

1 **High-level cognition is supported by at least second order**
2 **dynamic correlations in neural activity patterns**

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5 **Abstract**

6 Our thoughts arise from coordinated patterns of interactions between brain structures that change
7 with our ongoing experiences. High-order dynamic correlations in brain activity patterns reflect different
8 subgraphs of the brain’s connectome that display homologous lower-level dynamic correlations. We tested
9 the hypothesis that high-level cognition is supported by high-order dynamic correlations in brain activity
10 patterns. We developed an approach to estimating high-order dynamic correlations in timeseries data,
11 and we applied the approach to neuroimaging data collected as human participants either listened to a
12 ten-minute story or a temporally scrambled version of the story, or underwent a resting state scan. We
13 trained across-participants pattern classifiers to decode (in held-out data) when in the session each activity
14 snapshot was collected. We found that classifiers trained to decode from high-order dynamic correlations
15 yielded better performance on data collected as participants listened to the (unscrambled) story. By
16 contrast, classifiers trained to decode data from scrambled versions of the story or during the resting
17 state scan yielded the best performance when they were trained using first-order dynamic correlations
18 or raw activity patterns. We suggest that as our thoughts become more complex, they are supported by
19 higher-order patterns of dynamic network interactions throughout the brain.

20 **Introduction**

21 A central goal in cognitive neuroscience is to elucidate the *neural code*: the mapping between (a) mental
22 states or cognitive representations and (b) neural activity patterns. One means of testing models of the
23 neural code is to ask how accurately that model is able to “translate” neural activity patterns into known
24 (or hypothesized) mental states or cognitive representations (e.g., Haxby et al., 2001; Huth et al., 2016, 2012;
25 Kamitani & Tong, 2005; Mitchell et al., 2008; Nishimoto et al., 2011; Norman et al., 2006; Pereira et al.,
26 2018; Tong & Pratte, 2012). Training decoding models on different types of neural features (Fig. 1a) can
27 also help to elucidate which specific aspects of neural activity patterns are informative about cognition—
28 and, by extension, which types of neural activity patterns might comprise the neural code. For example,
29 prior work has used region of interest analyses to estimate the anatomical locations of specific neural
30 representations (e.g., Etzel et al., 2009), or to compare the relative contributions to the neural code of

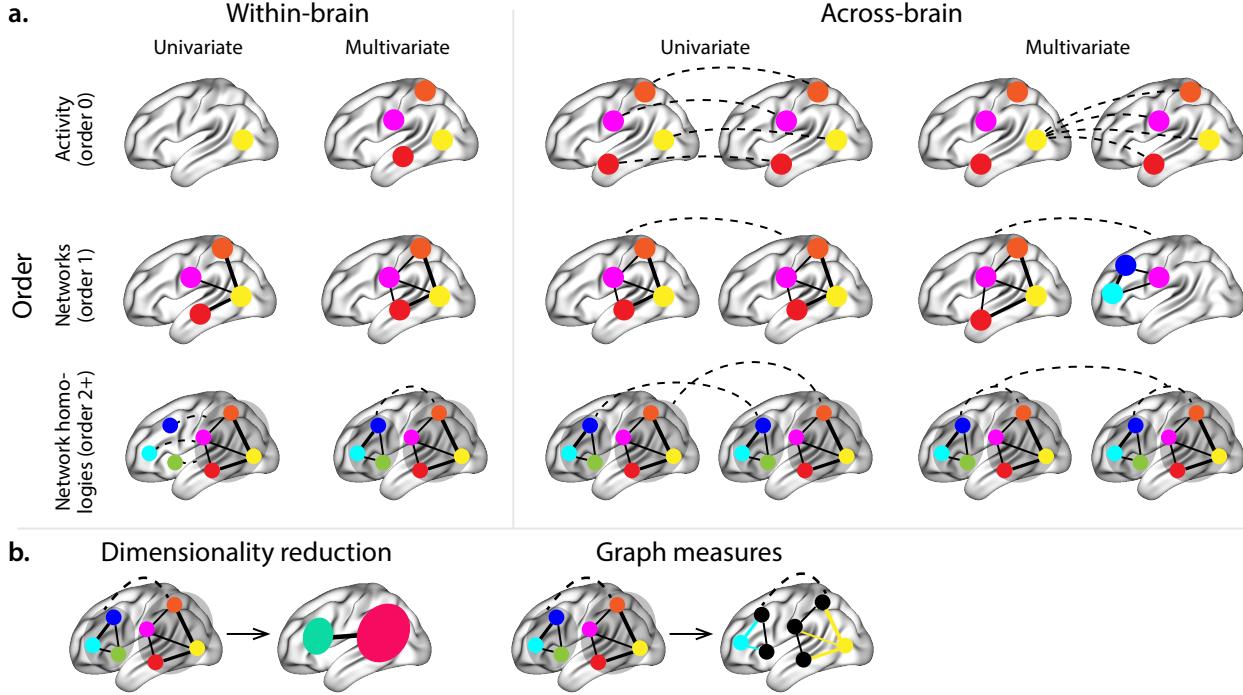


Figure 1: Neural patterns. a. A space of neural analyses Within-brain analyses are carried out within a single brain, whereas across-brain analyses compare neural patterns across two or more individuals' brains. Univariate analyses characterize the activities of individual units (e.g., nodes, small networks, hierarchies of networks, etc.), whereas multivariate analyses characterize the patterns of activities across units. Order 0 patterns involve individual nodes; order 1 patterns involve node-node interactions; order 2 (and higher) patterns relate to interactions between homologous networks. Each of these patterns may be static (e.g., averaging over time) or dynamic. **b. Summarizing neural patterns.** To efficiently compute with complex neural patterns, it can be useful to characterize the patterns using summary measures. Dimensionality reduction algorithms project the patterns onto lower-dimensional spaces whose dimensions reflect weighted combinations of the dimensions in the original space. Graph measures characterize each unit's participation in its associated network.

31 multivariate activity patterns versus patterns of dynamic correlations between neural activity patterns (e.g.,
 32 Fong et al., 2019; Manning et al., 2018). An emerging theme in this literature is that cognition is mediated
 33 by complex dynamic interactions between brain structures (Bassett et al., 2006; Demertzi et al., 2019; Sporns
 34 & Honey, 2006; Turk-Browne, 2013).

35 Studies of the neural code to date have primarily focused on univariate or multivariate neural pat-
 36 terns (for review see Norman et al., 2006), or (more recently) on patterns of dynamic first-order corre-
 37 lations (i.e., interactions between pairs of brain structures; Fong et al., 2019; Manning et al., 2018). We
 38 wondered what the future of this line of work might hold. For example, is the neural code mediated by
 39 higher-order interactions between brain structures? Second-order correlations reflect *homologous* patterns of
 40 correlation. In other words, if the changing patterns of correlations between two regions, *A* and *B*, are similar
 41 to those between two other regions, *C* and *D*, this would be reflected in the second-order correlations be-

42 tween ($A-B$) and ($C-D$). In this way, second-order correlations identify similarities and differences between
43 subgraphs of the brain’s connectome. Analogously, third-order correlations reflect homologies between
44 second-order correlations— i.e., homologous patterns of homologous interactions between brain regions.
45 More generally, higher-order correlations reflect homologies between patterns of lower-order correlations.
46 We can then ask: which “orders” of interaction are most reflective of high-level cognitive processes?

47 Another central question pertains to the extent to which the neural code is carried by activity patterns
48 that directly reflect ongoing cognition (e.g., following Haxby et al., 2001; Norman et al., 2006), versus the
49 dynamic properties of the network structure itself, independent of specific activity patterns in any given
50 set of regions (e.g., following Bassett et al., 2006). For example, graph measures such as centrality and
51 degree (Bullmore & Sporns, 2009) may be used to estimate how a given brain structure is “communicating”
52 with other structures, independently of the specific neural representations carried by those structures.
53 If one considers a brain region’s position in the network (e.g., its eigenvector centrality) as a dynamic
54 property, one can compare how the positions of different regions are correlated, and/or how those patterns
55 of correlations change over time. We can also compute higher-order patterns in these correlations to
56 characterize homologous subgraphs in the connectome that display similar changes in their constituent
57 brain structures’ interactions with the rest of the brain.

58 To gain insights into the above aspects of the neural code, we developed a computational framework
59 for estimating dynamic high-order correlations in timeseries data. This framework provides an important
60 advance, in that it enables us to examine patterns in higher-order correlations that are computationally
61 intractable to estimate via conventional methods. Given a multivariate timeseries, our framework provides
62 timepoint-by-timepoint estimates of the first-order correlations, second-order correlations, and so on (up
63 to tenth-order correlations in this manuscript). Our approach combines a kernel-based method for com-
64 puting dynamic correlations in timeseries data with a dimensionality reduction step (Fig. 1b) that projects
65 the resulting dynamic correlations into a low-dimensional space. We explored two dimensionality reduc-
66 tion approaches: principle components analysis (PCA; Pearson, 1901), which preserves an approximately
67 invertible transformation back to the original data; and a second non-invertible algorithm that explored
68 patterns in eigenvector centrality (Landau, 1895). This latter approach characterizes correlations between
69 each feature dimension’s relative *position* in the network in favor of the specific activity histories of different
70 features.

71 We validated our approach using synthetic data where the underlying correlations were known. We
72 then applied our framework to a neuroimaging dataset collected as participants listened to either an audio
73 recording of a ten-minute story or a temporally scrambled version of the story, or underwent a resting state
74 scan (Simony et al., 2016). We used a subset of the data to train across-participant classifiers to decode

75 listening times using a blend of neural features (comprising neural activity patterns, as well as different
76 orders of correlations between those patterns that were inferred using our computational framework).
77 We found that both the PCA-based and eigenvector centrality-based approaches yielded neural patterns
78 that could be used to decode accurately. Both approaches also yielded the best decoding accuracy for
79 data collected during (intact) story listening when high-order (PCA: second-order; eigenvector centrality:
80 fourth-order) dynamic correlation patterns were included as features. When we trained classifiers on the
81 scrambled stories or resting state data, only lower-order dynamic patterns were informative to the decoders.
82 Taken together, our results indicate that high-level cognition is supported by high-order dynamic patterns
83 of communication between brain structures.

