

¹ High-level cognition during story listening is reflected in
² high-order dynamic correlations in neural activity patterns

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⁵ **Abstract**

Our thoughts arise from coordinated patterns of interactions between brain structures that change with our ongoing experiences. High-order dynamic correlations in neural activity patterns reflect different subgraphs of the brain's functional connectome that display homologous lower-level dynamic correlations. Here we test the hypothesis that high-level cognition is reflected in high-order dynamic correlations in brain activity patterns. We develop an approach to estimating high-order dynamic correlations in timeseries data, and we apply the approach to neuroimaging data collected as human participants either listen to a ten-minute story or listen to a temporally scrambled version of the story. We train across-participant pattern classifiers to decode (in held-out data) when in the session each neural activity snapshot was collected. We find that classifiers trained to decode from high-order dynamic correlations yield the best performance on data collected as participants listened to the (unscrambled) story. By contrast, classifiers trained to decode data from scrambled versions of the story yielded the best performance when they were trained using first-order dynamic correlations or non-correlational activity patterns. We suggest that as our thoughts become more complex, they are reflected in 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: i.e., 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.,^{1–9}. Training decoding models on different
²⁵ types of neural features (Fig. 1a) can also help to elucidate which specific aspects of neural activity patterns
²⁶ are informative about cognition and, by extension, which types of neural activity patterns might compose
²⁷ the neural code. For example, prior work has used region of interest analyses to estimate the anatomical
²⁸ locations of specific neural representations e.g.,¹⁰, or to compare the relative contributions to the neural
²⁹ code of multivariate activity patterns versus dynamic correlations between neural activity patterns e.g.,^{11,12}.

30 An emerging theme in this literature is that cognition is mediated by dynamic interactions between brain
31 structures^{13–25}.

32 [Figure 1 about here.]

33 Studies of the neural code to date have primarily focused on univariate or multivariate neural patterns for
34 review see², or (more recently) on patterns of dynamic first-order correlations i.e., interactions between pairs
35 of brain structures;^{11,12,18,20–22}. What might the future of this line of work hold? For example, is the neural
36 code implemented through higher-order interactions between brain structures e.g., see²⁶? Second-order
37 correlations reflect homologous patterns of correlation. In other words, if the dynamic patterns of correla-
38 tions between two regions, *A* and *B*, are similar to those between two other regions, *C* and *D*, this would
39 be reflected in the second-order correlations between (*A*-*B*) and (*C*-*D*). In this way, second-order corre-
40 lations identify similarities and differences between subgraphs of the brain’s connectome. Analogously,
41 third-order correlations reflect homologies between second-order correlations—i.e., homologous patterns of
42 homologous interactions between brain regions. More generally, higher-order correlations reflect homolo-
43 gies between patterns of lower-order correlations. We can then ask: which “orders” of interaction are most
44 reflective of high-level cognitive processes?

45 One reason one might expect to see homologous networks in a dataset is related to the notion that network
46 dynamics reflect ongoing neural computations or cognitive processing e.g.,²⁷. If the nodes in two brain
47 networks are interacting (within each network) in similar ways then, according to our characterization
48 of network dynamics, we refer to the similarities between those patterns of interaction as higher-order
49 correlations. When higher-order correlations are themselves changing over time, we can also attempt to
50 capture and characterize those high-order dynamics.

51 Another central question pertains to the extent to which the neural code is carried by activity patterns that
52 directly reflect ongoing cognition e.g., following^{1,2}, versus the dynamic properties of the network structure
53 itself, independent of specific activity patterns in any given set of regions e.g., following¹⁶. For example,
54 graph measures such as centrality and degree²⁸ may be used to estimate how a given brain structure is
55 “communicating” with other structures, independently of the specific neural representations carried by
56 those structures. If one considers a brain region’s position in the network (e.g., its eigenvector centrality) as
57 a dynamic property, one can compare how the positions of different regions are correlated, and/or how those
58 patterns of correlations change over time. We can also compute higher-order patterns in these correlations
59 to characterize homologous subgraphs in the connectome that display similar changes in their constituent
60 brain structures’ interactions with the rest of the brain.

61 To gain insights into the above aspects of the neural code, we developed a computational framework

62 for estimating dynamic high-order correlations in timeseries data. This framework provides an important
63 advance, in that it enables us to examine patterns of higher-order correlations that are computationally
64 intractable to estimate via conventional methods. Given a multivariate timeseries, our framework pro-
65 vides timepoint-by-timepoint estimates of the first-order correlations, second-order correlations, and so
66 on. Our approach combines a kernel-based method for computing dynamic correlations in timeseries
67 data with a dimensionality reduction step (Fig. 1b) that projects the resulting dynamic correlations into
68 a low-dimensional space. We explored two dimensionality reduction approaches: principle components
69 analysis PCA,²⁹, which preserves an approximately invertible transformation back to the original data e.g.,
70 this follows related approaches taken by^{30–32}; and a second non-invertible algorithm for computing dy-
71 namic patterns in eigenvector centrality³³. This latter approach characterizes correlations between each
72 feature dimension’s relative position in the network (at each moment in time) in favor of the specific activity
73 histories of different features also see^{26,34,35}.

74 We validated our approach using synthetic data where the underlying correlations were known. We
75 then applied our framework to a neuroimaging dataset collected as participants listened to either an audio
76 recording of a ten-minute story, listened to a temporally scrambled version of the story, or underwent a
77 resting state scan³⁶. Temporal scrambling has been used in a growing number of studies, largely by Uri
78 Hasson’s group, to identify brain regions that are sensitive to higher-order and longer-timescale information
79 (e.g., cross-sensory integration, rich narrative meaning, complex situations, etc.) versus regions that are
80 primarily sensitive to low-order (e.g., sensory) information. For example,³⁷ argues that when brain areas
81 are sensitive to fine versus coarse temporal scrambling, this indicates that they are “higher order” in the
82 sense that they process contextual information pertaining to further-away timepoints. By contrast, low-level
83 regions, such as primary sensory cortices, do not meaningfully change their responses (after correcting for
84 presentation order) even when the stimulus is scrambled at fine timescales.

