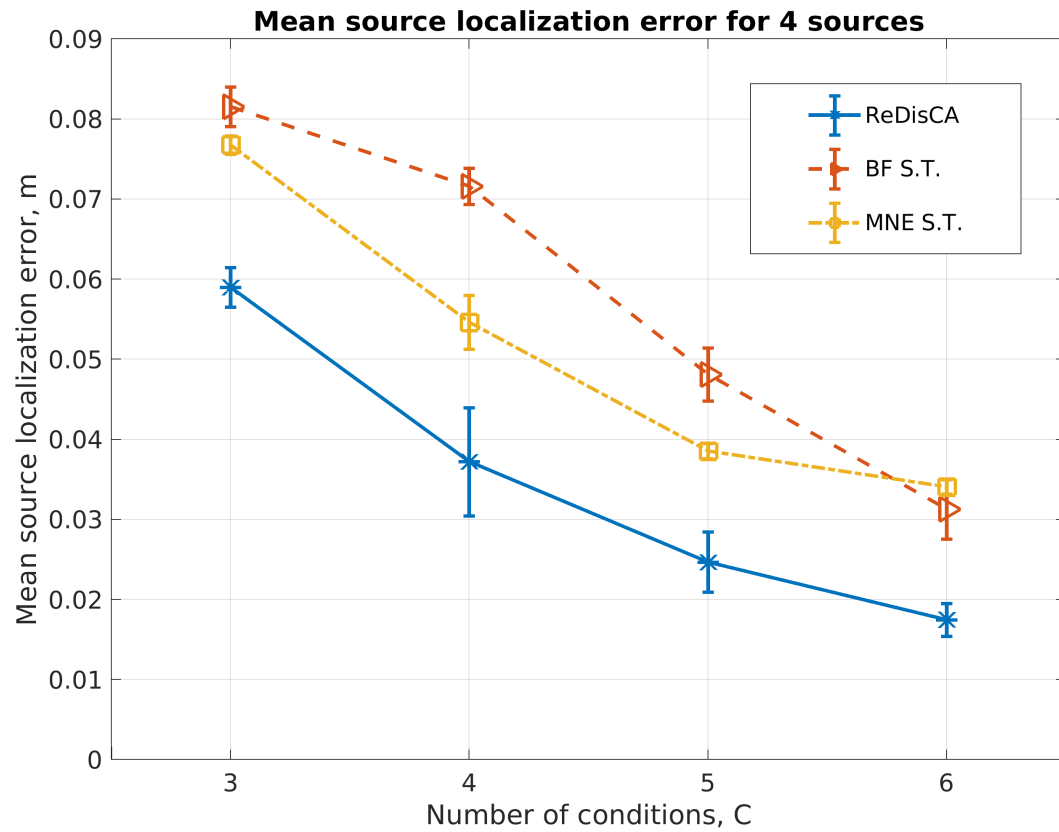


Figure 6: Average median localization error of 4 simultaneously active sources (each with its own RDM) as a function of the conditions count  $C$  for three methods ReDisCA, beamformer-powered single trial RSA, and MNE-powered single trial RSA. As expected the increase in the number of conditions leads to the decrease of source localization error. ReDisCA furnishes the best performance for all  $C$ , the mean median error appears to be less than 2 cm for  $C = 6$  conditions.

567 and described in [22]. In that data the N170 was elicited in a face perception task with stim-  
 568 uli from [51]. In this task, an image of a face, car, scrambled face, or scrambled car was  
 569 presented on each trial in the center of the screen, and participants responded whether the  
 570 stimulus was an “object” (face or car) or a “texture” (scrambled face or scrambled car).  
 571 The data were preprocessed and three ICA components corresponding to ocular and cardiac  
 572 artifacts were removed from the data. Then, the ERP were computed by averaging responses  
 573 within each of the stimulus types. The dataset comprises the EEG data from 40 subjects. In  
 574 our analysis for demonstration purposes we used single subject data recorded from the first  
 575 participant with index ”1”.

576 The second dataset is an Elekta Neuromag 306 MEG dataset from the first run of the  
 577 RSA study by [27]. In this open-access article, the authors employed source space RSA and  
 578 demonstrated distinct differences in the timing, brain regions involved, and dynamics of visual  
 579 processing of faces and tools during the categorization stage. They found that face-specific  
 580 spatiotemporal patterns were linked to bilateral activation of ventral occipito-temporal areas  
 581 during the feature binding stage at 140–170 ms. In contrast, tool-specific binding-related  
 582 activity was observed within the 210–220 ms window, located in the intraparietal sulcus of  
 583 the left hemisphere. Brain activity common to both categories began at 250 ms and included  
 584 widely distributed assemblies within the parietal, temporal, and prefrontal regions. A more  
 585 detailed description of the spatial-temporal dynamics can be found in Figure 3 of [27]. In  
 586 our analysis we used the data recorded from the first subject labeled as ”AD”.

#### 587 4.2.1. *ReDisCA of a low-density EEG dataset*

588 We first applied ReDisCA to explore the spatial-temporal structure of the response to  
 589 meaningful versus meaningless stimuli that were formed as the scrambled versions of the  
 590 original images. For that, we formed the theoretical RDM shown in Figure 7.a. Then,  
 591 scanning over time windows of duration  $T = 150$  ms and calculating the  $p$ -values we obtain  
 592 their color-coded map shown in Figure 7.b with rows corresponding to the components and  
 593 columns encode time. We then visualized uncorrected  $p$ -values corresponding to the first  
 594 component and identified the time interval corresponding to a continuous segment of  $p <$   
 595  $0.05$ . As can be seen from Figure 7.d we found such a segment at around  $t = 400$  ms.  
 596 The corresponding pattern is visualized in panel c) and has highly pronounced occipital  
 597 topography. This result is in agreement with observations made in a high-density EEG-  
 598 based study [37] that demonstrates a statistically significant difference between meaningful  
 599 and meaningless stimuli occurring in the time window around 300-500 ms and is localized to  
 600 the occipital area of the scalp. ReDisCA missed the first peak at around 100 ms reported by  
 601 [37] but that could be explained by a smaller number of electrodes in the current dataset as  
 602 compared to the one analyzed in [37]. At the same time, our analysis of an MEG dataset, see  
 603 Figure 15 in Section 4.2.2, shows a significantly different activation of ReDisCA component  
 604 starting at 160 ms and contrasting the meaningful vs. meaningless visual stimuli. This  
 605 component has dominantly occipital topography.

606 A significant component aligned with the theoretical meaningful vs. meaningless RDM  
 607 was observed over 3 adjacent time windows. Figure 8 shows the discovered topographic pat-  
 608 terns of the first ReDisCA component, the corresponding time courses of this component  
 609 observed within the four different conditions as well as the observed (or empirical) color-  
 610 coded RDM in the bottommost panel. As we can see the yellow and violet timecourses