84 Methods

85 Our general approach to comprises four general steps (Fig. 2). First, we derive a kernel-based approach
86 to computing dynamic pairwise correlations in a T (timepoints) by K (features) multivariate timeseries,
87 \mathbf{X}_0 . This yields a T by $O(K^2)$ matrix of dynamic correlations, \mathbf{Y}_1 , where each row comprises the upper
88 triangle of the correlation matrix at a single timepoint, reshaped into a row vector (this reshaped vector is
89 $(\frac{K^2-K}{2})$ -dimensional). Second, we apply a dimensionality reduction step to project the matrix of dynamic
90 correlations back onto a K -dimensional space. This yields a T by K matrix, \mathbf{X}_1 , that reflects an approximation
91 of the dynamic correlations reflected in the original data. Third, we use repeated applications of the kernel-
92 based dynamic correlation step to \mathbf{X}_n and the dimensionality reduction step to the resulting \mathbf{Y}_{n+1} to estimate
93 high-order dynamnic correlations. Each application of these steps to a T by K time series \mathbf{X}_n yields a T by K
94 matrix, \mathbf{X}_{n+1} , that reflects the dynamic correlations between the columns of \mathbf{X}_n . In this way, we refer to n as
95 the *order* of the timeseries, where \mathbf{X}_0 (order 0) denotes the original data and \mathbf{X}_n denotes n^{th} -order dynamic
96 correlations between the columns of \mathbf{X}_0 . Finally, we use a cross-validation-based decoding approach to
97 evaluate how well information contained in a given order (or weighted mixture of orders) may be used
98 to decode relevant cognitive states. If including a given \mathbf{X}_n in the feature set yields higher classification
99 accuracy on held-out data, we interpret this as evidence that the given cognitive states are reflected in
100 patterns of n^{th} -order correlations. All of the code used to produce the figures and results in this manuscript,
101 along with links to the corresponding datasets, may be found at github.com/ContextLab/timecorr-paper. In
102 addition, we have released a Python toolbox for computing dynamic high-order correlations in timeseries
103 data; our toolbox may be found at timecorr.readthedocs.io. **JRM NOTE: CHECK LINK**

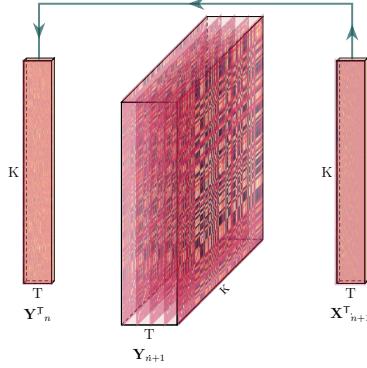


Figure 2: **Estimating dynamic high-order correlations.** Given a T by K matrix of multivariate timeseries data, \mathbf{Y}_n (where $n \in \mathbb{N}, n \geq 0$), we use Equation 5 to compute a timeseries of K by K correlation matrices, \mathbf{Y}_{n+1} . We then approximate \mathbf{Y}_{n+1} with the T by K matrix \mathbf{X}_{n+1} . This process may be repeated to scalably estimate iteratively higher-order correlations in the data. Note that the transposes of \mathbf{Y}_n and \mathbf{X}_{n+1} are displayed in the figure for compactness.

104 Kernel-based approach for computing dynamic correlations

Given a matrix of observations, we can compute the (static) Pearson's correlation between any pair of columns, $\mathbf{X}(\cdot, i)$ and $\mathbf{X}(\cdot, j)$ using (Pearson, 1901):

$$\text{corr}(\mathbf{X}(\cdot, i), \mathbf{X}(\cdot, j)) = \frac{\sum_{t=1}^T (\mathbf{X}(t, i) - \bar{\mathbf{X}}(\cdot, i))(\mathbf{X}(t, j) - \bar{\mathbf{X}}(\cdot, j))}{\sqrt{\sum_{t=1}^T \sigma_{\mathbf{X}(\cdot, i)}^2 \sigma_{\mathbf{X}(\cdot, j)}^2}}, \text{ where} \quad (1)$$

$$\bar{\mathbf{X}}(\cdot, k) = \sum_{t=1}^T \mathbf{X}(t, k), \text{ and} \quad (2)$$

$$\sigma_{\mathbf{X}(\cdot, k)}^2 = \sum_{t=1}^T (\mathbf{X}(t, k) - \bar{\mathbf{X}}(\cdot, k))^2 \quad (3)$$

- 105 We can generalize this formula to compute time-varying correlations by incorporating a *kernel function* that
 106 takes a time t as input, and returns how much the observed data at each timepoint $\tau \in [-\infty, \infty]$ contributes
 107 to the estimated instantaneous correlation at time t (Fig. 3).

Given a kernel function $\kappa_t(\cdot)$ for timepoint t , evaluated at timepoints $\tau \in [1, \dots, T]$, we can update the

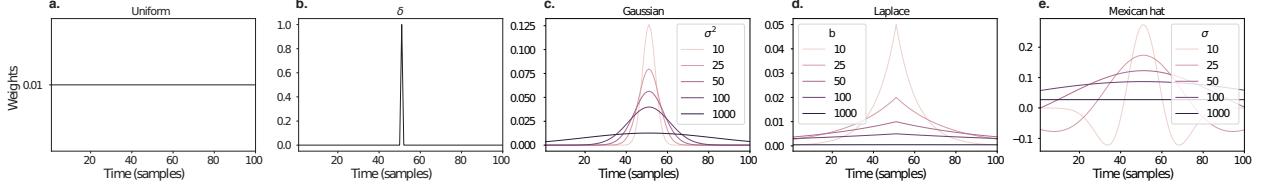


Figure 3: **Examples of kernel functions.** Each panel displays per-timepoint weights at $t = 50$, evaluated for 100 timepoints ($\tau \in [1, \dots, 100]$). **a. Uniform kernel.** The weights are timepoint-invariant; observations at all timepoints are weighted equally, and do not change as a function of τ . This is a special case of weight function that reduces dynamic correlations to static correlations. **b. Dirac δ kernel.** Only the observation at timepoint t is given a non-zero weight (of 1). **c. Gaussian kernels.** Each kernel's weights fall off in time according to a Gaussian probability density function centered on time t . Weights derived using several different example width parameters (σ^2) are displayed. **d. Laplace kernels.** Each kernel's weights fall off in time according to a Laplace probability density function centered on time t . Weights derived using several different example width parameters (b) are displayed. **e. Mexican hat (Ricker wavelet) kernels.** Each kernel's weights fall off in time according to a Ricker wavelet centered on time t . This function highlights the *contrasts* between local versus surrounding activity patterns in estimating dynamic correlations. Weights derived using several different example width parameters (σ) are displayed.

static correlation formula in Equation 2 to estimate the *instantaneous correlation* at timepoint t :

$$\text{timecorr}_{\kappa_t}(\mathbf{X}(\cdot, i), \mathbf{X}(\cdot, j)) = \frac{\sum_{\tau=1}^T (\mathbf{X}(\tau, i) - \tilde{\mathbf{X}}_{\kappa_t}(i))(\mathbf{X}(\tau, j) - \tilde{\mathbf{X}}_{\kappa_t}(j))}{\sqrt{\sum_{\tau=1}^T \tilde{\sigma}_{\kappa_t}^2(\mathbf{X}(\cdot, i))\tilde{\sigma}_{\kappa_t}^2(\mathbf{X}(\cdot, j))}}, \text{ where} \quad (4)$$

$$\tilde{\mathbf{X}}_{\kappa_t}(t, k) = \sum_{\tau=1}^T \kappa_t(\tau, k) \mathbf{X}(\tau, k), \quad (5)$$

$$\tilde{\sigma}_{\kappa_t}^2(\mathbf{X}(\cdot, k)) = \sum_{\tau=1}^T (\mathbf{X}(\tau, k) - \tilde{\mathbf{X}}_{\kappa_t}(t, k))^2. \quad (6)$$

108 Here $\text{timecorr}(\mathbf{X}(\cdot, i), \mathbf{X}(\cdot, j), \kappa_t)$ reflects the correlation at time t between columns i and j of \mathbf{X} , estimated using
 109 the kernel κ_t . We evaluate Equation 5 in turn each pair of columns in \mathbf{X} and for kernels centered on each
 110 timepoint in the timeseries, respectively, to obtain a T by K by K timeseries of dynamic correlations, \mathbf{Y} . For
 111 convenience, we then reshape the upper triangles of each timepoint's correlation matrix into a row vector
 112 to obtain an equivalent T by $\frac{K^2-K}{2}$ matrix.

113 Dynamic inter-subject functional connectivity (DISFC)

Equation 5 provides a means of taking a single observation matrix, \mathbf{X}_n and estimating the dynamic correlations from moment to moment, \mathbf{Y}_{n+1} . Suppose that one has access to a set of multiple observation matrices that reflect the same phenomenon. For example, one might collect neuroimaging data from several experimental participants, as each participant performs the same task (or sequence of tasks). Let $\mathbf{X}_n^1, \mathbf{X}_n^2, \dots, \mathbf{X}_n^P$ reflect the T by K observation matrices ($n = 0$) or reduced correlation matrices ($n > 0$) for each of

P participants in an experiment. We can use *inter-subject functional connectivity* (ISFC; Simony et al., 2016) to compute the degree of stimulus-driven correlations reflected in the multi-participant dataset at a given timepoint t using:

$$\bar{\mathbf{C}}(t) = M \left(R \left(\frac{1}{2P} \sum_{p=1}^P Z(Y_n^p(t))^T + Z(Y_n^p(t)) \right) \right), \quad (7)$$

where M extracts and vectorizes the diagonal and upper triangle of a symmetric matrix, Z is the Fisher z-transformation (Zar, 2010):

$$Z(r) = \frac{\log(1+r) - \log(1-r)}{2} \quad (8)$$

R is the inverse of Z :

$$R(z) = \frac{\exp(2z-1)}{\exp(2z+1)}, \quad (9)$$

and $\mathbf{Y}_n^p(t)$ denotes the correlation matrix (Eqn. 2) between each column of \mathbf{X}_n^p and each column of the average \mathbf{X}_n from all *other* participants, $\bar{\mathbf{X}}_n^{ \setminus p}$:

$$\bar{\mathbf{X}}_n^{ \setminus p} = R \left(\frac{1}{P-1} \sum_{q \in \setminus p} Z(\mathbf{X}_n^q) \right), \quad (10)$$

where $\setminus p$ denotes the set of all participants other than participant p . In this way, the T by $\frac{K^2-K}{2}$ DISFC matrix $\bar{\mathbf{C}}$ provides a time-varying extension of the ISFC approach developed by Simony et al. (2016).