85 We used a subset of the story listening and rest data to train across-participant classifiers to decode
86 listening times (of groups of participants) using a blend of neural features (comprising neural activity
87 patterns, as well as different orders of dynamic correlations between those patterns that were inferred
88 using our computational framework). We found that both the PCA-based and eigenvector centrality-based
89 approaches yielded neural patterns that could be used to decode accurately (i.e., well above chance). Both
90 approaches also yielded the best decoding accuracy for data collected during (intact) story listening when
91 high-order (PCA: second-order; eigenvector centrality: fourth-order) dynamic correlation patterns were
92 included as features. When we trained classifiers on the scrambled stories or resting state data, only
93 (relatively) lower-order dynamic patterns were informative to the decoders. Taken together, our results
94 indicate that high-level cognition is supported by high-order dynamic patterns of communication between

95 brain structures.

96 Results

97 We sought to understand whether high-level cognition is reflected in dynamic patterns of high-order correla-
98 tions. To that end, we developed a computational framework for estimating the dynamics of stimulus-driven
99 high-order correlations in multivariate timeseries data (see Dynamic inter-subject functional connectivity
100 (DISFC) and Dynamic higher-order correlations). We evaluated the efficacy of this framework at recovering
101 known patterns in several synthetic datasets (see Synthetic data: simulating dynamic first-order corre-
102 lations and Synthetic data: simulating dynamic higher-order correlations). We then applied the framework
103 to a public fMRI dataset collected as participants listened to an auditorily presented story, listened to a
104 temporally scrambled version of the story, or underwent a resting state scan (see Functional neuroimaging
105 data collected during story listening). We used the relative decoding accuracies of classifiers trained on
106 different sets of neural features to estimate which types of features reflected ongoing cognitive processing.

107 Recovering known dynamic first-order correlations

108 We generated synthetic datasets that differed in how the underlying first-order correlations changed over
109 time. For each dataset, we applied Equation 4 with a variety of kernel shapes and widths. We assessed how
110 well the true underlying correlations at each timepoint matched the recovered correlations (Fig. 2). For every
111 kernel and dataset we tested, our approach recovered the correlation dynamics we embedded into the data.
112 However, the quality of these recoveries varied across different synthetic datasets in a kernel-dependent
113 way.

114 [Figure 2 about here.]

115 In general, wide monotonic kernel shapes (Laplace, Gaussian), and wider kernels (within a shape),
116 performed best when the correlations varied gradually from moment-to-moment (Figs. 2a, c, and d). In the
117 extreme, as the rate of change in correlations approaches 0 (Fig. 2a), an infinitely wide kernel would exactly
118 recover the Pearson's correlation (e.g., compare Eqns. 1 and 4).

119 When the correlation dynamics were unstructured in time (Fig. 2b), a Dirac δ kernel (infinitely narrow)
120 performed best. This is because, when every timepoint's correlations are independent of the correlations at
121 every other timepoint, averaging data over time dilutes the available signal. Following a similar pattern,
122 holding kernel shape fixed, narrower kernel parameters better recovered randomly varying correlations.

123 **Recovering known dynamic higher-order correlations**

124 Following our approach to evaluating our ability to recover known dynamic first-order correlations from
125 synthetic data, we generated an analogous second set of synthetic datasets that we designed to exhibit
126 known dynamic first-order and second-order correlations (see Synthetic data: simulating dynamic higher-
127 order correlations). We generated a total of 400 datasets (100 datasets for each category) that varied in how
128 the first-order and second-order correlations changed over time. We then repeatedly applied Equation 4
129 using the overall best-performing kernel from our first-order tests (a Laplace kernel with a width of 20;
130 Fig. 2) to assess how closely the recovered dynamic correlations matched the dynamic correlations we had
131 embedded into the datasets.

132 Overall, we found that we could reliably recover both first-order and second-order correlations from the
133 synthetic data (Fig. 3). When the correlations were stable for longer intervals, or changed gradually (constant,
134 ramping, and event datasets), recovery performance was relatively high, and we were better able to recover
135 dynamic first-order correlations than second-order correlations. This is because errors in our estimation
136 procedure at lower orders necessarily propagate to higher orders (since lower-order correlations are used to
137 estimate higher-order correlations). Conversely, when the correlations were particularly unstable (random
138 datasets), we better recovered second-order correlations. This is because noise in our data generation
139 procedure propagates from higher orders to lower orders (see Synthetic data: simulating dynamic high-
140 order correlations).

141 [Figure 3 about here.]

142 We also examined the impact of the data duration (Fig. S3) and complexity (number of zero-order features;
143 Fig. S4) on our ability to accurately recover ground truth first-order and second-order dynamic correlations.
144 In general, we found that our approach better recovers ground truth dynamic correlations from longer
145 duration timeseries data. We also found that our approach tends to best recover data generated using fewer
146 zero-order features (i.e., lower complexity), although this tendency was not strictly monotonic. Further,
147 because our data generation procedure requires $O(K^4)$ memory to generate a second-order timeseries with K
148 zero-order features, we were not able to fully explore how the number of zero-order features affects recovery
149 accuracy as the number of features gets larger (e.g., as it approaches the number of features present in the
150 fMRI data we examine below). Although we were not able to formally test this to our satisfaction, we expect
151 that accurately estimating dynamic high-order correlations would require data with many more zero-order
152 features than we were able to simulate. Our reasoning is that high-order correlations necessarily involve
153 larger numbers of lower-order features, so achieving adequate “resolution” high-order timeseries might
154 require many low-order features.

155 Taken together, our explorations using synthetic data indicated that we are able to partially, but not
156 perfectly, recover ground truth dynamic first-order and second-order correlations. This suggests that our
157 modeling approach provides a meaningful (if noisy) estimate of high-order correlations. We next turned
158 to analyses of human fMRI data to examine whether the recovered dynamics might reflect the dynamics of
159 human cognition during a naturalistic story-listening task.