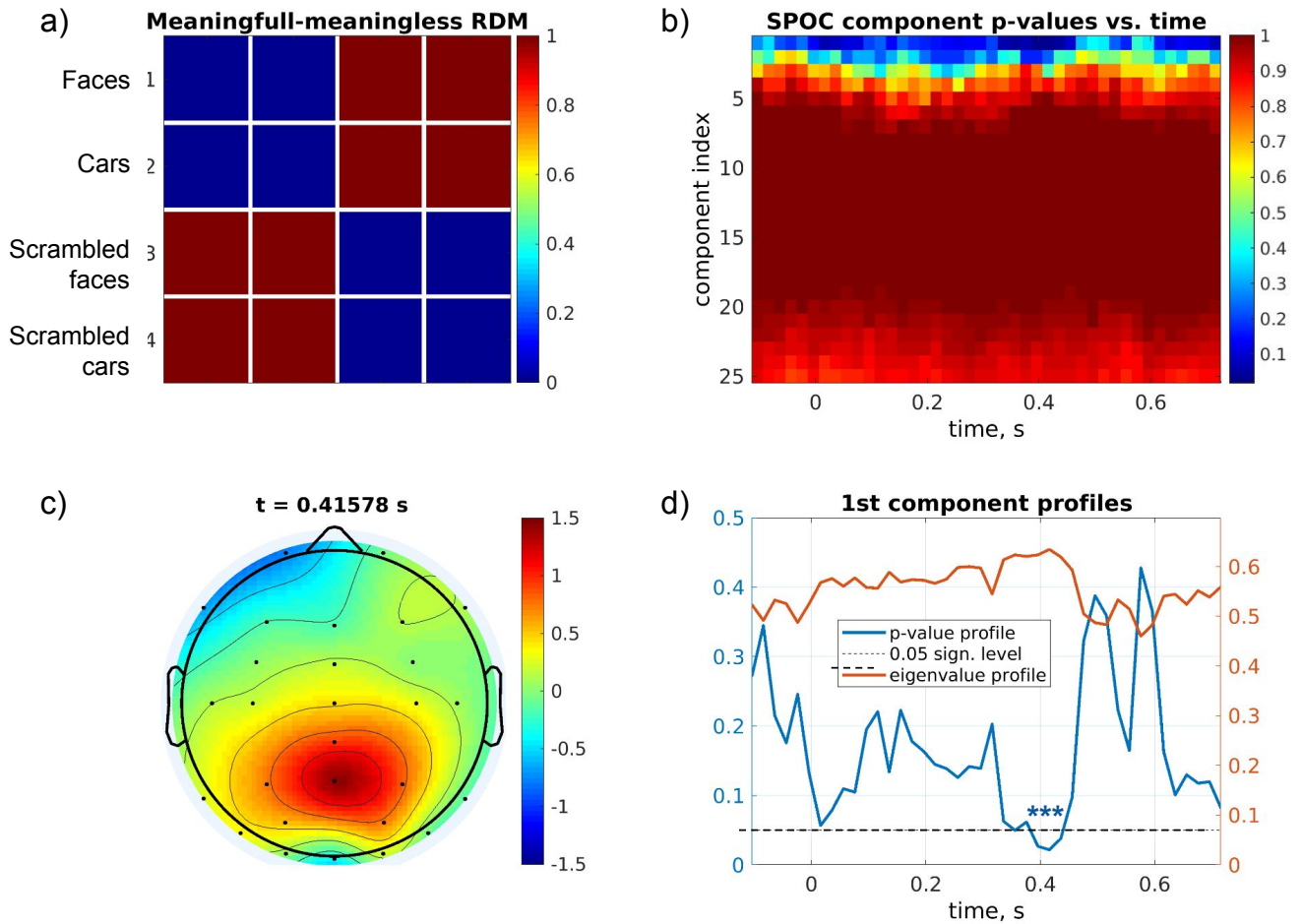


Figure 7: Meaningful vs meaningless stimuli perception analysis. a) Theoretical RDM contrasting the two types of stimuli. b) Color-coded map of component  $p$ -values, each row corresponds to a component and columns encode time. c) Topography (pattern) of the first and the only significant component during the time interval around  $t = 400$  ms. d) Temporal profiles of the uncorrected  $p$ -values corresponding to the first component. The significant segment is marked with asterisks.



611 corresponding to the meaningless stimuli appear disentangled from the red and blue ones ob-  
 612 served during the presentation of meaningful pictures. The topography of the first significant  
 613 ReDisCA component ( $p < 0.05$ ) remains highly similar over the three consecutive time win-  
 614 dows. Interestingly, the time series of this ERP component observed during the presentation  
 615 of faces (blue) exhibits longer-lasting traces as compared to that corresponding to the activity  
 616 during the presentation of cars (red curve) which is consistent with the findings reported in  
 617 several studies exploring neural correlates of face perception in humans [18]. Consequently,  
 618 the observed RDMs indeed appear to closely resemble the target RDM, see Figure 7.a used  
 619 for the described inquiry. Comparing the evolution of the topography of the first (the only  
 620 one found significant) ReDisCA component we can observe its gradual displacement in the  
 621 sagittal plane moving downwards with time followed by deepening (the topography widens)  
 622 of the source at the last time stamp. This may correspond to the traveling wave patterns  
 623 found in the visual area [52, 4].

624 We proceeded by examining the activity associated with particular meaningful stimuli  
 625 using the RDMs displayed in Figure 9.a for faces and Figure 9.b for cars, respectively. These  
 626 RDMs guide our search towards a component with a distinct activity in one condition (face  
 627 or car) different from that observed in the remaining three conditions. Additionally, unlike  
 628 what may be the case in the decoding-based multivariate pattern analysis approaches, the  
 629 RDMs prescribe the activity during the remaining three conditions to be similar. Although a  
 630 classifier can be built to enforce a compact representation within each of the classes, the RSA  
 631 offers a greater flexibility in imposing the geometric constraints on the discovered activity  
 632 using non-binary RDM matrices. See the analysis reported in Figures 16 and 17 in Section  
 633 4.2.2.

634 According to the large volume of studies N170 ERP component is considered to be face  
 635 specific and occurs at around 170 ms latency. We have therefore selected the time window  
 636 of duration  $T = 100$  ms centered at 200 ms and applied ReDisCA to it using the theoretical  
 637 RDM shown in Figure 9.a. Figure 10 shows ReDisCA's output and as we can see from the  
 638 top panel of 10 the first and the only significant ReDisCA component has topography corre-  
 639 sponding to a source in the right fusiform gyrus, the area known to be crucial to perception of  
 640 facial information and differentially activated in response to regular or scrambled face stimuli  
 641 [16, 27].

642 The corresponding ERP components obtained by filtering the multichannel ERP with  
 643 a spatial filter derived by ReDisCA are presented in the panel below the topography. We  
 644 indeed can observe a burst of activity around 170 ms in the "face" condition while in the other  
 645 three conditions the response curves do not have such a burst and are very closely aligned  
 646 implementing the requirement imposed by the RDM matrix. In agreement with other studies,  
 647 the discovered face-related ERP components remain active over a long duration of response.  
 648 The observed RDM is shown in the bottommost panel. We can see that it aligns well with  
 649 the theoretical RDM and exhibits a high correlation coefficient of 0.82.

650 Finally, we performed similar processing but using the theoretical RDM from Figure 9.b  
 651 designed to highlight response components specific to the processing of car images. We have  
 652 found two significant components with  $p < 0.01$  shown in Figure 11. The first components  
 653 appear to have a lower occipital topography with the time course exhibiting deflection at  
 654 around 150 ms that is specific to the second condition (car images). This reflects activity in  
 655 the ventral visual pathway during the image perception task. The traces of this ReDisCA

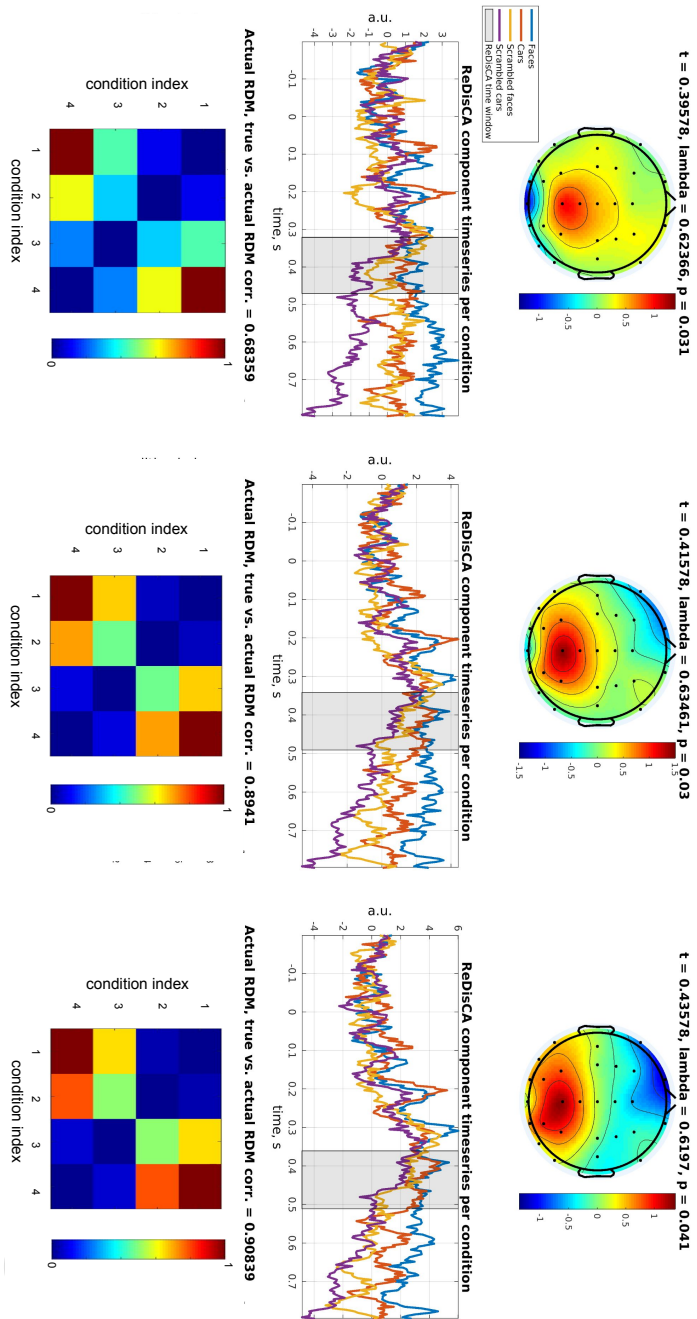


Figure 8: Meaningful vs. meaningless stimuli perception analysis. Topography, spatially filtered timeseries and the observed RDMs for the three consecutive time slices at around  $t = 400$  ms, see also Figure 7.d