116 Low-dimensional representations of dynamic correlations

Given a T by $\frac{K^2-K}{2}$ matrix of dynamic correlations, \mathbf{Y}_n , we propose two general approaches to computing a T by K low-dimensional representation of these correlations, \mathbf{X}_n . The first approach uses dimensionality reduction algorithms to project \mathbf{Y}_n onto a K -dimensional space. The second approach uses graph measures to characterize the relative positions of each feature ($k \in [1, \dots, K]$) in the network defined by the correlation matrix at each timepoint.

122 Dimensionality reduction-based approaches to computing \mathbf{X}_n

The modern library of dimensionality reduction algorithms include Principal Components Analysis (PCA; Pearson, 1901), Probabilistic PCA (PPCA; Tipping & Bishop, 1999), Exploratory Factor Analysis (EFA;

125 Spearman, 1904), Independent Components Analysis (ICA; Comon et al., 1991; Jutten & Herault, 1991),
126 *t*-Stochastic Neighbor Embedding (*t*-SNE; van der Maaten & Hinton, 2008), Uniform Manifold Approximation and Projection (UMAP; McInnes & Healy, 2018), non-negative matrix factorization (NMF; Lee &
127 Seung, 1999), Topographic Factor Analysis (TFA) Manning et al. (2014), Hierarchical Topographic Factor
128 analysis (HTFA) Manning et al. (2018), Topographic Latent Source Analysis (TLSA) Gershman et al. (2011),
129 Dictionary learning (J. Mairal et al., 2009; J. B. Mairal et al., 2009), deep autoencoders (Hinton & Salakhutdinov, 2006), among others. While complete characterizations of each of these algorithms is beyond the scope
130 of the present manuscript, the general intuition driving these approaches is to compute the T by I matrix,
131 \mathbf{X} , that is closest to the original T by J matrix, \mathbf{Y} , where (typically) $I \ll J$. The different approaches place
132 different constraints on what properties \mathbf{X} must satisfy and which aspects of the data are compared (and
133 how) to characterize the match between \mathbf{X} and \mathbf{Y} .

136 Applying dimensionality reduction algorithms to \mathbf{Y} yields a \mathbf{X} whose columns reflect weighted combinations
137 (or nonlinear transformations) of the original columns of \mathbf{Y} . This has two main consequences. First,
138 with each repeated dimensionality reduction, the resulting \mathbf{X}_n has lower and lower fidelity (with respect to
139 what the “true” \mathbf{Y}_n might have looked like without using dimensionality reduction to maintain scalability).
140 In other words, computing \mathbf{X}_n is a lossy operation. Second, whereas each columns of \mathbf{Y}_n may always be
141 mapped directly onto specific pairs of columns of \mathbf{Y}_{n-1} , the columns of \mathbf{X}_n reflect weighted combinations
142 and/or nonlinear transformations of the columns of \mathbf{Y}_n . Many dimensionality reduction algorithms are
143 invertible (or approximately invertible). However, attempting to map a given \mathbf{X}_n back onto the original
144 feature space of \mathbf{Y}_0 will usually require $O(TK^{2n})$ space and therefore quickly becomes intractable as n or K
145 grow large.

146 **Graph measure approaches to computing \mathbf{X}_n**

147 The above dimensionality reduction approaches to approximating a given \mathbf{Y}_n with a lower-dimensional
148 \mathbf{X}_n preserve a (potentially recombined and transformed) mapping back to the original data in \mathbf{Y}_0 . We
149 also explore graph measure approaches that forgo a preserved mapping back to the original data in favor
150 of preserving each feature’s relative *position* in the broader network of interactions and connections. To
151 illustrate the distinction between the two general approaches we explore, suppose a network comprises
152 nodes A , B , and C . If A and B exhibit uncorrelated activity patterns, the functional connection between
153 them will be (by definition) close to 0. However, if A and B each interact with C in similar ways, we might
154 attempt to capture those similarities using a measure that reflects the how A and B interact in the network.

155 In general, graph measures take as input a matrix of interactions (e.g., using the above notation, an K

156 by K correlation matrix or binarized correlation matrix reconstituted from a single timepoint's row of \mathbf{Y})
157 and return as output a set of K measures describing how each node (feature) sits within that correlation
158 matrix with respect to the rest of the population. Widely used measures include betweenness centrality (the
159 proportion of shortest paths between each pair of nodes in the population that involves the given node in
160 question; e.g., Barthélemy, 2004; Freeman, 1977; Geisberger et al., 2008; Newman, 2005; Opsahl et al., 2010);
161 diversity and dissimilarity (characterizations of how differently connected a given node is from others in
162 the population; e.g., Lin, 2009; Rao, 1982; Ricotta & Szeidl, 2006); Eigenvector centrality and pagerank
163 centrality (measures of how influential a given node is within the broader network; e.g., Bonacich, 2007;
164 Halu et al., 2013; Lohmann et al., 2010; Newman, 2008); transfer entropy and flow coefficients (a measure
165 of how much information is flowing from a given node to other nodes in the network; e.g., Honey et
166 al., 2007; Schreiber, 2000); k -coreness centrality (a measure of the connectivity of a node within its local
167 sub-graph; e.g., Alvarez-Hamelin et al., 2005; Christakis & Fowler, 2010); within-module degree (a measure
168 of how many connections a node has to its close neighbors in the network; e.g., Rubinov & Sporns, 2010);
169 participation coefficient (a measure of the diversity of a node's connections to different sub-graphs in the
170 network; e.g., Rubinov & Sporns, 2010); and sub-graph centrality (a measure of a node's participation in
171 all of the network's sub-graphs; e.g., Estrada & Rodríguez-Velázquez, 2005); among others.

172 For a given graph measure, $\eta : \mathbb{R}^{K \times K} \rightarrow \mathbb{R}^K$, we can use η to transform each row of \mathbf{Y}_n in a way that
173 characterizes the corresponding graph properties of each column. This results in a new T by K matrix, \mathbf{X}_n ,
174 that reflects how the features reflected in the columns of \mathbf{Y}_n participate in the network during each timepoint
175 (row).

176 Dynamic higher-order correlations

177 Because \mathbf{X}_n has the same shape as the original data \mathbf{X}_0 , approximating \mathbf{Y}_n with a lower-dimensional \mathbf{X}_n
178 enables us to estimate high-order dynamic correlations in a scalable way. Given a T by K input matrix, the
179 output of Equation 5 requires $O(TK^2)$ space to store. Repeated applications of Equation 5 (i.e., computing
180 dynamic correlations between the columns of the outputted dynamic correlation matrix) each require
181 exponentially more space; in general the n^{th} -order dynamic correlations of a T by K timeseries occupies
182 $O(TK^{2n})$ space. However, when we approximate or summarize the output of Equation 5 with a T by K matrix
183 (as described above), it becomes feasible to compute even very high-order correlations in high-dimensional
184 data. Specifically, approximating the n^{th} -order dynamic correlations of a T by K timeseries requires only
185 $O(TK^2)$ additional space— the same as would be required to compute first-order dynamic correlations. In
186 other words, the space required to store $n + 1$ multivariate timeseries reflecting up to n^{th} order correlations

187 in the original data scales linearly with n using our approach (Fig. 2).

188 Data

189 We examined two types of data: synthetic data and human functional neuroimaging data. We constructed
190 and leveraged the synthetic data to evaluate our general approach. Specifically, we tested how well
191 Equation 5 could be used to recover known dynamic correlations using different choices of kernel (κ ; Fig. 3),
192 for each of several synthetic datasets that exhibited different temporal properties. We applied our approach
193 to a functional neuroimaging dataset to test the hypothesis that ongoing cognitive processing is reflected
194 in high-order dynamic correlations. We used an across-participant classification test to estimate whether
195 dynamic correlations of different orders contain information about which timepoint in a story participants
196 were listening to.

197 Synthetic data

198 We constructed a total of 40 multivariate timeseries, collectively reflecting a total of 4 different patterns of
199 dynamic correlations (i.e., 10 datasets reflecting each type of dynamic pattern). Each timeseries comprised
200 50 features (dimensions) that varied over 300 timepoints. The observations at each timepoint were drawn
201 from a zero-mean multivariate Gaussian distribution with a covariance matrix defined for each timepoint
202 as described below. We drew the observations at each timepoint independently from the draws at all other
203 timepoints; in other words, for each observation $s_t \sim \mathcal{N}(\mathbf{0}, \Sigma_t)$ at timepoint t , $p(s_t) = p(s_t | p_{\setminus t})$.

Constant. We generated data with stable underlying correlations to evaluate how Equation 5 characterized correlation “dynamics” when the ground truth correlations were static. We constructed 10 multivariate timeseries, whose observations were each drawn from a single (stable) Gaussian distribution. For each dataset, we constructed a random covariance matrix, Σ_m :

$$\mathbf{C}(i, j) \sim \mathcal{N}(0, 1) \tag{11}$$

$$\Sigma_m = \mathbf{C}\mathbf{C}^\top, \text{ where} \tag{12}$$

204 $i, j \in [1, 2, \dots, 50]$. In other words, all of the observations (for each of the 300 timepoints) within each dataset
205 were drawn from a multivariate Gaussian distribution with the same covariance matrix, and the 10 datasets
206 each used a different covariance matrix.

207 **Random.** We generated a second set of 10 synthetic datasets whose observations at each timepoint were
208 drawn from a Gaussian distribution with a new randomly constructed (using Eqn. 12) covariance matrix.
209 Because each timepoint’s covariance matrix was drawn independently of the covariance matrices for all
210 other timepoints, these datasets provided a test of reconstruction accuracy in the absence of any meaningful
211 underlying temporal structure in the dynamic correlations underlying the data.