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

161 We used across-participant temporal decoders to identify cognitively relevant neural patterns in fMRI data
162 (see Forward inference and decoding accuracy). The dataset we examined collected by³⁶ comprised four
163 experimental conditions that exposed participants to stimuli that varied systematically in how cognitively
164 engaging they were. The intact experimental condition (intact) had participants listen to an audio recording
165 of a 10-minute story. The paragraph-scrambled experimental condition (paragraph) had participants listen
166 to a temporally scrambled version of the story, where the paragraphs occurred out of order (but where
167 the same total set of paragraphs were presented over the full listening interval). All participants in this
168 condition experienced the scrambled paragraphs in the same order. The word-scrambled experimental
169 condition (word) had participants listen to a temporally scrambled version of the story where the words
170 in the story occurred in a random order. All participants in the word condition experienced the scrambled
171 words in the same order. Finally, in a rest experimental condition (rest), participants lay in the scanner with
172 no overt stimulus, with their eyes open (blinking as needed). This public dataset provided a convenient
173 means of testing our hypothesis that different levels of cognitive processing and engagement are reflected
174 in different orders of brain activity dynamics.

175 [Figure 4 about here.]

176 In brief, we computed timeseries of dynamic high-order correlations that were similar across participants
177 in each of two randomly assigned groups: a training group and a test group. We then trained classifiers
178 on the training group's data to match each sample from the test group with a stimulus timepoint. Each
179 classifier comprised a weighted blend of neural patterns that reflected up to n^{th} -order dynamic correlations
180 (see Feature weighting and testing). We repeated this process for $n \in \{0, 1, 2, \dots, 10\}$. Our examinations of
181 synthetic data suggested that none of the kernels we examined were “universal” in the sense of optimally
182 recovering underlying correlations regardless of the temporal structure of those correlations. We found a
183 similar pattern in the (real) fMRI data, whereby different kernels yielded different decoding accuracies, but
184 no single kernel emerged as the clear “best.” In our analyses of neural data, we therefore averaged our

185 decoding results over a variety of kernel shapes and widths in order to identify results that were robust to
186 specific kernel parameters (see Identifying robust decoding results).

187 Our approach to estimating dynamic high-order correlations entails mapping the high-dimensional
188 feature space of correlations (represented by a T by $O(K^2)$ matrix) onto a lower-dimensional feature space
189 (represented by a T by K matrix). We carried out two sets of analyses that differed in how this mapping was
190 computed. The first set of analyses used PCA to find a low-dimensional embedding of the original dynamic
191 correlation matrices (Fig. 4a,b). The second set of analyses characterized correlations in dynamics of each
192 feature's eigenvector centrality, but did not preserve the underlying activity dynamics (Fig. 4c,d).

193 [Figure 5 about here.]

194 Both sets of temporal decoding analyses yielded qualitatively similar results for the auditory (non-rest)
195 conditions of the experiment (Fig. 4: pink, green, and teal lines; Fig. 5: three leftmost columns). The highest
196 decoding accuracy for participants who listened to the intact (unscrambled) story was achieved using high-
197 order dynamic correlations (PCA: second-order; eigenvector-centrality: fourth-order). Scrambled versions
198 of the story were best decoded by lower-order correlations (PCA/paragraph: first-order; PCA/word: order
199 zero; eigenvector centrality/paragraph: order zero; eigenvector centrality/word: order zero). The two sets
200 of analyses yielded different decoding results on resting state data (Fig. 4: purple lines; Fig. 5: rightmost
201 column). We note that, while the resting state times could be decoded reliably, the accuracies were only very
202 slightly above chance. We speculate that the decoders might have picked up on attentional drift, boredom,
203 or tiredness; we hypothesize that these all increased throughout the resting state scan. The decoders might
204 be picking up on aspects of these loosely defined cognitive states that are common across individuals. The
205 PCA-based approach achieved the highest resting state decoding accuracy using order zero features (non-
206 correlational, activation-based), whereas the eigenvector centrality-based approach achieved the highest
207 resting state decoding accuracy using second-order correlations. Taken together, these analyses indicate
208 that high-level cognitive processing (while listening to the intact story) is reflected in the dynamics of high-
209 order correlations in brain activity, whereas lower-level cognitive processing (while listening to scrambled
210 versions of the story that lack rich meaning) is reflected in the dynamics of lower-order correlations and
211 non-correlational activity dynamics. Further, these patterns are associated both with the underlying activity
212 patterns (characterized using PCA) and also with the changing relative positions that different brain areas
213 occupy in their associated networks (characterized using eigenvector centrality).

214 [Figure 6 about here.]

215 Having established that patterns of high-order correlations are informative to decoders, we next won-
216 dered which specific networks of brain regions contributed most to these patterns. As a representative

example, we selected the kernel parameters that yielded decoding accuracies that were the most strongly correlated (across conditions and orders) with the average accuracies across all of the kernel parameters we examined. Using Figure 4c as a template, the best-matching kernel was a Laplace kernel with a width of 50 (Fig. 9d; also see Fig. S9). We used this kernel to compute a single K by K n^{th} -order DISFC matrix for each experimental condition. We then used Neurosynth³⁸ to compute the terms most highly associated with the most strongly correlated pairs of regions in each of these matrices (Fig. 6; see Reverse inference).

For all of the story listening conditions (intact, paragraph, and word; top three rows of Fig. 6), we found that first- and second-order correlations were most strongly associated with auditory and speech processing areas. During intact story listening, third-order correlations reflected integration with visual areas, and fourth-order correlations reflected integration with areas associated with high-level cognition and cognitive control, such as the ventrolateral prefrontal cortex. However, when participants listened to temporally scrambled stories, these higher-order correlations instead involved interactions with additional regions associated with speech and semantic processing (second and third rows of Fig. 6). By contrast, we found a much different set of patterns in the resting state data (Fig. 6, bottom row). First-order resting state correlations were most strongly associated with regions involved in counting and numerical understanding. Second-order resting state correlations were strongest in visual areas; third-order correlations were strongest in task-positive areas; and fourth-order correlations were strongest in regions associated with autobiographical and episodic memory. We carried out analogous analyses to create maps (and decode the top associated Neurosynth terms) for up to fifteenth-order correlations (Figs. S5, S6, S7, and S8). Of note, examining fifteenth-order correlations between 700 nodes using conventional methods would have required storing roughly $\frac{700^{2 \times 15}}{2} \approx 1.13 \times 10^{85}$ floating point numbers—assuming single-precision (32 bits each), this would require roughly 32 times as many bits as there are molecules in the known universe! Although these fifteenth-order correlations do appear (visually) to have some well-formed structure, we provide this latter example primarily as a demonstration of the efficiency and scalability of our approach.