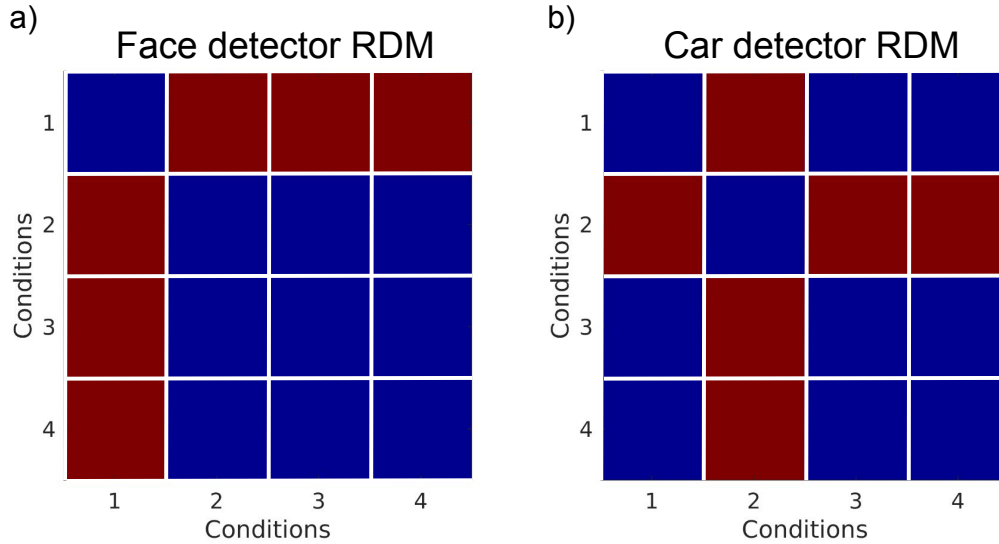


Figure 9: Theoretical RDMs corresponding to faces (a) and cars (b)

656 component appear to be remarkably similar in the other three conditions not only during the  
 657 target interval but also over the entire response duration. The observed and the theoretical  
 658 RDM appear highly correlated with a correlation coefficient greater than 0.99.

659 Interestingly, the second component has a pronounced topography that may reflect the  
 660 activity in the dorsal visual pathway that is known to accompany visual perception of objects  
 661 and is hypothesized to reflect the neural processes of formation of spatial relations between  
 662 the objects within the scene that is then fed to the ventral visual stream [3]. It may also be  
 663 related to identifying the car as a graspable tool as far as the steering wheel is concerned [2].

664 Based on the above we can conclude that the reported real data analysis results obtained  
 665 with a direct application of ReDisCA to the averaged ERP data appear to align well with the  
 666 existing knowledge in the field of neuroimaging related to visual perception of faces and cars  
 667 and differentiation between meaningful and meaningless stimuli including not only spatial  
 668 but also temporal structure of this process.

669 These findings obtained with ReDisCA appear to be in line with what's already known in  
 670 the field of neuroimaging regarding the brain processes underlying visual perception. This in-  
 671 cludes distinguishing between meaningful and meaningless stimuli, delineation of face-specific  
 672 and car-specific activation considering both the spatial and temporal aspects of this cognitive  
 673 process.

#### 674 4.2.2. *ReDisCA of the MEG visual stimuli categorization dataset*

675 To enable a comparison to a more traditional source space RSA we applied ReDisCA to  
 676 the MEG dataset from [27] corresponding to the first run of their experiment.

677 Similarly to [27], we divided the responses within each category into two equal parts and  
 678 labeled them numerically as 1 and 2, resulting in total 6 subcategories labeled "face 1", "face

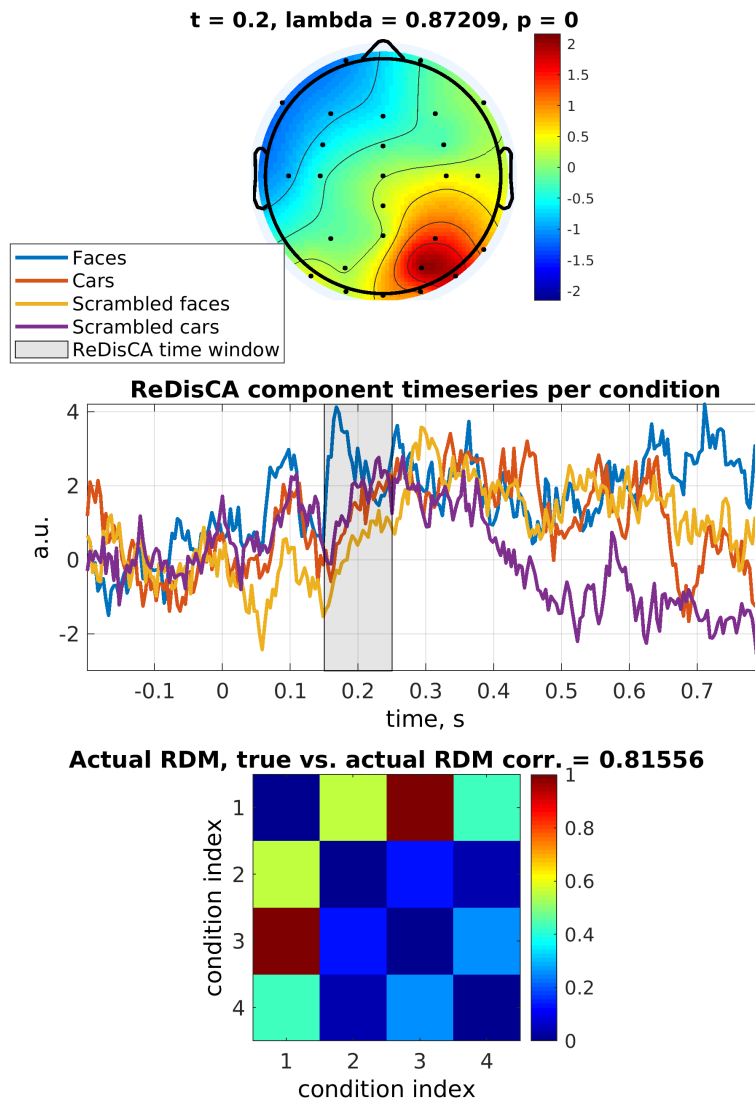


Figure 10: ReDisCA of face-specific responses using the RDM depicted in Figure 9.a. The top panel shows the topography (pattern) of the first and the only significant ReDisCA component. The topography corresponds to a source in the right fusiform gyrus, the area pivotal to the perception of facial information. In the central panel the corresponding ERP components in the four conditions are displayed. The observed RDM is shown in the bottommost panel and exhibits a high correlation coefficient of 0.82 with the theoretical RDM.

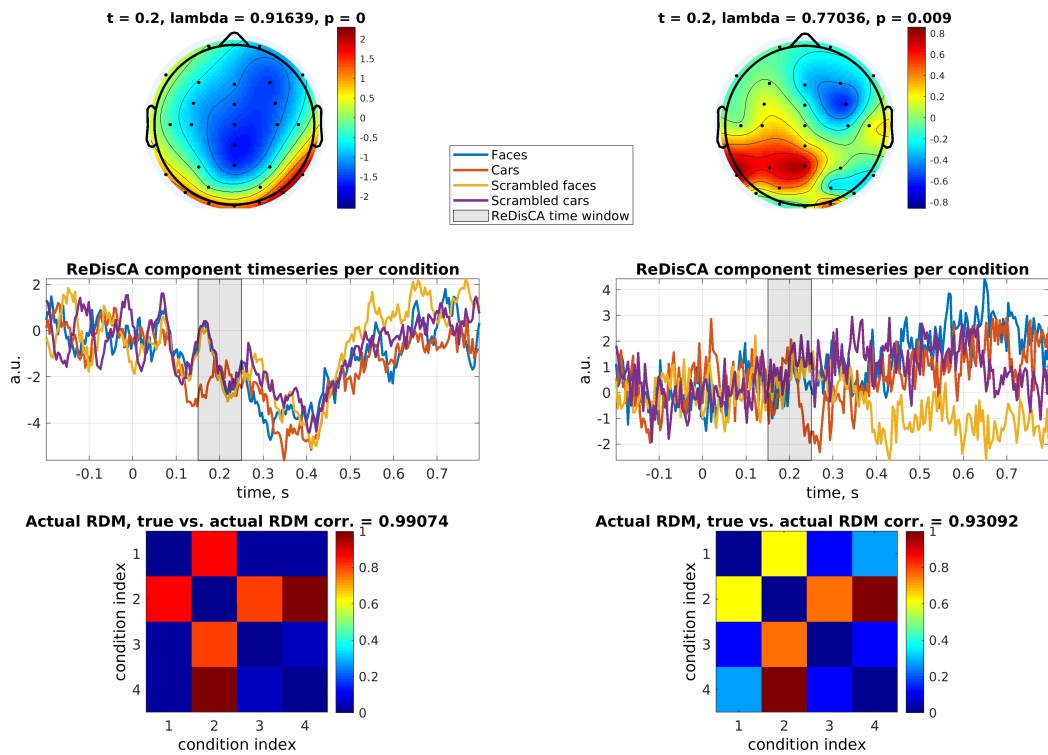


Figure 11: Two significant components discovered by ReDisCA using car detector RDM (Figure 9.b) applied at  $t = 170$  ms latency.