Ramping. We generated a third set of 10 synthetic datasets whose underlying correlations changed gradually over time. For each dataset, we constructed two *anchor* correlation matrices using Equation 12, Σ_{start} and Σ_{end} . For each of the 300 timepoints in each dataset, we drew the observations from a multivariate Gaussian distribution whose covariance matrix at each timepoint $t \in [0, \dots, 299]$ was given by

$$\Sigma_t = \left(1 - \frac{1-t}{299}\right)\Sigma_{\text{start}} + \frac{t}{299}\Sigma_{\text{end}}. \quad (13)$$

212 The gradually changing correlations underlying these datasets allow us to evaluate the recovery of dynamic
213 correlations when each timepoint’s correlation matrix is unique (as in the random datasets), but where the
214 correlation dynamics are structured.

215 **Event.** We generated a fourth set of 10 synthetic datasets whose underlying correlation matrices exhibited
216 prolonged intervals of stability, interspersed with abrupt changes. For each dataset, we used Equation ??
217 to generate 5 random covariance matrices. We constructed a timeseries where each set of 60 consecutive
218 samples was drawn from a Gaussian with the same covariance matrix. These datasets were intended to
219 simulate a system that undergoes occasional abrupt state changes.

220 Functional neuroimaging data collected during story listening

221 We examined an fMRI dataset collected by Simony et al. (2016) that the authors have made publically
222 available at arks.princeton.edu/ark:/88435/dsp015d86p269k. The dataset comprises neuroimaging data
223 collected as participants listened to an audio recording of a story (intact condition; 36 participants), listened
224 to time scrambled recordings of the same story (17 participants in the paragraph-scrambled condition
225 listened to the paragraphs in a randomized order and 36 in the word-scrambled condition listened to
226 the words in a randomized order), or lay resting with their eyes open in the scanner (rest condition; 36
227 participants). Full neuroimaging details may be found in the original paper for which the data were
228 collected (Simony et al., 2016).

229 **Hierarchical topographic factor analysis (HTFA).** Following our prior related work, we used HTFA (Manning et al., 2018) to derive a compact representation of the data. In brief, this approach approximates the
230 timeseries of voxel activations (44,415 voxels) using a much smaller number of radial basis function (RBF)
231 nodes (in this case 700 nodes). This provides a convenient representation for examining full-brain network
232 dynamics. All of the analyses we carried out on the neuroimaging dataset were performed in this lower-
233 dimensional space. In other words, each participant’s data matrix, Y_0 , was a number-of-timepoints by 700
234 matrix of HTFA-derived factor weights (where the row and column labels were matched across partici-
235 pants). Code for carrying out HTFA on fMRI data may be found as part of the BrainIAK toolbox (Capota et
236 al., 2017), which may be downloaded at brainiak.org.
237

238 **Temporal decoding**

239 We sought to identify neural patterns that reflected participants’ ongoing cognitive processing of incoming
240 stimulus information. As reviewed by Simony et al. (2016), one way of homing in on these stimulus-driven
241 neural patterns is to compare activity patterns across individuals (e.g., using ISFC analyses). In particular,
242 neural patterns will be similar across individuals, to the extent that the neural patterns under consideration
243 are stimulus driven, and to the extent that the corresponding cognitive representations are reflected in similar
244 spatial patterns across people. Following this logic, we used an across-participants temporal decoding test
245 developed by Manning et al. (2018) to assess the degree to which different neural patterns reflected ongoing
246 stimulus-driven cognitive processing across people. The approach entails using a subset of the data to
247 train a classifier to decode which stimulus timepoint (i.e., moment in the story participants listened to). We
248 use decoding (forward inference) accuracy on held-out data, from held-out participants, as a proxy for the
249 extent to which the inputted neural patterns reflected stimulus-driven cognitive processing in a similar way
250 across individuals.

251 **Forward inference and decoding accuracy**

252 We used an across-participants correlation-based classifier to decode which stimulus timepoint matched a
253 given neural pattern. We first divided the participants into two groups: a template group, $\mathcal{G}_{\text{template}}$, and a
254 to-be-decoded group, $\mathcal{G}_{\text{decode}}$. We used Equation 7 to compute a DISFC matrix for each group ($\bar{\mathbf{C}}_{\text{template}}$ and
255 $\bar{\mathbf{C}}_{\text{decode}}$, respectively). We then correlated the rows of $\bar{\mathbf{C}}_{\text{template}}$ and $\bar{\mathbf{C}}_{\text{decode}}$ to form a number-of-timepoints by
256 number-of-timepoints decoding matrix, Λ . In this way, the rows of Λ reflected timepoints from the template
257 group, while the columns reflected timepoints from the to-be-decoded group. We assigned temporal labels
258 to each row $\bar{\mathbf{C}}_{\text{decode}}$ using the row of $\bar{\mathbf{C}}_{\text{template}}$ to which it was most highly correlated. We then repeated

259 this decoding procedure, but using $\mathcal{G}_{\text{decode}}$ as the template group and $\mathcal{G}_{\text{template}}$ as the to-be-decoded group.
260 Given the true timepoint labels (for each group), we defined the *decoding accuracy* as the proportion of
261 correctly decoded timepoints, across both groups.

262 **Feature weighting and testing**

263 We sought to examine which types of neural features (i.e., activations, first-order dynamic correlations, and
264 higher-order dynamic correlations) were informative to the temporal decoders. Using the notation above,
265 these features correspond to $\mathbf{Y}_0, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$, and so on (we examined up to tenth order correlations, or \mathbf{X}_{10}).

266 One challenge to fairly evaluating high-order correlations is that if the kernel used in Equation 5 is
267 wider than a single timepoint, each repeated application of the equation will result in further temporal
268 blur. Because our primary assessment metric is temporal decoding accuracy, this unfairly biases against
269 detecting meaningful signal in higher-order correlations (relative to lower-order correlations). We attempted
270 to mitigate temporal blur in estimating each \mathbf{X}_n by using a Dirac δ function kernel (which places all of its
271 mass over a single timepoint; Fig. 3b) to compute each lower-order correlation ($\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n-1}$). We then used
272 a (potentially wider, as described below) kernel to compute \mathbf{X}_n from \mathbf{X}_{n-1} . In this way, temporal blurring
273 was applied only in the last step of computing \mathbf{X}_n . We note that, because each \mathbf{X}_n is a low-dimensional
274 representation of the corresponding \mathbf{Y}_n , the higher-order correlations we estimated reflect true correlations
275 in the data with lower-fidelity than estimates of lower-order correlations.

276 After computing each $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n-1}$ for each participant, we divided participants into two equally sized
277 groups (± 1 for odd numbers of participants): $\mathcal{G}_{\text{train}}$ and $\mathcal{G}_{\text{test}}$. We then further subdivided $\mathcal{G}_{\text{train}}$ into $\mathcal{G}_{\text{train}_1}$
278 and $\mathcal{G}_{\text{train}_2}$. We then computed Λ temporal correlation matrices for each type of neural feature, using $\mathcal{G}_{\text{train}_1}$
279 and $\mathcal{G}_{\text{train}_2}$. This resulted in $n + 1$ Λ matrices (one for the original timeseries of neural activations, and one
280 for each of n orders of dynamic correlations). Our objective was to find a set of weights of each of these Λ
281 matrices such that the weighted average of the $n + 1$ matrices yielded the highest decoding accuracy. We
282 used quasi-Newton gradient ascent (Nocedal & Wright, 2006), using decoding accuracy as the objective
283 function to be maximized, to find an optimal set of training data-derived weights, $\phi_{0,1,\dots,n}$, where $\sum_{i=0}^n \phi_i = 1$
284 and where $\phi_i \geq 0 \forall i \in [0, 1, \dots, n]$.

285 After estimating an optimal set of weights, we computed a new set of $n + 1$ Λ matrices correlating the
286 DISFC patterns from $\mathcal{G}_{\text{train}}$ and $\mathcal{G}_{\text{test}}$ at each timepoint. We use the resulting decoding accuracy of $\mathcal{G}_{\text{test}}$
287 timepoints to estimate how informative the set up neural features containing up to n^{th} order correlations
288 were.

289 We used a permutation-based procedure to form a stable estimate of decoding accuracy for each set of

290 neural features. In particular, we computed the decoding accuracy for each of 10 random group assignments
291 of $\mathcal{G}_{\text{train}}$ and $\mathcal{G}_{\text{test}}$. We report the mean accuracy (and 95% confidence intervals) for each set of neural features.

292 **Identifying robust decoding results**

293 The temporal decoding procedure we use to estimate which neural features support ongoing cognitive
294 processing is governed by many parameters. For example, Equation 5 requires defining a kernel function,
295 which can take on different shapes and widths. For a fixed set of neural features, each of these parameters
296 can yield different decoding accuracies. Further, the best decoding accuracy for a given timepoint may be
297 reliably achieved by one set of parameters, whereas the best decoding accuracy for another timepoint might
298 be reliably achieved by a different set of parameters, and the best decoding accuracy across *all* timepoints
299 might be reliably achieved by still another different set of parameters. Rather than attempting to maximize
300 decoding accuracy, we sought to discover the trends in the data that were robust to specific classifier
301 parameters choices. Specifically, we sought to characterize how decoding accuracy varied (under different
302 experimental conditions) as a function of which neural features were considered.

303 To identify decoding results that were robust to specific classifier parameter choices, we repeated our
304 decoding analyses that substituted in a variety of kernel shapes and widths for Equation 5. We examined
305 Gaussian (Fig. 3c), Laplace (Fig. 3d), and Mexican Hat (Fig. 3e) kernels, each with widths of 5, 10, 20, and
306 50 samples. We then report the average decoding accuracies across all of these parameter choices. This
307 enabled us to (roughly) factor out performance characteristics that were parameter dependent (within the
308 space of parameters we examined).