Discussion

We tested the hypothesis that high-level cognition is reflected in high-order brain network dynamics e.g., see^{19,26}. We examined high-order network dynamics in functional neuroimaging data collected during a story listening experiment. When participants listened to an auditory recording of the story, participants exhibited similar high-order brain network dynamics. By contrast, when participants instead listened to temporally scrambled recordings of the story, only lower-order brain network dynamics were similar across participants. Our results indicate that higher orders of network interactions support higher-level aspects of

²⁴⁸ cognitive processing (Fig. 7).

²⁴⁹ [Figure 7 about here.]

²⁵⁰ The notion that cognition is reflected in (and possibly mediated by) patterns of first-order network dy-
²⁵¹ namics has been suggested by or proposed in myriad empirical studies and reviews e.g.,^{11,12,17,18,20–22,24,25,32,39–42}.
²⁵² Our study extends this line of work by finding cognitively relevant higher-order network dynamics that
²⁵³ reflect ongoing cognition. Our findings also complement other work that uses graph theory and topology
²⁵⁴ to characterize how brain networks reconfigure during cognition e.g.,^{16,26,30,31,34,35,43}.

²⁵⁵ An open question not addressed by our study pertains to how different structures integrate incoming
²⁵⁶ information with different time constants. For example, one line of work suggests that the cortical surface
²⁵⁷ comprises a structured map such that nearby brain structures process incoming information at similar
²⁵⁸ timescales. Low-level sensory areas integrate information relatively quickly, whereas higher-level regions
²⁵⁹ integrate information relatively slowly^{37,44–49}. A similar hierarchy appears to play a role in predicting future
²⁶⁰ events⁵⁰. Other related work in human and mouse brains indicates that the temporal response profile of a
²⁶¹ given brain structure may relate to how strongly connected that structure is with other brain areas⁵¹. Further
²⁶² study is needed to understand the role of temporal integration at different scales of network interaction,
²⁶³ and across different anatomical structures. Importantly, our analyses do not speak to the physiological
²⁶⁴ basis of higher-order dynamics, and could reflect nonlinearities, chaotic patterns, non-stationarities, and/or
²⁶⁵ multistability, etc. However, our decoding analyses do indicate that higher-order dynamics are consistent
²⁶⁶ across individuals, and therefore unlikely to reflect non-stimulus-driven dynamics that are unlikely to be
²⁶⁷ similar across individuals.

²⁶⁸ One limitation of our approach relates to how noise propagates in our estimation procedure. Specifi-
²⁶⁹ cally, our procedure for estimating high-order dynamic correlations depends on estimates of lower-order
²⁷⁰ dynamic correlations. This means that our measures of which higher-order patterns are reliable and stable
²⁷¹ across experimental conditions are partially confounded with the stability of lower-order patterns. Prior
²⁷² work suggests that the stability of what we refer to here as first-order dynamics likely varies across the
²⁷³ experimental conditions we examined³⁶. Therefore a caveat to our claim that richer stimuli evoke more
²⁷⁴ stable higher-order dynamics is that our approach assumes that those high-order dynamics reflect relations
²⁷⁵ or interactions between lower-order features.

²⁷⁶ Another potential limitation of our approach relates to recent work suggesting that the brain undergoes
²⁷⁷ rapid state changes, for example across event boundaries e.g.,^{44,52} used hidden semi-Markov models to es-
²⁷⁸ timate state-specific network dynamics also see⁵³. Our general approach might be extended by considering
²⁷⁹ putative state transitions. For example, rather than weighting all timepoints using a similar kernel (Eqn. 4),

280 the kernel function could adapt on a timepoint-by-timepoint basis such that only timepoints determined to
281 be in the same “state” were given non-zero weight.

282 Identifying high-order network dynamics associated with high-level cognition required several impor-
283 tant methods advances. First, we used kernel-based dynamic correlations to extended the notion of (static)
284 inter-subject functional connectivity³⁶ to a dynamic measure of inter-subject functional connectivity (DISFC)
285 that does not rely on sliding windows e.g., as in¹¹, and that may be computed at individual timepoints. This
286 allowed us to precisely characterize stimulus-evoked network dynamics that were similar across individ-
287 uals. Second, we developed a computational framework for efficiently and scalably estimating high-order
288 dynamic correlations. Our approach uses dimensionality reduction algorithms and graph measures to
289 obtain low-dimensional embeddings of patterns of network dynamics. Third, we developed an analysis
290 framework for identifying robust decoding results by carrying out our analyses using a range of parameter
291 values and identifying which results were robust to specific parameter choices. By showing that high-level
292 cognition is reflected in high-order network dynamics, we have elucidated the next step on the path towards
293 understanding the neural basis of cognition.

294 Methods

295 Our general approach to efficiently estimating high-order dynamic correlations comprises four general
296 steps (Fig. 8). First, we derive a kernel-based approach to computing dynamic pairwise correlations in
297 a T (timepoints) by K (features) multivariate timeseries, \mathbf{X}_0 . This yields a T by $O(K^2)$ matrix of dynamic
298 correlations, \mathbf{Y}_1 , where each row comprises the upper triangle and diagonal of the correlation matrix at
299 a single timepoint, reshaped into a row vector (this reshaped vector is $(\frac{K^2-K}{2} + K)$ -dimensional). Second,
300 we apply a dimensionality reduction step to project the matrix of dynamic correlations back onto a K -
301 dimensional space. This yields a T by K matrix, \mathbf{X}_1 , that reflects an approximation of the dynamic correlations
302 reflected in the original data. Third, we use repeated applications of the kernel-based dynamic correlation
303 step to \mathbf{X}_n and the dimensionality reduction step to the resulting \mathbf{Y}_{n+1} to estimate high-order dynamic
304 correlations. Each application of these steps to a T by K time series \mathbf{X}_n yields a T by K matrix, \mathbf{X}_{n+1} , that
305 reflects the dynamic correlations between the columns of \mathbf{X}_n . In this way, we refer to n as the order of the
306 timeseries, where \mathbf{X}_0 (order 0) denotes the original data and \mathbf{X}_n denotes (approximated) n^{th} -order dynamic
307 correlations between the columns of \mathbf{X}_0 . Finally, we use a cross-validation-based decoding approach to
308 evaluate how well information contained in a given order (or weighted mixture of orders) may be used
309 to decode relevant cognitive states. If including a given \mathbf{X}_n in the feature set yields higher classification
310 accuracy on held-out data, we interpret this as evidence that the given cognitive states are reflected in

311 patterns of n^{th} -order correlations.