679 2", "tool 1", "tool 2", "nons. 1", and "nons. 2". In each of the subcategory we had 80  
 680 epochs and 480 epochs in total. Since ReDisCA operates on the averaged evoked responses,  
 681 we averaged the single-trial responses to obtain six evoked response field (ERF) matrices,  
 682 one for each subcategory. Each ERF response is a  $204 \times 1500$  matrix, reflecting the activity of 204  
 683 planar gradiometers over 1500 ms, with 500 ms of pre-stimulus and 1000 ms of post-stimulus  
 684 intervals.

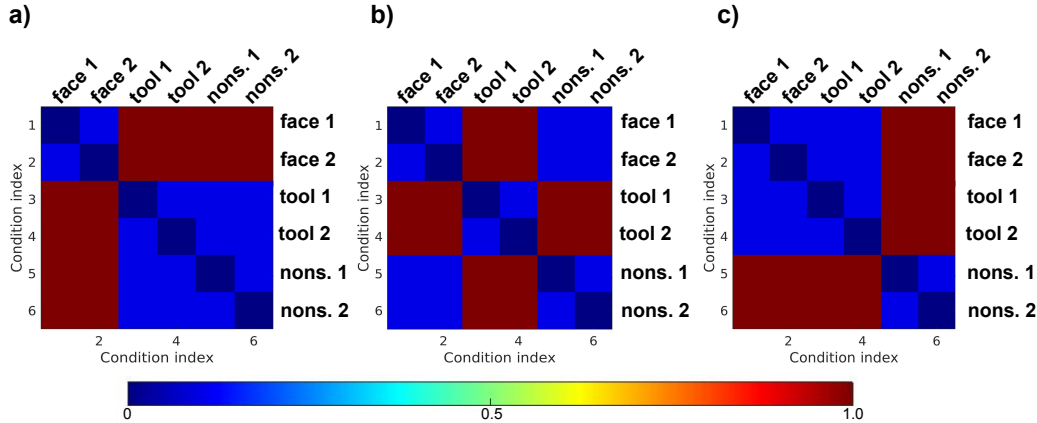


Figure 12: Three theoretical RDM matrices used for analysis of [27] dataset.

685 We have then applied ReDisCA to these six ERFs aiming to elucidate the components  
 686 supporting cortical processing of each of the 3 categories. We used the theoretical RDM ma-  
 687 trices shown in Figure 12 for each of the three categories. This time we applied ReDisCA to  
 688 the entire 1500 ms time-window at once. We then used the spatial filters derived by ReDisCA  
 689 and computed the time series associated with each of the representation dissimilarity compo-  
 690 nents. In our presentation here we considered only the first three statistically significant  
 691 ReDisCA components.

692 The top row of Figure 13 shows the temporal profiles for each of the 6 categories ("face  
 693 1", "face 2", ..., "nons. 2", see the legend) for the face-specific theoretical RDM from Figure  
 694 12.a. Panels a)-c) of Figure 13 correspond to the first three ReDisCA components. The  
 695 title of each panel contains the component's  $p$ -value. The bottom row of plots in Figure  
 696 13 depicts spatial patterns associated with each ReDisCA component discovered using the  
 697 face-specific theoretical RDM.

698 To determine the intervals of significant difference in component activation time series  
 699 between categories, we performed randomization tests. This involved permuting the sub-  
 700 category labels of individual epochs, computing surrogate averages, and applying the corre-  
 701 sponding spatial filters. We then corrected for multiple comparisons using the family-wise  
 702 error rate (FWER) principle operationalized by the maximum statistics computed over the  
 703 entire time interval. The results of the statistical testing are shown with red and blue asterisk  
 704 lines located above and below the time series plots in the top panels of Figures 13 - 15. For  
 705 the reader's convenience and to facilitate a comparison of ReDisCA results with the source  
 706 space RSA findings reported in [27], we have also indicated the starting times of the major

707 significance intervals in each of the time series plots.

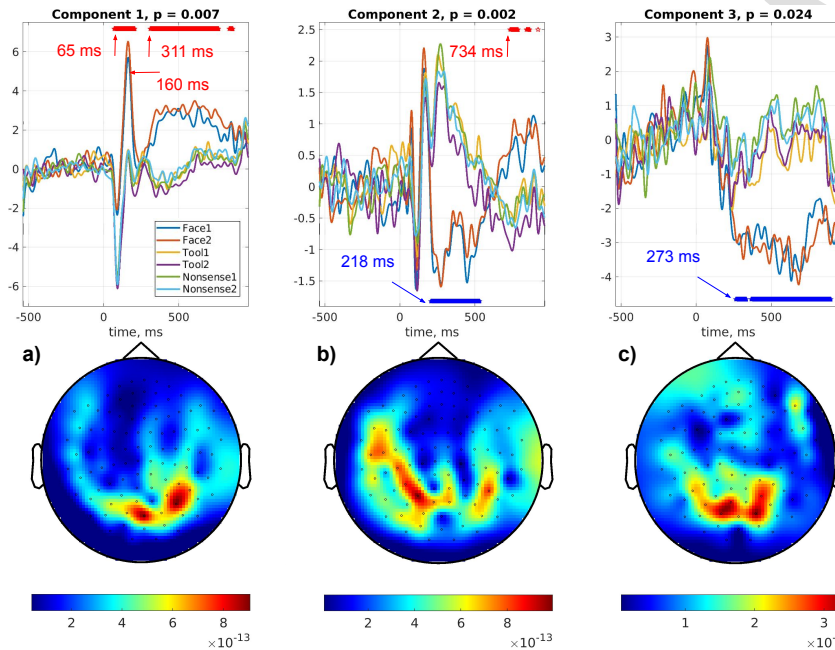


Figure 13: ReDisCA applied to the data from [27] with the face-specific theoretical RDM, see Figure 12.a. Panels a)-c) correspond to the first three ReDisCA components. Within each panel the top plot shows temporal profiles for each of the 6 subcategories ("face 1", "face 2", "tools 1", "tools 2", "nons. 1" and "nons. 2"), see the legend and the title for the associated  $p$ -value. The bottom plot shows the component's spatial pattern.

708 Similarly we have applied ReDisCA using the other two theoretical RDMs from Figures  
709 12.b and 12.c and generated Figures 14 and 15 with ReDisCA results.

710 The first face category-related ReDisCA component, shown in Figure 13.a exhibits the  
711 early differential response to faces starting at 65 ms, see [55] for a review of possible reasons.  
712 The response curve has a prominent peak at 160 ms. This peak differentiates the neural  
713 response to face stimuli from the responses to the other categories. The spatial topography  
714 shown in the bottom panel of Figure 13.a has maximum over the central and right occipital  
715 sensors. This topography likely corresponds to the neuronal sources in the occipital pole,  
716 inferior occipital and the right fusiform gyrus. Notably, this ReDisCA component rises again  
717 with the significance interval starting at 311 ms. This component aligns well with the blue  
718 face-related decoding trace shown in Figure 3 of [27]. The second ReDisCA component,  
719 see Figure 13.b, demonstrates prominent activation of the parietal cortex with the first sig-  
720 nificance interval starting at 218 ms. This topography may reflect sources located in the  
721 middle temporal posterior cortex. The last ReDisCA component shows late and sustained  
722 processing of face-related information starting at 273 ms by neuronal populations located  
723 in the bilateral occipital regions involving some activation of the frontal lobes which may  
724 reflect fronto-temporal interactions associated with visual processing [45]. This component  
725 augments the first ReDisCA component but does not exhibit early response to the face stim-

726 uli.