309 **Reverse inference**

310 The dynamic patterns we examine comprise high-dimensional correlation patterns at each timepoint. To
311 help interpret the resulting patterns in the context of other studies, we created summary maps by computing
312 the across-timepoint average pairwise correlations at each order of analysis (first order, second order, etc.,
313 up to fifteenth order correlations). We selected the 10 strongest (absolute value) correlations at each order.
314 Each correlation is between the dynamic activity patterns (or patterns of dynamic high-order correlations)
315 measured at two RBF nodes (see *Hierarchical Topographic Factor Analysis*). Therefore, the 10 strongest
316 correlations involved up to 20 RBF nodes. Each RBF defines a spatial function whose activations range
317 from 0 to 1. We thresholded each RBF at 0.999 to construct a map of spherical components that denoted the
318 endpoints of the 10 strongest correlations. We then carried out a meta analysis using Neurosynth (Rubin et
319 al., 2017) to identify the 10 terms most commonly associated with the given map. This resulted in a set of

320 10 terms associated with the average dynamic correlation patterns at each order.

321 Results

322 We sought to understand whether high-level cognition is supported by dynamic patterns of high-order
323 correlations. To that end, we developed a computational framework for estimating the dynamics of high-
324 order correlations in multivariate timeseries data (see *Dynamic inter-subject functional connectivity (DISFC)*
325 and *Dynamic higher-order correlations*). We evaluated the efficacy of this framework at recovering known
326 patterns in several synthetic datasets (see *Synthetic data*). We then applied the framework to a public fMRI
327 dataset collected as participants listened to an auditorily presented story, a temporally scrambled version
328 of the story, or underwent a resting state scan (see *Functional neuroimaging data collected during story listening*).
329 We used the relative decoding accuracies of classifiers trained on different sets of neural features to estimate
330 which types of features reflected ongoing cognitive processing.

331 Recovering known dynamic correlations from synthetic data

332 We generated synthetic datasets that differed in how the underlying correlations changed over time. For
333 each dataset, we applied Equation 5 with a variety of kernel shapes and widths. We assessed how well
334 the true underlying correlations at each timepoint matched the recovered correlations (Fig. 4). For every
335 kernel and dataset we tested, our approach recovered the correlation dynamics we embedded into the data.
336 However, the quality of these recoveries varied across different synthetic datasets in a kernel-dependent
337 way.

338 In general, wide monotonic kernels (Laplace, Gaussian) performed best when the correlations varied
339 gradually from moment-to-moment (Figs. 4a, c, and d). **TODO: Say something about kernel widths within**
340 **a shape.** In the extreme, as the rate of change in correlations approaches 0 (Fig. 4a), an infinitely wide kernel
341 would exactly recover the Pearson's correlation (e.g., compare Eqns. 2 and 5).

342 When the correlation dynamics were unstructured in time (Fig. 4b), a Dirac δ kernel (infinitely narrow)
343 performed best. This is because, when every timepoint's correlations are independent of the correlations in
344 every other timepoint, averaging data over time dilutes the available signal. **TODO: Say something about**
345 **kernel widths within a shape.**

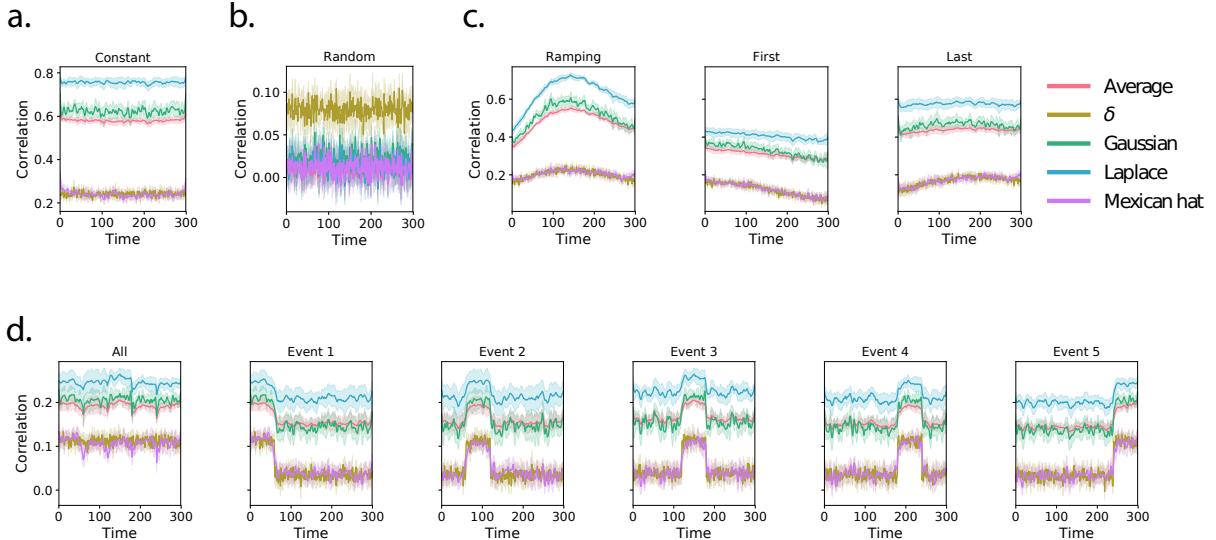


Figure 4: Recovering known dynamic correlations from synthetic data. Each panel displays the average correlations between the vectorized upper triangles of the recovered correlation matrix at each timepoint and either the true underlying correlation at each timepoint or a reference correlation matrix. (The averages are taken across 10 different randomly generated synthetic datasets of the given category.) Error ribbons denote 95% confidence intervals (taken across datasets). Different colors denote different kernel shapes, whereas the shading within each color type denotes kernel widths. For a complete description of each synthetic dataset, see *Synthetic data*. **a. Constant correlations.** These datasets have a stable (unchanging) underlying correlation matrix. **b. Random correlations.** These datasets are generated using a new independently drawn correlation matrix at each new timepoint. **c. Ramping correlations.** These datasets are generated by smoothly varying the underlying correlations between the randomly drawn correlation matrices at first and last timepoints. The left panel displays the correlations between the recovered dynamic correlations and the underlying ground truth correlations. The middle panel compares the recovered correlations with the *first* timepoint’s correlation matrix. The right panel compares the recovered correlations with the *last* timepoint’s correlation matrix. **d. Event-based correlations.** These datasets are each generated using five randomly drawn correlation matrices that each remain stable for a fifth of the total timecourse. The left panel displays the correlations between the recovered dynamic correlations and the underlying ground truth correlations. The right panels compare the recovered correlations with the correlation matrices unique to each event.

346 **Cognitively relevant dynamic high-order correlations in fMRI data**

347 We used across-participant temporal decoders to identify cognitively relevant neural patterns in fMRI data
348 (see *Forward inference and decoding accuracy*). The dataset we examined (collected by Simony et al., 2016)
349 comprised four experimental conditions that exposed participants to stimuli that varied systematically in
350 how cognitively engaging they were. The *intact* experimental condition had participants listen to an audio
351 recording of a 10-minute story. The *paragraph*-scrambled experimental condition had participants listen to a
352 temporally scrambled version of the story, where the paragraphs occurred out of order (but where the same
353 total set of paragraphs were presented over the full listening interval). All participants in this condition
354 experienced the scrambled paragraphs in the same order. The *word*-scrambled experimental condition had
355 participants listen to a temporally scrambled version of the story where the words in the story occurred in a
356 random order. All participants in the word conditions experienced the scrambled words in the same order.
357 Finally, in a *rest* experimental condition participants lay in the scanner with no overt stimulus, with their
358 eyes open (blinking as needed). This dataset provided a convenient means of testing our hypothesis that
359 different levels of cognitive engagement might be supported by different orders of complex brain activity
360 dynamics.

361 In brief, we computed timeseries of dynamic high-order correlations that were similar across participants
362 in each of two randomly assigned groups: a training group and a test group. We then trained classifiers
363 on the training group's data to match each sample from the test group with a stimulus timepoint. Each
364 classifier comprised a weighted blend of neural patterns that reflected up to n^{th} -order dynamic correlations
365 (see *Feature weighting and testing*). We repeated this process for $n \in \{0, 1, 2, \dots, 10\}$. Our examinations of
366 synthetic data suggested that none of the kernels we examined were "universal" in the sense of optimally
367 recovering underlying correlations regardless of the structure of those correlations. In our analyses of neural
368 data, we therefore averaged our decoding results over a variety of kernel shapes and widths in order to
369 identify results that were robust to specific kernel parameters (also see *Identifying robust decoding results*).

370 Our approach to estimating dynamic high-order correlations requires mapping the high-dimensional
371 feature space of correlations (a T by $O(K^2)$ matrix) onto a lower-dimensional T by K matrix. We carried out
372 two sets of analyses that differed in how this mapping was computed. The first set of analyses used PCA
373 to find a low-dimensional embedding of the original dynamic correlation matrices (Fig. 5a,b). The second
374 set of analyses characterized correlations in dynamics of each feature's eigenvector centrality, but did not
375 preserve the underlying activity dynamics (Fig. 5c,d).