312 All of the code used to produce the figures and results in this manuscript, along with links to the
 313 corresponding datasets, may be found at github.com/ContextLab/timecorr-paper. In addition, we have
 314 released a Python toolbox for computing dynamic high-order correlations in timeseries data; our toolbox
 315 may be found at timecorr.readthedocs.io.

316 [Figure 8 about here.]

317 **Kernel-based approach for computing dynamic correlations**

Given a T by K matrix of observations, \mathbf{X} , we can compute the (static) Pearson's correlation between any pair of columns, $\mathbf{X}(\cdot, i)$ and $\mathbf{X}(\cdot, j)$ using²⁹:

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

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

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

318 We can generalize this formula to compute time-varying correlations by incorporating a kernel function that
 319 takes a time t as input, and returns how much the observed data at each timepoint $\tau \in [-\infty, \infty]$ contributes
 320 to the estimated instantaneous correlation at time t Fig. 9; also see⁵⁴ for a similar approach.

321 [Figure 9 about here.]

Given a kernel function $\kappa_t(\cdot)$ for timepoint t , evaluated at timepoints $\tau \in [1, \dots, T]$, we can update the static correlation formula in Equation 1 to estimate the instantaneous correlation at timepoint t :

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

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

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

322 Here $\text{timecorr}_{\kappa_t}(\mathbf{X}(\cdot, i), \mathbf{X}(\cdot, j))$ reflects the correlation at time t between columns i and j of \mathbf{X} , estimated using
 323 the kernel κ_t . We evaluate Equation 4 in turn for each pair of columns in \mathbf{X} and for kernels centered on each

³²⁴ timepoint in the timeseries, respectively, to obtain a T by K by K timeseries of dynamic correlations, \mathbf{Y} . For
³²⁵ convenience, we then reshape the upper triangles and diagonals of each timepoint's symmetric correlation
³²⁶ matrix into a row vector to obtain an equivalent T by $(\frac{K^2-K}{2} + K)$ matrix.

³²⁷ **Dynamic inter-subject functional connectivity (DISFC)**

Equation 4 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;^{36,55} to compute the stimulus-driven correlations reflected in the multi-participant dataset at a given timepoint t using:

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

where M extracts and vectorizes the upper triangle and diagonal of a symmetric matrix, Z is the Fisher z -transformation⁵⁶:

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

R is the inverse of Z :

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

and $\mathbf{Y}_{n+1}^p(t)$ denotes the correlation matrix at timepoint t (Eqn. 4) between each column of \mathbf{X}_n^p and each column of the average \mathbf{X}_n from all other participants, $\bar{\mathbf{X}}_n^{\setminus p}$:

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

³²⁸ where $\setminus p$ denotes the set of all participants other than participant p . In this way, the T by $(\frac{K^2-K}{2} + K)$ DISFC
³²⁹ matrix $\bar{\mathbf{C}}$ provides a time-varying extension of the ISFC approach developed by³⁶.

330 **Low-dimensional representations of dynamic correlations**

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

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

337 The modern toolkit of dimensionality reduction algorithms include Principal Components Analysis PCA;²⁹,
338 Probabilistic PCA PPCA;⁵⁷, Exploratory Factor Analysis EFA;⁵⁸, Independent Components Analysis ICA;^{59,60},
339 t -Stochastic Neighbor Embedding t -SNE;⁶¹, Uniform Manifold Approximation and Projection UMAP;⁶²,
340 non-negative matrix factorization NMF;⁶³, Topographic Factor Analysis TFA;⁶⁴, Hierarchical Topographic
341 Factor analysis HTFA;¹¹, Topographic Latent Source Analysis TLSA;⁶⁵, dictionary learning^{66,67}, and deep
342 auto-encoders⁶⁸, among others. While complete characterizations of each of these algorithms is beyond the
343 scope of the present manuscript, the general intuition driving these approaches is to compute the T by K
344 matrix, \mathbf{X} , that is closest to the original T by J matrix, \mathbf{Y} , where (typically) $K \ll J$. The different approaches
345 place different constraints on what properties \mathbf{X} must satisfy and which aspects of the data are compared
346 (and how) in order to optimize how well \mathbf{X} approximates \mathbf{Y} .

347 Applying dimensionality reduction algorithms to \mathbf{Y} yields an \mathbf{X} whose columns reflect weighted combi-
348 nations (or nonlinear transformations) of the original columns of \mathbf{Y} . This has two main consequences. First,
349 with each repeated dimensionality reduction, the resulting \mathbf{X}_n has lower and lower fidelity (with respect to
350 what the “true” \mathbf{Y}_n might have looked like without using dimensionality reduction to maintain tractability).
351 In other words, computing \mathbf{X}_n is a lossy operation. Second, whereas each column of \mathbf{Y}_n may be mapped
352 directly onto specific pairs of columns of \mathbf{X}_{n-1} , the columns of \mathbf{X}_n reflect weighted combinations and/or
353 nonlinear transformations of the columns of \mathbf{Y}_n . Many dimensionality reduction algorithms are invertible
354 (or approximately invertible). However, attempting to map a given \mathbf{X}_n back onto the original feature space
355 of \mathbf{X}_0 will usually require $O(TK^2)$ space and therefore becomes intractable as n or K grow large.