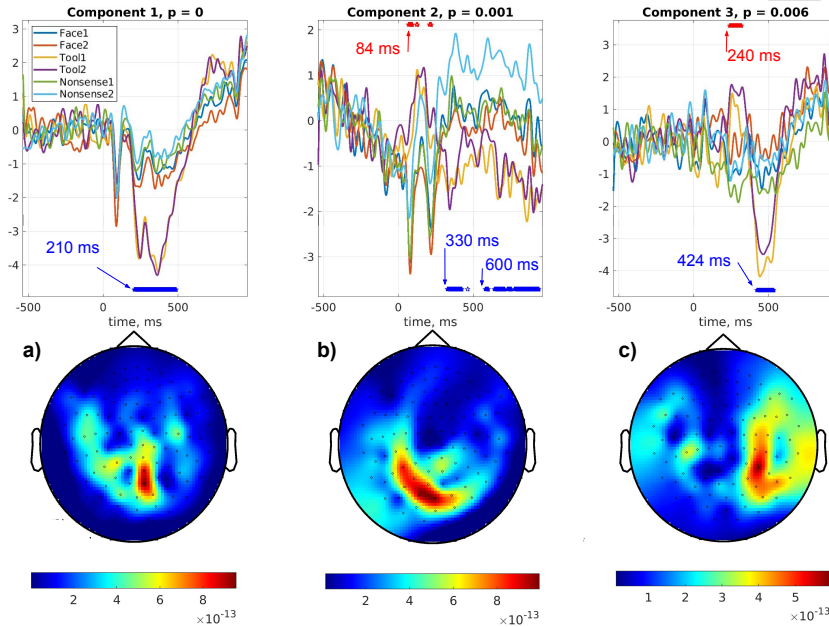


Figure 14: ReDisCA applied to the data from [27] with the tool-specific theoretical RDM, see Figure 12.b.

727 Figure 14 shows the results of ReDisCA with the tool-specific theoretical RDM from  
 728 Figure 12.b. ReDisCA component 1 (Figure 14.a) shows a prominent response to the "tool  
 729 1" and "tool 2" stimuli that occurs at 210 ms and appears to be localized to the central  
 730 occipito-parietal region also involving the planar gradientometers located over the left (and  
 731 compactly over the right) central sulcus areas. Later activation involves the extended parietal  
 732 and occipital regions (Component 2, Figure 14.b) localized to the mid-occipital and left  
 733 parietal cortices. Interestingly, ReDisCA's Component 3 shows activity starting later at  
 734 around 240 ms and stemming from the right and left sensory-motor cortices and sources in  
 735 the temporal lobe with the prevalence of the right side in contrast to Component 1. These  
 736 observations align well with those in [27] where the authors also observed responses at similar  
 737 latency with the left sensory-motor cortex (ReDisCA's component 1) leading the right one  
 738 (ReDisCA's component 3), see the tools-related curves in Figure 3 of [27] for the IPS, VPM  
 739 and the MTp cortices.

740 Next, we explore ReDisCA's components contrasting the perception of the meaningful  
 741 ("face" and "tool") and the meaningless ("nons.") visual stimuli, see Figure 12.c for the cor-  
 742 responding theoretical RDM. In Figure 15.a and Figure 15.b we can see the two components  
 743 that can be assigned to the ventral and dorsal visual pathways correspondingly. The activity  
 744 response to the meaningful stimuli occurred as early as 160 ms in the occipito-parietal region  
 745 (Component 1) followed by the prominent response along the dorsal visual pathway (Com-  
 746 ponent 2). Early (182 ms) and short-lasting as well as the late (675 ms) differential response  
 747 between the meaningful and the meaningless stimuli gets isolated into a single component



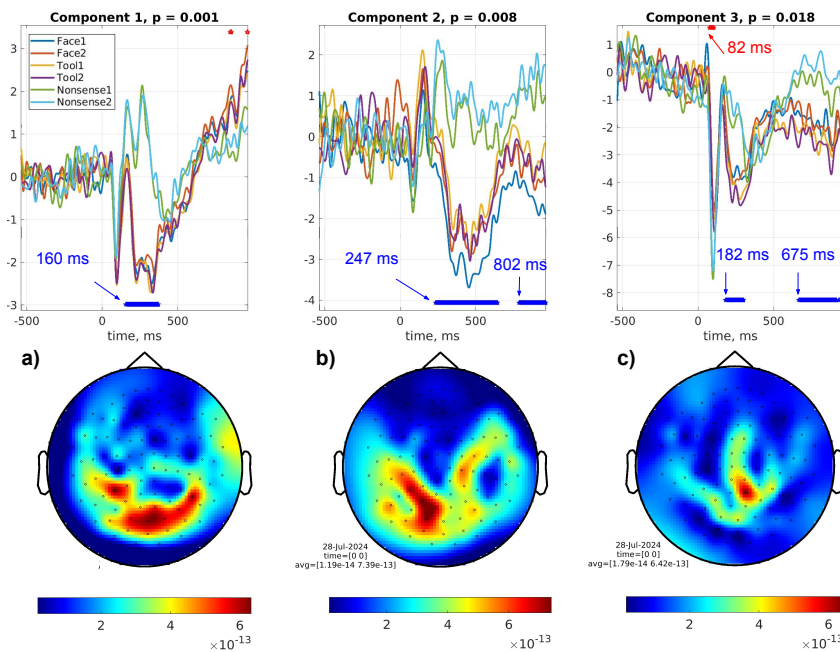


Figure 15: ReDisCA applied to the data from [27] with the RDM contrasting meaningful ("face", "tool") vs. meaningless ("nons.") categories, see Figure 12.c.

748 with a focal mid-parietal topography, see Component 3 in Figure 15.c.

749 In the final example we used ReDisCA to impose specific geometric relationships between  
 750 the resultant components. To do so we used the non-binary RDM shown in Figure 16.a which  
 751 forces ReDisCA to look for the components whose activation is similar within each of the  
 752 three categories (faces, tools, and visually meaningless images). Simultaneously, it imposes  
 753 geometric relations on the activation of the sought components, requiring that the distance  
 754 between each meaningful category and the meaningless one is less than the distance between  
 755 the two meaningful categories, see Figure 16.b. Since ReDisCA currently searches for one-  
 756 dimensional components, the responses to the two meaningful stimuli (faces and tools) will  
 757 be positioned on the opposite sides relative to the responses to the nonsensical visual stimuli.

758 The three components with the lowest  $p$ -values are shown in Figure 17 in the order they  
 759 were returned by ReDisCA.

760 From 17.a we can observe the rise of the response magnitude in the "tools" condition that  
 761 is significantly different from the response in the "faces" condition (that remains nearly flat  
 762 over this interval) as shown by the asterisks on the top of the plot. The significant difference  
 763 starts at 202 ms which nearly exactly matches the results reported in Figure 3 of [27]. As  
 764 evident from the topography, the observed response is produced by dominantly left parietal  
 765 sources and possibly sources from the left sensory-motor cortex. Component 2 shows the  
 766 development of this response in the visual areas of the cortex which again aligns well with  
 767 the late (around 260-350 ms) activity of the fusiform gyrus (FG) in response to the images  
 768 of "tools". The last component reflects face-specific activity that peaks early at around  
 769 160 ms, then mixes with the activity in the other subcategories and then in the second window

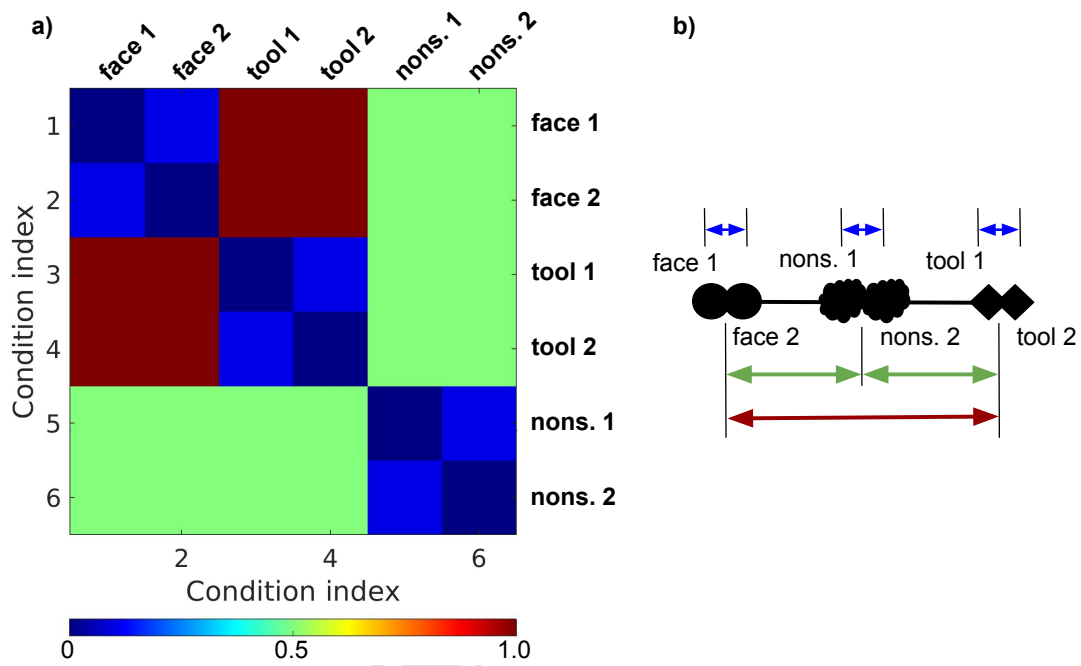


Figure 16: a) The non-binary theoretical RDM matrix used to impose the specific geometric relationship on the component time series. b) This matrix requires that the responses to "face" and "tool" categories are maximally separated while both are equally distanced from the response to the nonsensical images. The distances in a) and b) are identically color-coded.