376 Both sets of temporal decoding analyses yielded qualitatively similar results for the auditory (non-
377 rest) conditions of the experiment (Fig. 5: pink, yellow, and teal lines). The highest decoding accuracy

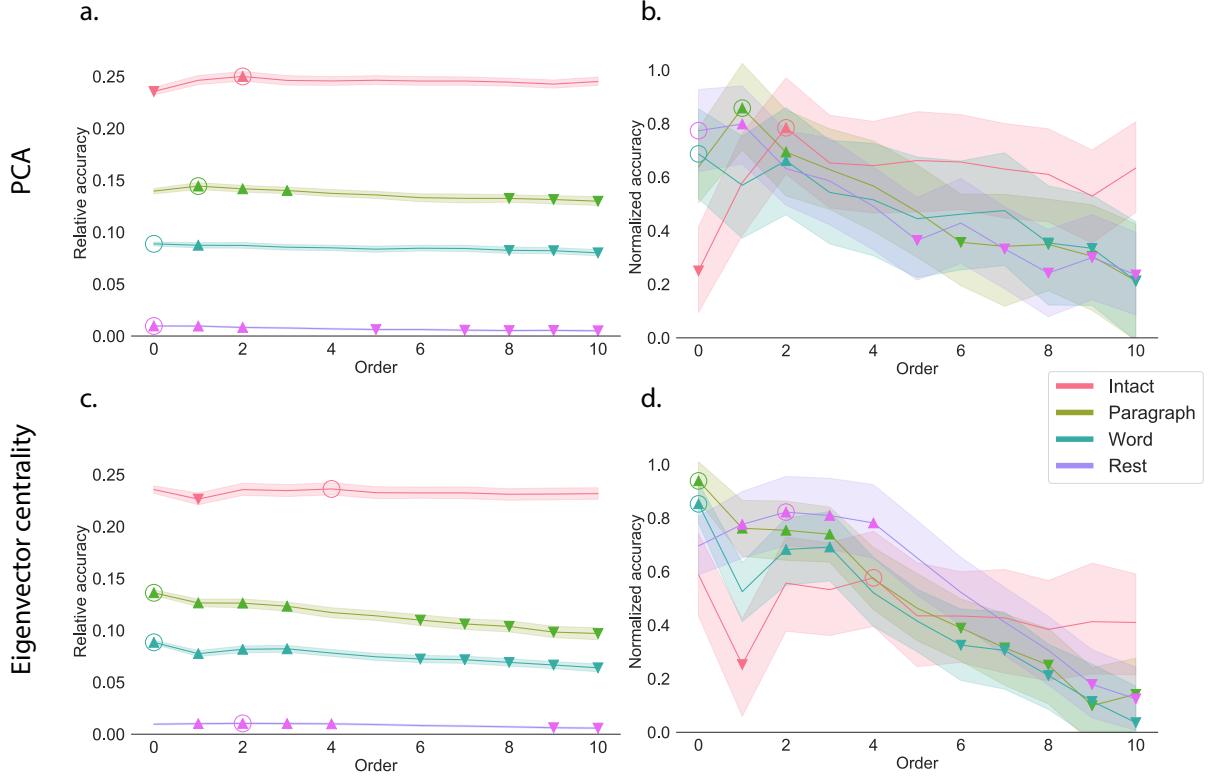


Figure 5: Across-participant decoding accuracy varies with correlation order and cognitive engagement.

a. Decoding accuracy as a function of order: PCA. Order (x-axis) refers to the maximum order of dynamic correlations that were available to the classifiers (see *Feature weighting and testing*). The reported across-participant decoding accuracies are averaged over all kernel shapes and widths (see *Identifying robust decoding results*). The y-values are displayed relative to chance accuracy (intact: $\frac{1}{300}$; paragraph: $\frac{1}{272}$; word: $\frac{1}{300}$; rest: $\frac{1}{400}$). The error bars denote 95% confidence intervals across cross-validation folds (i.e., random assignments of participants to the training and test sets). The colors denote the experimental condition. Arrows denote sets of features that yielded reliably higher (upwards facing) or lower (downward facing) decoding accuracy than the mean of all other features (via a two-tailed test, thresholded at $p < 0.05$). The circled values represent the maximum decoding accuracy within each experimental condition.

b. Normalized decoding accuracy as a function of order: PCA. This panel displays the same results as Panel a, but here each curve has been normalized to have a maximum value of 1 and a minimum value of 0 (including the upper and lower bounds of the respective 95% confidence intervals). Panels a and b used PCA to project each high-dimensional pattern of dynamic correlations onto a lower-dimensional space.

c. Decoding accuracy as a function of order: eigenvector centrality. This panel is in the same format as Panel a, but here eigenvector centrality has been used to project the high-dimensional patterns of dynamic correlations onto a lower-dimensional space.

d. Normalized decoding accuracy as a function of order: eigenvector centrality. This panel is in the same format as Panel b, but here eigenvector centrality has been used to project the high-dimensional patterns of dynamic correlations onto a lower-dimensional space.

378 for participants who listened to the intact (unscrambled) story was achieved using high-order dynamic
379 correlations (PCA: second-order; eigenvector-centrality: fourth-order). Scrambled versions of the story were
380 best decoded by lower-order correlations (PCA/paragraph: first-order; PCA/word: order zero; eigenvector
381 centrality/paragraph: order zero; eigenvector centrality/word: order zero). The two sets of analyses yielded
382 different decoding results on resting state data (Fig. 5: purple lines). We note could be decoded only very
383 slightly above chance; we speculate that the decoders might have picked up on attentional drift, boredom,
384 or tiredness; we hypothesize these all increase throughout the resting state scan. Our decoders might
385 be picking up on aspects of these loosely defined cognitive states that are common across individuals. The
386 PCA-based approach achieved the highest resting state decoding accuracy using order zero features (non-
387 correlational activation-based), whereas the eigenvector centrality-based approach achieved the highest
388 resting state decoding accuracy using second-order correlations. Taken together, these analyses indicate
389 that high-level cognitive processing (while listening to the intact story) is reflected in the dynamics of high-
390 order correlations in brain activity, whereas lower-level cognitive processing (while listening to scrambled
391 versions of the story that lack rich meaning) is reflected in the dynamics of lower-order correlations and
392 non-correlational activity dynamics. Further, these patterns are associated both with the underlying activity
393 patterns (characterized using PCA) and also with the changing relative positions that different brain areas
394 occupy in their associated networks (characterized using eigenvector centrality).

395 Having established that patterns of high-order correlations are informative to decoders, we next won-
396 dered which specific networks of brain regions contributed most to these patterns. As a representative
397 example, we selected the kernel parameters that yielded decoding accuracies that best matched the average
398 accuracies across all of the kernel parameters we examined. Using Figure ??c as a template, the best-
399 matching kernel was a Laplace kernel with a width of 50 (Fig. 3d). We used this kernel to compute a single
400 K by K n^{th} -order correlation matrix for each experimental condition, along with the Neurosynth (Rubin et
401 al., 2017) terms most highly associated with each of these matrices (Fig. 6; see *Reverse inference*).

402 For all of the story listening conditions (intact, paragraph, and word), we found that first- and second-
403 order correlations were most strongly associated with auditory and speech processing. During intact story
404 listening, third-order correlations reflected integration with visual areas, and fourth-order correlations
405 reflected integration with areas associated with high-level cognition and cognitive control, such as the ven-
406 tralateral prefrontal cortex. However, during listening to temporally scrambled stories, these higher-order
407 correlations instead involved interactions with additional regions associated with speech and semantic pro-
408 cessing. By contrast, we found a much different set of patterns in the resting state data. First-order resting
409 state correlations were most strongly associated with regions involved in counting and numerical under-
410 standing. Second-order resting state correlations were strongest in visual areas; third-order correlations

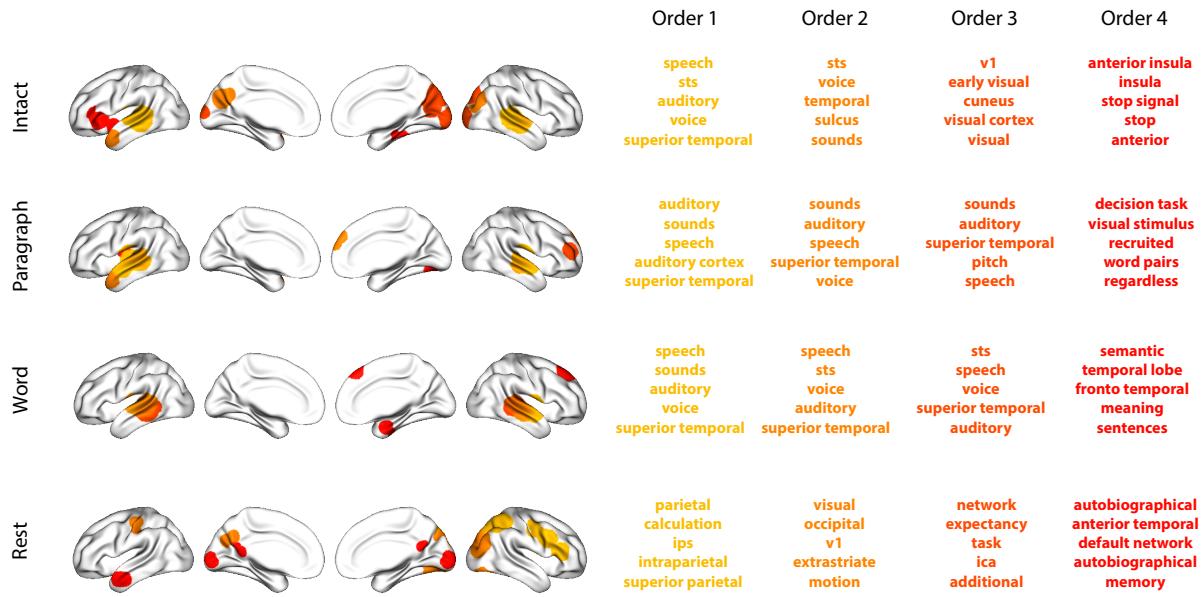


Figure 6: Top terms associated with the endpoints of the strongest correlations. Each color corresponds to one order of correlations, averaged across participants and time. The inflated brain plots display the locations of the endpoints of the 10 strongest (absolute value) correlations at each order, projected onto the cortical surface (Combrisson et al., 2019). The lists of terms on the right display the top five Neurosynth terms (Rubin et al., 2017) decoded from the corresponding brain maps for each order. Each row displays data from a different experimental condition. Additional maps and their corresponding Neurosynth terms may be found in the *Supplementary materials* (intact: Figure S1; paragraph: Figure S2; word: Figure S3; rest: Figure S4).