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

357 The above dimensionality reduction approaches to approximating a given \mathbf{Y}_n with a lower-dimensional
358 \mathbf{X}_n preserve a (potentially recombined and transformed) mapping back to the original data in \mathbf{X}_0 . We also
359 explore graph measures that instead characterize each feature’s relative position in the broader network of

360 interactions and connections. To illustrate the distinction between the two general approaches we explore,
361 suppose a network comprises nodes A and B , along with several other nodes. If A and B exhibit uncorrelated
362 activity patterns, then by definition the functional connection (correlation) between them will be close to
363 0. However, if A and B each interact with other nodes in similar ways, we might attempt to capture those
364 similarities between A 's and B 's interactions with those other members of the network.

365 In general, graph measures take as input a matrix of interactions (e.g., using the above notation, a K
366 by K correlation matrix or binarized correlation matrix reconstituted from a single timepoint's row of \mathbf{Y}),
367 and return as output a set of K measures describing how each node (feature) sits within that correlation
368 matrix with respect to the rest of the population. Widely used measures include betweenness centrality the
369 proportion of shortest paths between each pair of nodes in the population that involves the given node in
370 question; e.g.,^{69–73}; diversity and dissimilarity characterizations of how differently connected a given node
371 is from others in the population; e.g.,^{74–76}; eigenvector centrality and pagerank centrality measures of how
372 influential a given node is within the broader network; e.g.,^{77–80}; transfer entropy and flow coefficients a
373 measure of how much information is flowing from a given node to other nodes in the network; e.g.,^{81,82};
374 k -coreness centrality a measure of the connectivity of a node within its local subgraph; e.g.,^{83,84}; within-
375 module degree a measure of how many connections a node has to its close neighbors in the network;
376 e.g.,⁸⁵; participation coefficient a measure of the diversity of a node's connections to different subgraphs
377 in the network; e.g.,⁸⁵; and subgraph centrality a measure of a node's participation in all of the network's
378 subgraphs; e.g.,⁸⁶; among others.

379 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
380 characterizes the corresponding graph properties of each column. This results in a new T by K matrix,
381 \mathbf{X}_n , that reflects how the features reflected in the columns of \mathbf{X}_{n-1} participate in the network during each
382 timepoint (row).

383 **Dynamic higher-order correlations**

384 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
385 enables us to estimate high-order dynamic correlations in a scalable way. Given a T by K input matrix, the
386 output of Equation 4 requires $O(TK^2)$ space to store. Repeated applications of Equation 4 (i.e., computing
387 dynamic correlations between the columns of the outputted dynamic correlation matrix) each require
388 exponentially more space; in general the n^{th} -order dynamic correlations of a T by K timeseries occupies
389 $O(TK^{2^n})$ space. However, when we approximate or summarize the output of Equation 4 with a T by K matrix
390 (as described above), it becomes feasible to compute even very high-order correlations in high-dimensional

391 data. Specifically, approximating the n^{th} -order dynamic correlations of a T by K timeseries requires only
392 $O(TK^2)$ additional space— the same as would be required to compute first-order dynamic correlations. In
393 other words, the space required to store $n + 1$ multivariate timeseries reflecting up to n^{th} order correlations
394 in the original data scales linearly with n using our approach (Fig. 8).

395 **Data**

396 We examined two types of data: synthetic data and human functional neuroimaging data. We constructed
397 and leveraged the synthetic data to evaluate our general approach for a related validation approach see⁸⁷.
398 Specifically, we tested how well Equation 4 could be used to recover known dynamic correlations using
399 different choices of kernel (κ ; Fig. 9), for each of several synthetic datasets that exhibited different temporal
400 properties. We also simulated higher-order correlations and tested how well Equation 4 could recover these
401 correlations using the best kernel from the previous synthetic data analyses. We then applied our approach
402 to a functional neuroimaging dataset to test the hypothesis that ongoing cognitive processing is reflected
403 in high-order dynamic correlations. We used an across-participant classification test to estimate whether
404 dynamic correlations of different orders contain information about which timepoint in a story participants
405 were listening to.

406 **Synthetic data: simulating dynamic first-order correlations**

407 We constructed a total of 400 different multivariate timeseries, collectively reflecting a total of 4 qualitatively
408 different patterns of dynamic first-order correlations (i.e., 100 datasets reflecting each type of dynamic pat-
409 tern). Each timeseries comprised 50 features (dimensions) that varied over 300 timepoints. The observations
410 at each timepoint were drawn from a zero-mean multivariate Gaussian distribution with a covariance matrix
411 defined for each timepoint as described below. We drew the observations at each timepoint independently
412 from the draws at all other timepoints; in other words, for each observation $s_t \sim \mathcal{N}(\mathbf{0}, \Sigma_t)$ at timepoint t ,
413 $p(s_t) = p(s_t | s_{\setminus t})$.

Constant. We generated data with stable underlying correlations to evaluate how Equation 4 characterized correlation “dynamics” when the ground truth correlations were static. We constructed 100 multivariate timeseries whose observations were each drawn from a single (stable) Gaussian distribution. For each

dataset (indexed by m), we constructed a random covariance matrix, Σ_m :

$$\Sigma_m = \mathbf{C}\mathbf{C}^\top, \text{ where} \quad (11)$$

$$\mathbf{C}(i, j) \sim \mathcal{N}(0, 1), \text{ and where} \quad (12)$$

414 $i, j \in [1, 2, \dots, 50]$. In other words, all of the observations (for each of the 300 timepoints) within each dataset
415 were drawn from a multivariate Gaussian distribution with the same covariance matrix, and the 100 datasets
416 each used a different covariance matrix.

417 **Random.** We generated a second set of 100 synthetic datasets whose observations at each timepoint were
418 drawn from a Gaussian distribution with a new randomly constructed (using Eqn. 11) covariance matrix.
419 Because each timepoint's covariance matrix was drawn independently from the covariance matrices for all
420 other timepoints, these datasets provided a test of reconstruction accuracy in the absence of any meaningful
421 underlying temporal structure in the dynamic correlations underlying the data.