770 starting at 356 ms becomes prominently distinct from the response in the other categories.

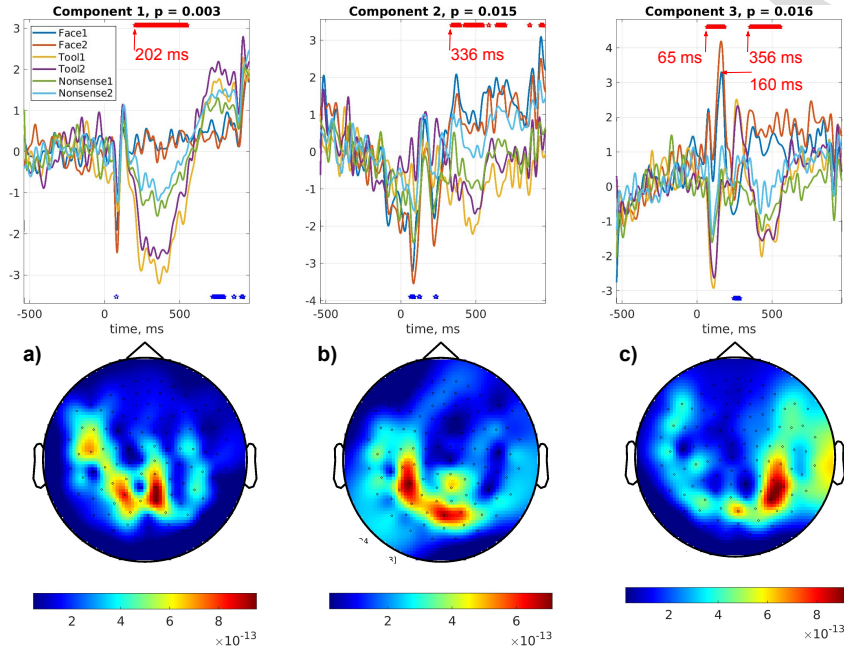


Figure 17: Representational dissimilarity components in the dataset by [27] obtained using non-binary theoretical RDM shown in Figure 16.

771 We have also performed MUSIC scan in order to highlight the cortical areas whose source  
 772 topographies fall into the representational dissimilarity subspace identified by ReDisCA. To  
 773 do so we have utilized the forward model built using the individual MRI as described in [27]  
 774 and applied equation (14) to compute the subspace correlation  $\rho_m^{MUSIC}$  between the pair of  
 775 topographies corresponding to a freely oriented dipole at each  $m$ -th cortical location and the  
 776 representational dissimilarity subspace identified by ReDisCA spanned by the topographies  
 777 shown in Figure 17.

778 In Figure 18 we can observe involvement of the dominantly right fusiform gyrus, right  
 779 insula, left intraparietal sulcus and anterior central gyrus as cortical regions demonstrating  
 780 the requested geometric relationships imposed by the RDM in Figure 16.a In these regions  
 781 the response to faces and tools appears on the opposite sides w.r.t. their response to nonsense  
 782 stimuli as schematized in Figure 16.b and observed in the top panels of Figure 17.

783 Overall, application of ReDisCA to the MEG dataset exploring the neural processes  
 784 underlying visual categorization of faces and tools appears to support the main result of the  
 785 original study [27] and confirms that while perception of faces is dominantly accompanied by  
 786 the activity in the ventral visual stream, the images of tools elicit activity along the dorsal  
 787 visual path and also result in the activation of hand related sensory-motor areas associated  
 788 with the use of the tools.

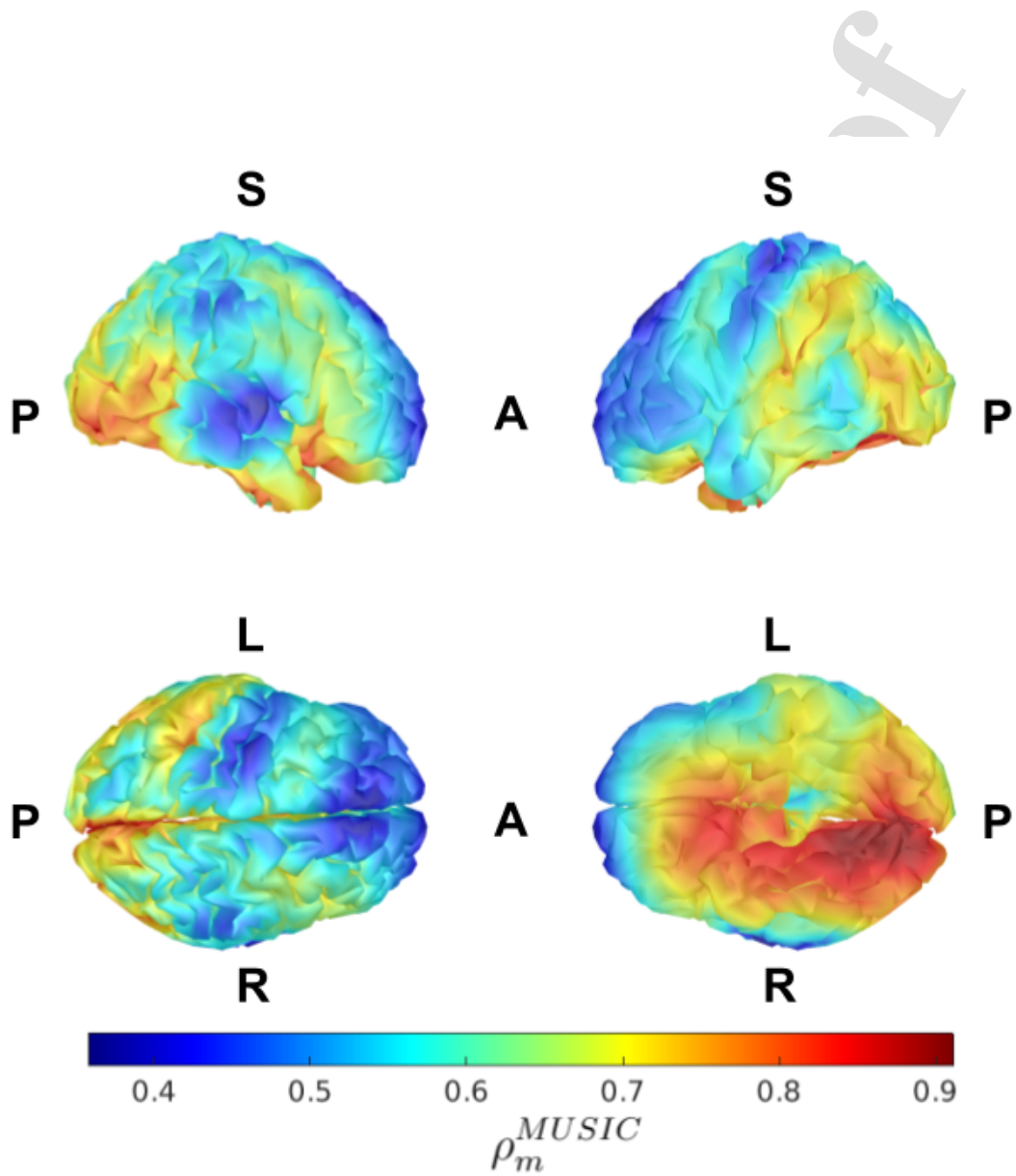


Figure 18: Cortical map reflecting the first principal angle between the dissimilarity subspace spanned by the topographies from Figure 17 and the subspaces spanned by the topographies of a freely oriented dipole at each cortical location, see equation (14). This highlights the potential contribution of the cortical sources to the multivariate activity pertinent to the user specified RDM. (14). Letters A,P,S,L,R - anterior, posterior, superior, left, right define the view angle.