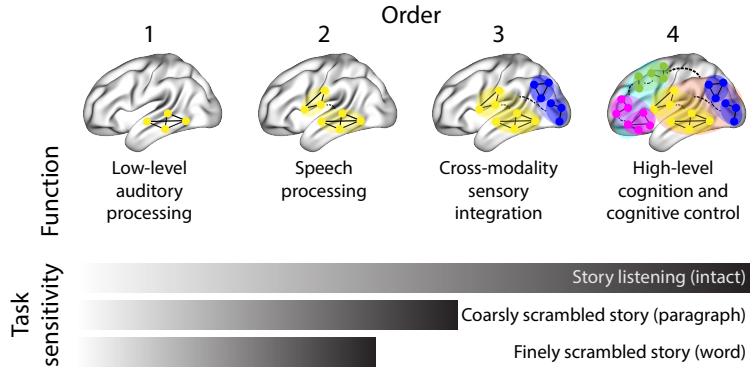


Figure 7: Proposed high-order network dynamics underlying high-level cognition. Higher orders of network interactions support higher-level aspects of cognitive processing. When tasks evoke richer, deeper, and/or higher-level processing, this is reflected in higher-order network interactions.

411 were strongest in task-positive areas; and fourth-order correlations were strongest in regions associated
 412 with autobiographical and episodic memory. We carried out analogous analyses to create maps (and de-
 413 code the top associated Neurosynth terms) for up to fifteenth-order correlations (Figs. S1, S2, S3, and S4).
 414 Of note, examining fifteenth-order correlations between 700 nodes using conventional methods would have
 415 required storing roughly $\frac{700^{2 \times 15}}{2} \approx 1.13 \times 10^{85}$ floating point numbers—assuming single-precision (32 bits
 416 each), this would require roughly 32 times as many bits as there are molecules in the known universe!
 417 Although these fifteenth-order correlations do appear (visually) to have some well-formed structure, we
 418 provide this latter example primarily as a demonstration of the efficiency and scalability of our approach.

419 Discussion

420 We tested the hypothesis that high-level cognition is supported by high-order brain network dynamics.
 421 We examined high-order network dynamics in functional neuroimaging data collected during a story
 422 listening experiment. When participants listened to an auditory recording of the story, participants exhibited
 423 similar high-order brain network dynamics. By contrast, when participants instead listened to temporally
 424 scrambled recordings of the story, only lower-order brain network dynamics were similar across participants.
 425 Our results indicate that higher orders of network interactions support higher-level aspects of cognitive
 426 processing (Fig.7).

427 Identifying higher-order network dynamics associated with high-level cognition required several im-
 428 portant methods advances. First, we used kernel-based dynamic correlations to extended the notion of
 429 (static) inter-subject functional connectivity (Simony et al., 2016) to a dynamic measure of inter-subject func-
 430 tional connectivity (DISFC) that does not rely on sliding windows, and that may be computed at individual

431 timepoints. This allowed us to precisely characterize stimulus-evoked network dynamics that were similar
432 across individuals. Second, we developed a computational framework for efficiently and scalably estimat-
433 ing high-order dynamic correlations. Our approach uses dimensionality reduction algorithms and graph
434 measures to obtain low-dimensional embeddings of patterns of network dynamics. Third, we developed
435 an analysis framework for identifying robust decoding results by carrying out our analyses using a range
436 of parameter values and then identifying which results were robust to specific parameter choices.

437 Relevant literature:

- 438 • ?: more complex concepts involve more complex network dynamics
- 439 • Demertzi et al. (2019): human consciousness is supported by dynamic complex patterns of brain
440 signal coordination. studied the brains of healthy vs minimally conscious patients; conscious patients
441 displayed richer and more structured patterns of network interactions
- 442 • Mack et al. (2017): richer task structure is supported by more complex (higher rank) brain patterns in
443 the prefrontal cortex
- 444 • ?: review of time-varying connectivity
- 445 • ?: higher variability in dynamic functional connectivity predicts worse attention. also, dynamic
446 functional connectivity improves attention predictions over static functional connectivity.
- 447 • ?: dynamic causal modelling: compute causal interaction dynamics in multivariate timeseries data.
448 important to consider causation in interpreting the direction of information flow reflected in the
449 patterns we identified through our analyses.
- 450 • ?: another review of time varying connectivity
- 451 • Roy et al. (2019): memories are distributed across functionally connected brain areas
- 452 • Fallon et al. (2019): the timescale of spontaneous resting state fMRI increases with structural connec-
453 tivity strength (in mouse and human brains)
- 454 • Liégeois et al. (2019): dynamic resting state functional connectivity best captures task-based phe-
455 notypes (processing speed, fluid intelligence), whereas static and dynamic functional connectivity
456 equally capture self-reported measures like loneliness and life satisfaction. suggest that different
457 timescales of connectivity dynamics reflect different aspects of behavior.
- 458 • Zheng et al. (2019): characterize brain connectomes at different geometric scales

- 459 • McIntosh & Jirsa (2019): neural processes reflect system interactions that occur on relatively low-
460 dimensional manifolds, thereby constraining possible functional configurations. (motivation for di-
461 mensionality reduction approach?)
- 462 • Toker & Sommer (2019): another approach to reducing dimensionality of network interactions, using
463 spectral clustering
- 464 • Zou et al. (2019): another review of complex network dynamics in timeseries data
- 465 • Shappell et al. (2019): state-based analyses of network dynamics using hidden semi-Markov models.
466 could be a useful direction for extended our work; for example, we could define kernel functions to
467 only integrate within an “event.” This could potentially improve resolution of event-specific network
468 dynamics.
- 469 • Cole et al. (2019): potential artifacts or spurious insights that affect standard functional connectivity
470 analyses (not sure this applies)
- 471 • ?: simulations for benchmarking time-varying connectivity methods (should we use this? seems
472 useful! could potentially replace synthetic data section)
- 473 • ?
- 474 • Sizemore et al. (2018)
- 475 • Reimann et al. (2017)
- 476 • Gonzalez-Castillo et al. (2019)
- 477 • Betzel et al. (2019)

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485 **Author contributions**

486 Concept: J.R.M. Implementation: T.H.C., L.L.W.O., and J.R.M. Analyses: L.L.W.O and J.R.M.

487 **References**

- 488 Alvarez-Hamelin, I., Dall'Asta, L., Barrat, A., & Vespignani, A. (2005). *k*-corr decomposition: a tool for the
489 visualiztion of large scale networks. *arXiv*, cs/0504107v2.
- 490 Barthélemy, M. (2004). Betweenness centrality in large complex networks. *European Physical Journal B*, 38,
491 163–168.
- 492 Bassett, D., Meyer-Lindenberg, A., Achard, S., Duke, T., & Bullmore, E. (2006, December). Adaptive
493 reconfiguration of fractal small-world human brain functional networks. *Proceedings of the National
494 Academy of Sciences, USA*, 103(51), 19518–23.
- 495 Betzel, R. F., Byrge, L., Esfahlani, F. Z., & Kennedy, D. P. (2019). Temporal fluctuations in the brain's modular
496 architecture during movie-watching. *bioRxiv*, doi.org/10.1101/750919.
- 497 Bonacich, P. (2007). Some unique properties of eigenvector centrality. *Social Networks*, 29(4), 555–564.
- 498 Bullmore, E., & Sporns, O. (2009). Complex brain networks: graph theoretical analysis of structural and
499 functional systems. *Nature Reviews Neuroscience*, 10(3), 186–198.
- 500 Capota, M., Turek, J., Chen, P.-H., Zhu, X., Manning, J. R., Sundaram, N., . . . Shin, Y. S. (2017). *Brain imaging
501 analysis kit*. Retrieved from <https://doi.org/10.5281/zenodo.59780>
- 502 Christakis, N. A., & Fowler, J. H. (2010). Social network sensors for early detection of contagious outbreaks.
503 *PLoS One*, 5(9), e12948.
- 504 Cole, M. W., Ito, T., Schultz, D., Mill, R., Chen, R., & Cocuzza, C. (2019). Task activations produce spurious
505 but systematic inflation of task functional connectivity estimates. *NeuroImage*, 189, 1–18.
- 506 Combrisson, E., Vallat, R., O'Reilly, C., Jas, M., Pascarella, A., l Saive, A., . . . Jerbi, K. (2019). Visbrain: a
507 multi-purpose GPU-accelerated open-source suite for multimodal brain data visualization. *Frontiers in
508 Neuroinformatics*, 13(14), 1–14.
- 509 Comon, P., Jutten, C., & Herault, J. (1991). Blind separation of sources, part II: Problems statement. *Signal
510 Processing*, 24(1), 11 - 20.

- 511 Demertzi, A., Tagliazucchi, E., Dehaene, S., Deco, G., Barttfeld, P., Raimondo, F., ... Sitt, J. D. (2019). Human
512 consciousness is supported by dynamic complex patterns of brain signal coordination. *Science Advances*,
513 5(2), eaat7603.
- 514 Estrada, E., & Rodríguez-Velázquez, J. A. (2005). Subgraph centrality in complex networks. *Physical Review*
515 *E*, 71(5), 056103.
- 516 Etzel, J. A., Gazzola, V., & Keysers, C. (2009). An introduction to anatomical ROI-based fMRI classification.
517 *Brain Research*, 1282, 114–125.
- 518 Fallon, J., Ward, P., Parkes, L., Oldham, S., Arnatkevičiūtė, A., Fornito, A., & Fulcher, B. D. (2019).
519 Timescales of spontaneous activity fluctuations relate to structural connectivity in the brain. *bioRxiv*,
520 doi.org/10.1101/655050.
- 521 Fong, A. H. C., Yoo, K., Rosenberg, M. D., Zhang, S., Li, C.-S. R., Scheinost, D., ... Chun, M. M. (2019).
522 Dynamic functional connectivity during task performance and rest predicts individual differences in
523 attention across studies. *NeuroImage*, 188, 14–25.
- 524 Freeman, L. C. (1977). A set of measures of centrality based on betweenness. *Sociometry*, 40(1), 35–41.
- 525 Geisberger, R., Sanders, P., & Schultes, D. (2008). Better approximation of betweenness centrality. *Proceedings*
526 *of the meeting on Algorithm Engineering and Experiments*, 90–100.
- 527 Gershman, S., Blei, D., Pereira, F., & Norman, K. (2011). A topographic latent source model for fMRI data.
528 *NeuroImage*, 57, 89–100.
- 529 Gonzalez-Castillo, J., Caballero-Gaudes, C., Topolski, N., Handwerker, D. A., Pereira, F., & Bandettini, P. A.
530 (2019). Imaging the spontaneous flow of thought: distinct periods of cognition contribute to dynamic
531 functional connectivity during rest. *NeuroImage*, 202(116129).
- 532 Halu, A., Mondragón, R. J., Panzarasa, P., & Bianconi, G. (2013). Multiplex PageRank. *PLoS One*, 8(10),
533 e78293.
- 534 Haxby, J. V., Gobbini, M. I., Furey, M. L., Ishai, A., Schouten, J. L., & Pietrini, P. (2001). Distributed and
535 overlapping representations of faces and objects in ventral temporal cortex. *Science*, 293, 2425–2430.
- 536 Hinton, G. E., & Salakhutdinov, R. R. (2006). Reducing the dimensionality of data with neural networks.
537 *Science*, 313(5786), 504–507.