Ramping. We generated a third set of 100 synthetic datasets whose underlying correlations changed gradually over time. For each dataset, we constructed two “anchor” covariance matrices using Equation 11, 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

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

422 The gradually changing correlations underlying these datasets allow us to evaluate the recovery of dynamic
423 correlations when each timepoint's correlation matrix is unique (as in the random datasets), but where the
424 correlation dynamics are structured and exhibit first-order autocorrelations (as in the constant datasets).

425 **Event.** We generated a fourth set of 100 synthetic datasets whose underlying correlation matrices exhibited
426 prolonged intervals of stability, interspersed with abrupt changes. For each dataset, we used Equation 11
427 to generate 5 random covariance matrices. We constructed a timeseries where each set of 60 consecutive
428 samples was drawn from a Gaussian with the same covariance matrix. These datasets were intended to
429 simulate a system that exhibits periods of stability punctuated by occasional abrupt state changes.

430 **Synthetic data: simulating dynamic high-order correlations**

431 We developed an iterative procedure for constructing timeseries data that exhibits known dynamic high-
432 order correlations. The procedure builds on our approach to generating dynamic first-order correlations.
433 Essentially, once we generate a timeseries with known first-order correlations, we can use the known first-
434 order correlations as a template to generate a new timeseries of second-order correlations. In turn, we can
435 generate a timeseries of third-order correlations from the second-order correlations, and so on. In general,
436 we can generate order n correlations given a timeseries of order $n - 1$ correlations, for any $n > 1$. Finally,
437 given the order n timeseries, we can reverse the preceding process to generate an order $n - 1$ timeseries, an
438 order $n - 2$ order timeseries, and so on, until we obtain an order 0 timeseries of simulated data that reflects
439 the chosen high-order dynamics.

440 The central mathematical operation in our procedure is the Kronecker product (\otimes). The Kronecker
441 product of a $K \times K$ matrix, m_1 , with itself (i.e., $m_1 \otimes m_1$) produces a new $K^2 \times K^2$ matrix, m_2 whose entries
442 reflect a scaled tiling of the entries in m_1 . If these tilings (scaled copies of m_1) are indexed by row and column,
443 then the tile in the i^{th} row and j^{th} column contains the entries of m_1 , multiplied by $m_1(i, j)$. Following this
444 pattern, the Kronecker product $m_2 \otimes m_2$ yields the $K^4 \times K^4$ matrix m_3 whose tiles are scaled copies of m_2 . In
445 general, repeated applications of the Kronecker self-product may be used to generate $m_{n+1} = m_n \otimes m_n$ for
446 $n > 1$, where m_{n+1} is a $K^{2^n} \times K^{2^n}$ matrix. After generating a first-order timeseries of dynamic correlations (see
447 Synthetic data: simulating dynamic first-order correlations), we use this procedure (applied independently
448 at each timepoint) to transform it into a timeseries of n^{th} -order correlations. When m_{n+1} is generated in this
449 way, the temporal structure of the full timeseries (i.e., constant, random, ramping, event) is preserved, since
450 changes in the original first-order timeseries are also reflected in the scaled tilings of itself that comprise the
451 higher-order matrices.

452 Given a timeseries of n^{th} -order correlations, we then need to work “backwards” in order to generate the
453 order-zero timeseries. If the n^{th} -order correlation matrix at a given timepoint is m_n , then we can generate an
454 order $n - 1$ correlation matrix (for $n > 1$) by taking a draw from $\mathcal{N}(0, m_n)$ and reshaping the resulting vector
455 to have square dimensions. To force the resulting matrix to be symmetric, we remove its lower triangle, and
456 replace the lower triangle with (a reflected version of) its upper triangle. Intuitively, the re-shaped matrix
457 will look like a noisy (but symmetric) version of the template matrix, m_{n-1} . (When $n = 1$, no re-shaping
458 is needed; the resulting K -dimensional vector may be used as the observation at the given timepoint.)
459 After independently drawing each timepoint’s order $n - 1$ correlation matrix from that timepoint’s order
460 n correlation matrix, this process can be applied repeatedly until $n = 0$. This results in a K -dimensional
461 timeseries of T observations containing the specified high-order correlations at orders 1 through n . Following

462 our approach to generating synthetic data exhibiting known first-order correlations, we constructed a total
463 of 400 additional multivariate timeseries, collectively reflecting a total of 4 qualitatively different patterns of
464 dynamic correlations (i.e., 100 datasets reflecting each type of dynamic pattern: constant, random, ramping,
465 and event). Each timeseries comprised 10 zero-order features (dimensions) that varied over 300 timepoints.
466 After applying our dynamic correlation estimation procedure, this yielded a 100-dimensional timeseries of
467 first-order features that could then be used to estimate dynamic second-order correlations. (We chose to
468 use $K = 10$ zero-order features for our higher order simulations in order to put the accuracy computations
469 displayed in Figs. 2 and 3 on a roughly even footing.)

470 **Functional neuroimaging data collected during story listening**

471 We examined an fMRI dataset collected by³⁶ that the authors have made publicly available at arks.princeton.edu/ark:/88435/ds
472 The dataset comprises neuroimaging data collected as participants listened to an audio recording of a story
473 (intact condition; 36 participants), listened to temporally scrambled recordings of the same story (17 partici-
474 pants in the paragraph-scrambled condition listened to the paragraphs in a randomized order and 36 in the
475 word-scrambled condition listened to the words in a randomized order), or lay resting with their eyes open
476 in the scanner (rest condition; 36 participants). Full neuroimaging details may be found in the original paper
477 for which the data were collected³⁶. Procedures were approved by the Princeton University Committee on
478 Activities Involving Human Subjects, and by the Western Institutional Review Board (Puyallup, WA). All
479 subjects were native English speakers with normal hearing and provided written informed consent.

480 **Hierarchical topographic factor analysis (HTFA).** Following our prior related work, we used HTFA¹¹
481 to derive a compact representation of the neuroimaging data. In brief, this approach approximates the
482 timeseries of voxel activations (44,415 voxels) using a much smaller number of radial basis function (RBF)
483 nodes in this case, 700 nodes, as determined by an optimization procedure described by¹¹. This provides
484 a convenient representation for examining full-brain network dynamics. All of the analyses we carried
485 out on the neuroimaging dataset were performed in this lower-dimensional space. In other words, each
486 participant's data matrix, \mathbf{X}_0 , was a number-of-timepoints by 700 matrix of HTFA-derived factor weights
487 (where the row and column labels were matched across participants). Code for carrying out HTFA on fMRI
488 data may be found as part of the BrainIAK toolbox⁸⁸, which may be downloaded at brainiak.org.