## 789 5. Discussion

790 Conceptually, ReDisCA extends the family of the previously developed methods for de-  
 791 composing multichannel EEG and MEG data and extracting the spatial-temporal compo-  
 792 nents with desired properties. One popular example is the Spatial Spectral Decomposition  
 793 (SSD) technique [41]. SSD seeks to maximize the power at a frequency band of interest while  
 794 simultaneously minimizing it within the side bands. For each specific triplet of frequency  
 795 bands (one central and two flanking) the SSD results in a set of spatial components whose  
 796 time series exhibit the frequency band selective property. In particular, the timecourses of  
 797 the SSD-derived spatial components are characterized by the maximal ratio of power within  
 798 the central band to that within the two flanking sub-bands which justifies the use of SSD  
 799 for extracting rhythmic components from multichannel EEG or MEG time series. Another  
 800 popular method is the Source Power Comodulation, or SPoC [9]. SPoC aims to find spa-  
 801 tial filters and patterns by using in the decomposition process a target behavioral variable  
 802 to emphasize the components whose instantaneous power profile correlates with the target  
 803 variable. Typically SPoC targets rhythmic activity and extracts its sources whose envelope  
 804 aligns well with the target variable. Notably, neither SSD nor SPoC or their early fore-  
 805 runner ICA require forward and inverse modeling machinery to extract target component  
 806 time series. Theoretically speaking, the design of either of these methods does not require  
 807 that the obtained components correspond to a specific neuronal source with a well-defined  
 808 location. In practice, however, the obtained patterns that pertain to individual components  
 809 exhibit remarkable alignment with the appropriate dipolar electromagnetic model and allow  
 810 for pinpointing a specific cortical location as a source of activity with the desired property.

811 In its current version ReDisCA operates with evoked response data recorded over sev-  
 812 eral experimental conditions and aims at finding spatial components (each potentially cor-  
 813 responding to a distinct neuronal source) whose activation time series exhibit the expected  
 814 representational structure. We have started with the Euclidean norm as a distance between  
 815 component activation time series. This continuous measure of dissimilarity not only allows  
 816 for an analytic solution of the subsequent optimization problem but appears superior [58, 15]  
 817 to the simplest forms of more intricate classification accuracy-based distances. Based on this  
 818 and using the standard notion of spatial filtering of multichannel EEG or MEG data we  
 819 devised ReDisCA as the approach for dissecting the evoked responses into a set of spatial  
 820 components with activation time series that adhere to the user-supplied target (or theoretical)  
 821 representational dissimilarity structure.

822 To achieve this we have formulated the specific constrained optimization problem (5). Its  
 823 solution gives us the spatial filters whose application to the multichannel evoked response  
 824 yields component activation timeseries with the expected target representational structure  
 825 encoded by the prespecified target RDM. These time series combined with the spatial patterns  
 826 corresponding to each of the spatial filters [17, 48, 23] give us spatial decomposition of the  
 827 multichannel evoked responses observed over the range of experimental conditions. The  
 828 goodness of fit is given by the corresponding generalized eigenvalue.

829 In contrast to the source space RSA [27] ReDisCA does not require inverse modeling  
 830 and does not perform an explicit and exhaustive scan over brain sources in the attempt to  
 831 pinpoint those whose empirical RDM is close enough to the target RDM. Conceptually the  
 832 role of the inverse modeling in ReDisCA is similar to that in the multivariate pattern analysis

833 of EEG or MEG data, see for example [7]. While the inverse modeling can be applied to  
 834 the patterns [17, 24] obtained from the regression weights it is not the essential step in the  
 835 analysis.

836 In simulations to compare ReDisCA to the source space RSA we fitted an electromag-  
 837 netic model to the signal subspace spanned by the topographies of the statistically significant  
 838 ReDisCA components, see equation (14) and matched the obtained locations against those  
 839 of the simulated sources. This allowed us to rigorously compare ReDisCA with the explicit  
 840 inverse modeling-driven RSA. ReDisCA has successfully identified the signal subspace cor-  
 841 responding to the simulated sources and provided higher ROC AUC scores as compared to  
 842 the source space RSA based on the exhaustive scan. Note that in our implementation of the  
 843 source space RSA we analyzed each cortical source separately, used MNE and LCMV beam-  
 844 former as inverse solvers and employed the L2-norm as the dissimilarity measure instead of  
 845 sLORETA and LDA classifier used in [27]. However, when matching these two techniques  
 846 against each other one has to keep in mind that ReDisCA uses less information and does not  
 847 require inverse modeling which makes it applicable to a broader collection of datasets and  
 848 modalities. For example, ReDisCA may be an interesting option to employ for the analysis  
 849 of ECoG data where forward and inverse modeling are less straightforward than it is with  
 850 non-invasive EEG or MEG data. Also, ReDisCA is directly applicable to the averaged evoked  
 851 responses time series and does not require the presence of single-trial data.

852 In the final example of real-data analysis we have visualized the representational dissim-  
 853 ilarity subspace discovered by ReDisCA. To this end we have performed MUSIC scan and  
 854 visualized the cosine of the first principal angle between the dissimilarity subspace and the  
 855 subspaces spanned by the topographies of a freely oriented dipole at each cortical location.  
 856 This highlights the potential contribution of the cortical sources to the multivariate activity  
 857 pertinent to the user specified RDM. More sophisticated analysis of the ReDisCA discov-  
 858 ered subspace can be performed using a variety of EEG and MEG inverse problem solving  
 859 approaches [14] including the advanced hierarchical Bayesian techniques aimed at recovery  
 860 of the underlying neuronal current source density e.g. [33, 50] or parametric approaches to  
 861 discover discrete sources [35] and their associated time series. Doing so one has to take into  
 862 account the importance of accurately modeling individual subject heads and tissue conduc-  
 863 tivity profiles [59] to improve the source localization accuracy. At the same time, ReDisCA,  
 864 a spatial decomposition method, as opposed to the source-space RSA, does not require the  
 865 inverse modeling and can be used to analyze the datasets with no detailed anatomic infor-  
 866 mation, see Section 4.2.1. Although at the expense of potentially important details, in such  
 867 a setting ReDisCA can be useful in non-invasive explorations of the representational drift  
 868 phenomenon [11] and in the analysis of psychiatric conditions e.g. [53].

869 Any RSA implementation benefits from the increase in the number of experimental condi-  
 870 tions. Although we demonstrated that ReDisCA outperformed conventional RSA approaches  
 871 for all tested counts of conditions (3,4,5,6), the practically useful results can be obtained from  
 872 datasets with no less than four conditions. MNE inverse solver appeared to be a better option  
 873 as compared to the LCMV beamformer for the number of conditions less than 6. ReDisCA  
 874 followed by the source localization procedure yielded almost a 2-fold reduction in the mean  
 875 source localization error as compared to the exhaustive scanning source space RSA. The ap-  
 876 proach reported in [27] where voxel time series obtained with sLORETA are combined into  
 877 ROIs followed by dimension reduction and LDA classification. This combination may poten-

878 tially improve the accuracy of the exhaustive scan-based RSA however, requires significantly  
 879 more computations and in contrast to ReDisCA is not directly applicable to the averaged  
 880 evoked responses time series.

881 We demonstrate that the optimization problem in ReDisCA is mathematically analogous  
 882 to that of SPoC, but it utilizes modified input data matrices. These matrices are calculated  
 883 as the difference between the evoked responses recorded for each pair of conditions. In  
 884 this context, the entries of the theoretical RDM formally take on the role of the behavioral  
 885 variable, as shown in Table 1.

886 In the future, ReDisCA can potentially adopt cross-validated Euclidean distances [58].  
 887 To cope with the inherent asymmetry one can use a symmetric version of it as  $d_{c.v.}^{ij} =$   
 888  $\frac{1}{2} \mathbf{w}^\top \left( \mathbf{R}_{[A][B]}^{ij} + \mathbf{R}_{[B][A]}^{ij} \right) \mathbf{w}$ , where  $\mathbf{R}_{[A][B]}^{ij} = \left( \mathbf{X}_{[A]}^{c_i} - \mathbf{X}_{[A]}^{c_j} \right) \left( \mathbf{X}_{[B]}^{c_i} - \mathbf{X}_{[B]}^{c_j} \right)^\top$  and  $\mathbf{R}_{[B][A]}^{ij} =$   
 889  $\left( \mathbf{X}_{[B]}^{c_i} - \mathbf{X}_{[B]}^{c_j} \right) \left( \mathbf{X}_{[A]}^{c_i} - \mathbf{X}_{[A]}^{c_j} \right)^\top$  with  $\mathbf{X}_{[A]}^{c_i}$  representing averaged responses corresponding to  
 890 condition  $c_i$  and obtained using base data partition A and  $\mathbf{X}_{[B]}^{c_i}$  - using validation partition  
 891 B. Investigation of the utility of this cross-validated distance in the ReDisCA setting is a  
 892 separate topic that needs to be addressed by future studies.