- 538 Honey, C. J., Kötter, R., Breakspear, M., & Sporns, O. (2007). Network structure of cerebral cortex shapes
539 functional connectivity on multiple time scales. *Proceedings of the National Academy of Science USA*, 104(24),
540 10240–10245.
- 541 Huth, A. G., de Heer, W. A., Griffiths, T. L., Theunissen, F. E., & Gallant, J. L. (2016). Natural speech reveals
542 the semantic maps that tile human cerebral cortex. *Nature*, 532, 453–458.
- 543 Huth, A. G., Nisimoto, S., Vu, A. T., & Gallant, J. L. (2012). A continuous semantic space describes
544 the representation of thousands of object and action categories across the human brain. *Neuron*, 76(6),
545 1210–1224.
- 546 Jutten, C., & Herault, J. (1991). Blind separation of sources, part I: An adaptive algorithm based on
547 neuromimetic architecture. *Signal Processing*, 24(1), 1–10.
- 548 Kamitani, Y., & Tong, F. (2005). Decoding the visual and subjective contents of the human brain. *Nature*
549 *Neuroscience*, 8, 679–685.
- 550 Landau, E. (1895). Zur relativen Wertbemessung der Turnierresultate. *Deutsches Wochenschach*, 11, 366–369.
- 551 Lee, D. D., & Seung, H. S. (1999). Learning the parts of objects by non-negative matrix factorization. *Nature*,
552 401, 788–791.
- 553 Liégeois, R., Li, J., Kong, R., Orban, C., De Ville, D. V., Ge, T., … Yeo, B. T. T. (2019). Resting brain
554 dynamics at different timescales capture distinct aspects of human behavior. *Nature Communications*,
555 10(2317), doi.org/10.1038/s41467-019-10317-7.
- 556 Lin, J. (2009). Divergence measures based on the Shannon entropy. *IEEE Transactions on Information Theory*,
557 37(1), 145–151.
- 558 Lohmann, G., Margulies, D. S., Horstmann, A., Pleger, B., Lepsien, J., Goldhahn, D., … Turner, R. (2010).
559 Eigenvector centrality mapping for analyzing connectivity patterns in fMRI data of the human brain.
560 *PLoS One*, 5(4), e10232.
- 561 Mack, M. L., Preston, A. R., & Love, B. C. (2017). Medial prefrontal cortex compresses concept representations
562 through learning. *bioRxiv*, doi.org/10.1101/178145.
- 563 Mairal, J., Ponce, J., Sapiro, G., Zisserman, A., & Bach, F. R. (2009). Supervised dictionary learning. *Advances*
564 *in Neural Information Processing Systems*, 1033–1040.
- 565 Mairal, J. B., Bach, F., Ponce, J., & Sapiro, G. (2009). Online dictionary learning for sparse coding. *Proceedings*
566 *of the 26th annual international conference on machine learning*, 689–696.

- 567 Manning, J. R., Ranganath, R., Norman, K. A., & Blei, D. M. (2014). Topographic factor analysis: a Bayesian
568 model for inferring brain networks from neural data. *PLoS One*, 9(5), e94914.
- 569 Manning, J. R., Zhu, X., Willke, T. L., Ranganath, R., Stachenfeld, K., Hasson, U., ... Norman, K. A. (2018).
570 A probabilistic approach to discovering dynamic full-brain functional connectivity patterns. *NeuroImage*,
571 180, 243–252.
- 572 McInnes, L., & Healy, J. (2018). UMAP: Uniform manifold approximation and projection for dimension
573 reduction. *arXiv*, 1802(03426).
- 574 McIntosh, A. R., & Jirsa, V. K. (2019). The hidden repertoire of brain dynamics and dysfunction. *Network
Neuroscience*, doi.org/10.1162/netn_a00107.
- 575 Mitchell, T., Shinkareva, S., Carlson, A., Chang, K., Malave, V., Mason, R., & Just, M. (2008). Predicting
576 human brain activity associated with the meanings of nouns. *Science*, 320(5880), 1191.
- 577 Newman, M. E. J. (2005). A measure of betweenness centrality based on random walks. *Social Networks*, 27,
578 39–54.
- 579 Newman, M. E. J. (2008). The mathematics of networks. *The New Palgrave Encyclopedia of Economics*, 2, 1–12.
- 580 Nishimoto, S., Vu, A., Naselaris, T., Benjamini, Y., Yu, B., & Gallant, J. (2011). Reconstructing visual
581 experience from brain activity evoked by natural movies. *Current Biology*, 21, 1 - 6.
- 582 Nocedal, J., & Wright, S. J. (2006). *Numerical optimization*. New York: Springer.
- 583 Norman, K. A., Newman, E., Detre, G., & Polyn, S. M. (2006). How inhibitory oscillations can train neural
584 networks and punish competitors. *Neural Computation*, 18, 1577–1610.
- 585 Opsahl, T., Agneessens, F., & Skvoretz, J. (2010). Node centrality in weighted networks: generalizing degree
586 and shortest paths. *Social Networks*, 32, 245–251.
- 587 Pearson, K. (1901). On lines and planes of closest fit to systems of points in space. *The London, Edinburgh,
588 and Dublin Philosophical Magazine and Journal of Science*, 2, 559-572.
- 589 Pereira, F., Lou, B., Pritchett, B., Ritter, S., Gershman, S. J., Kanwisher, N., ... Fedorenko, E. (2018). Toward
590 a universal decoder of linguistic meaning from brain activation. *Nature Communications*, 9(963), 1–13.
- 591 Rao, C. R. (1982). Diversity and dissimilarity coefficients: a unified approach. *Theoretical Population Biology*,
21(1), 24–43.

- 592 Reimann, M. W., Nolte, M., Scolamiero, M., Turner, K., Perin, R., Chindemi, G., ... Markram, H. (2017).
593 Cliques of neurons bound into cavities provide a missing link between structure and function. *Frontiers*
594 in *Computational Neuroscience*, 11(48), 1–16.
- 595 Ricotta, C., & Szeidl, L. (2006). Towards a unifying approach to diversity measures: Bridging the gap
596 between the Shannon entropy and Rao's quadratic index. *Theoretical Population Biology*, 70(3), 237–243.
- 597 Roy, D. S., Park, Y.-G., Ogawa, S. K., Cho, J. H., Choi, H., Kamensky, L., ... Tonegawa, S. (2019). Brain-
598 wide mapping of contextual fear memory engram ensembles supports the dispersed engram complex
599 hypothesis. *bioRxiv*, doi.org/10.1101/668483.
- 600 Rubin, T. N., Kyoejo, O., Gorgolewski, K. J., Jones, M. N., Poldrack, R. A., & Yarkoni, T. (2017). Decoding
601 brain activity using a large-scale probabilistic functional-anatomical atlas of human cognition. *PLoS*
602 *Computational Biology*, 13(10), e1005649.
- 603 Rubinov, M., & Sporns, O. (2010). Complex network measures of brain connectivity: uses and interpreta-
604 tions. *NeuroImage*, 52, 1059–1069.
- 605 Schreiber, T. (2000). Measuring information transfer. *Physical Review Letters*, 85(2), 461–464.
- 606 Shappell, H., Caffo, B. S., Pekar, J. J., & Lindquist, M. A. (2019). Improved state change estimation in
607 dynamic functional connectivity using hidden semi-Markov models. *NeuroImage*, 191, 243–257.
- 608 Simony, E., Honey, C. J., Chen, J., & Hasson, U. (2016). Uncovering stimulus-locked network dynamics
609 during narrative comprehension. *Nature Communications*, 7(12141), 1–13.
- 610 Sizemore, A. E., Giusti, C., Kahn, A., Vettel, J. M., Betzel, R. F., & Bassett, D. S. (2018). Cliques and cavities
611 in the human connectome. *Journal of Computational Neuroscience*, 44(1), 115–145.
- 612 Spearman, C. (1904). General intelligence, objectively determined and measured. *American Journal of*
613 *Psychology*, 15, 201–292.
- 614 Sporns, O., & Honey, C. J. (2006). Small worlds inside big brains. *Proceedings of the National Academy of*
615 *Science USA*, 103(51), 19219–19220.
- 616 Tipping, M. E., & Bishop, C. M. (1999). Probabilistic principal component analysis. *Journal of Royal Statistical*
617 *Society, Series B*, 61(3), 611–622.
- 618 Toker, D., & Sommer, F. T. (2019). Information integration in large brain networks. *PLoS Computational*
619 *Biology*, 15(2), e1006807.

- 620 Tong, F., & Pratte, M. S. (2012). Decoding patterns of human brain activity. *Annual Review of Psychology*, 63,
621 483–509.
- 622 Turk-Browne, N. B. (2013). Functional interactions as big data in the human brain. *Science*, 342, 580–584.
- 623 van der Maaten, L. J. P., & Hinton, G. E. (2008). Visualizing high-dimensional data using t-SNE. *Journal of
624 Machine Learning Research*, 9, 2579-2605.
- 625 Zar, J. H. (2010). *Biostatistical analysis*. Prentice-Hall/Pearson.
- 626 Zheng, M., Allard, A., Hagmann, P., & Serrano, M. A. (2019). Geometric renormalization unravels self-
627 similarity of the multiscale human connectome. *arXiv*, 1904.11793.
- 628 Zou, Y., Donner, R. V., Marwan, N., Donges, J. F., & Kurths, J. (2019). Complex network approaches to
629 nonlinear time series analysis. *Physics Reports*, 787, 1–97.