893 Feature-weighted RSA is a modification of RSA that allows to better align the observed  
 894 and the theoretical RDMs [21]. This is achieved by mixing the RDMs that pertain to the  
 895 individual features, e.g. voxels comprising an ROI, with optimal weights maximizing the  
 896 similarity of this mixed RDM and its theoretical target. In application to EEG and MEG data  
 897 the role of individual features is played by individual channels and therefore the adaptively  
 898 tuned weights may be considered as some sort of spatial filtering. At the same time, since  
 899 the weighted RDM matrix entries appear in the form of non-linearly transformed channel  
 900 data (squared distances, functions of classification accuracy, etc.) the coefficients of such a  
 901 mixing can not be transformed into electromagnetically meaningful patterns and are therefore  
 902 difficult to interpret [13].

903 In contrast, ReDisCA by design seeks for a linear spatial filter applied directly to the  
 904 channel data to isolate a source with the desired representational pattern. Because of this,  
 905 the weights vector can be easily converted to source topography, or pattern [24, 17], which  
 906 takes into account the spatial correlation structure present in the data. This guarantees that  
 907 the discovered spatial patterns can be used for implementing a rigorous source localization  
 908 procedure based on the notion of signal subspace as described for example in [40]. This  
 909 property positively distinguishes ReDisCA from the sensor space RSA approach described in  
 910 [37] where the authors using high-density EEG were able to highlight the detailed spatial and  
 911 temporal patterns of responses underlying various aspects of meaningfulness in the presented  
 912 visual stimuli. They achieved this using newly proposed differentiation analysis (DA) and  
 913 computed temporal and spatial profiles of the category differentiation index (CDI) that can  
 914 be used to make judgments about time windows and approximate spatial locations of the  
 915 pivotal sources. However, due to their empirical nature, the obtained spatial CDI maps can  
 916 not be rigorously fitted with an electromagnetic model and therefore are only tangentially  
 917 related to the underlying distribution of cortical sources whose activity exhibits the desired  
 918 representational properties.

919 ReDisCA is formulated to search for a single spatial vector, as indicated by Equation (5),  
 920 and evaluates the similarity of activation in the temporal dimension. This places specific

921 constraints on the size of the temporal window  $T$  to ensure ReDisCA's proper functioning.  
 922 It's crucial to recognize that the size of this window is contingent upon the frequency con-  
 923 tent of the investigated evoked response. Faster-changing signals permit more information  
 924 (pertaining to similarity/dissimilarity) within shorter time intervals.

925 Additionally, the window size is influenced by the number of sensors employed. In theory,  
 926 larger sensor arrays necessitate longer windows to ensure the correlation matrices are full  
 927 rank. Note, however, that typically, EEG and MEG data are projected into smaller sub-  
 928 spaces with dimensions 10-100. All subsequent operations are conducted within this reduced  
 929 dimensional space to guarantee the full rank of the resulting matrices. An alternative or  
 930 additional approach involves employing the Tikhonov regularization strategy when comput-  
 931 ing the inverse of the correlation matrix  $\bar{\mathbf{R}}$ . It's evident that reducing the subspace size  
 932 and increasing the regularization parameter, in addition to enhancing stability, adversely  
 933 impacts ReDisCA's spatial resolution. At the same time, as illustrated with the last example  
 934 described in Section 4.2.2 ReDisCA can be applied to the entire response duration window  
 935 and automatically provides the time-intervals where the sought representational dissimilar-  
 936 ity structure arises. Guidelines detailing these trade-offs must be developed in the future,  
 937 drawing upon both simulations and theoretical analyses followed by verification with real  
 938 data.

939 The approaches such as SSD, SPoC and now ReDisCA are designed to be applied to a  
 940 single subject. When the conclusion needs to be drawn from a cohort of subjects, special  
 941 steps need to be undertaken. For example, in the source space RSA approach reported in  
 942 [27] pooling across subjects is performed using the standard in the MEG approach based on  
 943 warping individual cortex geometries onto the canonical cortex followed by calculation of the  
 944 group level statistics. Given the superiority of ReDisCA demonstrated here as compared to  
 945 the explicit scan in detecting sources with specified RDMs, see Figures 4 and 5, the source  
 946 space estimates can be obtained by applying the individual inverse modeling to the patterns  
 947 discovered by ReDisCA followed by warping these individual results onto the canonical brain.  
 948 It is potentially possible to consider development of group-level approaches, conceptually  
 949 similar to those reported in [28, 20] and driven by ReDisCA functional (5).

950 ReDisCA's applications extend beyond EEG and MEG data analysis to potentially in-  
 951 clude the ROI-based examination of fMRI data. Interpreting the weights that scale individual  
 952 voxel RDMs, as introduced in [21], poses challenges in converting it into a pattern, as dis-  
 953 cussed in [17]. Here, the difficulty arises because the weights in [21] are applied to the  
 954 Representational Dissimilarity Matrices (RDMs) of individual voxels and not to the actual  
 955 voxel activations. Since the RDM elements are non-linear functions of voxel activation, the  
 956 weights in [21] can not be converted into within ROI activation patterns highlighting the  
 957 voxels that contribute most to the target RDM.

958 Employing ReDisCA within each ROI may resolve this challenge, by applying weights  
 959 to the activation of individual voxels rather than to their non-linear functions. This would  
 960 enable the subsequent transformation of ReDisCA weights into patterns [17, 46] which could  
 961 enhance the spatial resolution of fMRI-based functional mapping by clarifying the delineation  
 962 of an extended ROI into subregions contributing to the improved alignment with the target  
 963 RDM.

964 Moreover, ReDisCA can advance the methodology outlined in [32], where the RSA princi-  
 965 ple was used to analyze representations emerging in the layers of an artificial neural network.



966 An intriguing possibility arises when ReDisCA-derived weights align with those of a subse-  
967 quent neuron connected to the analyzed layer, signifying that the individual neuron appears  
968 to be tuned to track the representational structure encoded in the target RDM.

## 969 **6. Conclusion**

970 In conclusion, this study introduces and applies the novel technique of Representational  
971 Dissimilarity Component Analysis (ReDisCA) to overcome challenges associated with clas-  
972 sical Representational Similarity Analysis (RSA), particularly in EEG and MEG data. By  
973 estimating spatial-temporal components aligned with a target representational dissimilarity  
974 matrix (RDM), ReDisCA produces spatial filters and associated topographies that reveal  
975 "representationally relevant" sources. The application of these spatial filters to evoked re-  
976 sponse time series demonstrates superior performance in terms of source localization accuracy  
977 compared to conventional source space RSA, with significantly fewer computations. Our ap-  
978 proach does not require forward modeling and any geometric information but if these are  
979 available the obtained components permit rigorous fits with the electromagnetic model by  
980 means of a plethora of methods for solving the inverse problem. The methodology is validated  
981 through realistic simulations and applied to a real EEG and an MEG dataset, showcasing its  
982 potential for discovering representational structures without relying on the inverse modeling.  
983 In the discussion, we highlighted the limitations of ReDisCA, outlined potential directions  
984 for its further development, and identified novel applications.

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## 988 **8. Conflict of interest statement**

989 The authors declare that they have no conflicts of interest regarding the publication of  
990 this article.

## 991 **9. Ethics statement**

992 In this study we utilized two datasets recorded from human subjects and reported in  
993 separate previously published articles. The first ERP170 EEG dataset is described in [22].  
994 This study was approved by the Institutional Review Board at the University of California,  
995 Davis, and all participants provided informed consent. All materials are freely available  
996 at <https://doi.org/10.18115/D5JW4R>. The second MEG dataset was previously reported in  
997 [27] and collected in accordance with the recommendations of the Declaration of Helsinki  
998 with written informed consent from all subjects. The protocol was approved by the ethics  
999 committee of Moscow State University of Psychology and Education.

1000 .

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Data and Code Availability Statement

The code is available upon request by emailing at [ossadchi@gmail.com](mailto:ossadchi@gmail.com). The data used in the MS are publicly available at <https://osf.io/pfde9/>

Journal Pre-proof

# Representational dissimilarity component analysis (ReDisCA)

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Declaration of Interest Statement

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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