489 **Temporal decoding**

490 We sought to identify neural patterns that reflected participants' ongoing cognitive processing of incoming
491 stimulus information. As reviewed by³⁶, one way of homing in on these stimulus-driven neural patterns
492 is to compare activity patterns across individuals (e.g., using ISFC analyses). In particular, neural patterns
493 will be similar across individuals to the extent that the neural patterns under consideration are stimulus-
494 driven, and to the extent that the corresponding cognitive representations are reflected in similar spatial
495 patterns across people also see⁵⁵. Following this logic, we used an across-participant temporal decoding test
496 developed by¹¹ to assess the degree to which different neural patterns reflected ongoing stimulus-driven
497 cognitive processing across people (Fig. 10). The approach entails using a subset of the data to train a
498 classifier to decode stimulus timepoints (i.e., moments in the story participants listened to) from neural
499 patterns. We use decoding (forward inference) accuracy on held-out data, from held-out participants, as a
500 proxy for the extent to which the inputted neural patterns reflected stimulus-driven cognitive processing in
501 a similar way across individuals.

502 **Forward inference and decoding accuracy**

503 We used an across-participant correlation-based classifier to decode which stimulus timepoint matched
504 each timepoint's neural pattern (Fig. 10). We first divided the participants into two groups: a template group,
505 $\mathcal{G}_{\text{template}}$ (i.e., training data), and a to-be-decoded group, $\mathcal{G}_{\text{decode}}$ (i.e., test data). We used Equation 7 to
506 compute a DISFC matrix for each group ($\bar{\mathbf{C}}_{\text{template}}$ and $\bar{\mathbf{C}}_{\text{decode}}$, respectively). We then correlated the rows of
507 $\bar{\mathbf{C}}_{\text{template}}$ and $\bar{\mathbf{C}}_{\text{decode}}$ to form a number-of-timepoints by number-of-timepoints decoding matrix, Λ . In this
508 way, the rows of Λ reflected timepoints from the template group, while the columns reflected timepoints
509 from the to-be-decoded group. We used Λ to assign temporal labels to each row $\bar{\mathbf{C}}_{\text{decode}}$ using the row of
510 $\bar{\mathbf{C}}_{\text{template}}$ with which it was most highly correlated. We then repeated this decoding procedure, but using
511 $\mathcal{G}_{\text{decode}}$ as the template group and $\mathcal{G}_{\text{template}}$ as the to-be-decoded group. Given the true timepoint labels (for
512 each group), we defined the decoding accuracy as the average proportion of correctly decoded timepoints,
513 across both groups. We defined the relative decoding accuracy as the difference between the decoding
514 accuracy and chance accuracy (i.e., $\frac{1}{T}$).

515 **Feature weighting and testing**

516 We sought to examine which types of neural features (i.e., activations, first-order dynamic correlations, and
517 higher-order dynamic correlations) were informative to the temporal decoders. Using the notation above,
518 these features correspond to $\mathbf{X}_0, \mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3$, and so on.

519

[Figure 10 about here.]

520 One challenge to fairly evaluating high-order correlations is that if the kernel used in Equation 4 is
 521 wider than a single timepoint, each repeated application of the equation will result in further temporal
 522 blur. Because our primary assessment metric is temporal decoding accuracy, this unfairly biases against
 523 detecting meaningful signal in higher-order correlations (relative to lower-order correlations). We attempted
 524 to mitigate temporal blur in estimating each \mathbf{X}_n by using a Dirac δ function kernel (which places all of its
 525 mass over a single timepoint; Fig. 9b, 10a) to compute each lower-order correlation ($\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n-1}$). We
 526 then used a new (potentially wider, as described below) kernel to compute \mathbf{X}_n from \mathbf{X}_{n-1} . In this way,
 527 temporal blurring was applied only in the last step of computing \mathbf{X}_n . We note that, because each \mathbf{X}_n is a
 528 low-dimensional representation of the corresponding \mathbf{Y}_n , the higher-order correlations we estimated reflect
 529 true correlations in the data with lower-fidelity than estimates of lower-order correlations. Therefore, even
 530 after correcting for temporal blurring, our approach is still biased against finding meaningful signal in
 531 higher-order correlations.

532 After computing each $\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_{n-1}$ for each participant, we divided participants into two equally sized
 533 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 $\mathcal{G}_{\text{train}_1}$
 534 and $\mathcal{G}_{\text{train}_2}$. We then computed Λ (temporal correlation) matrices for each type of neural feature, using $\mathcal{G}_{\text{train}_1}$
 535 and $\mathcal{G}_{\text{train}_2}$. This resulted in $n + 1$ Λ matrices (one for the original timeseries of neural activations, and one
 536 for each of n orders of dynamic correlations). Our objective was to find a set of weights for each of these
 537 Λ matrices such that the weighted average of the $n + 1$ matrices yielded the highest decoding accuracy.
 538 We used quasi-Newton gradient ascent⁸⁹, using decoding accuracy (for $\mathcal{G}_{\text{train}_1}$ and $\mathcal{G}_{\text{train}_2}$) as the objective
 539 function to be maximized, to find an optimal set of training data-derived weights, $\phi_{0,1,\dots,n}$, where $\sum_{i=0}^n \phi_i = 1$
 540 and where $\phi_i \geq 0 \forall i \in [0, 1, \dots, n]$.

541 After estimating an optimal set of weights, we computed a new set of $n + 1$ Λ matrices correlating the
 542 DISFC patterns from $\mathcal{G}_{\text{train}}$ and $\mathcal{G}_{\text{test}}$ at each timepoint. We use the resulting decoding accuracy of $\mathcal{G}_{\text{test}}$
 543 timepoints (using the weights in $\phi_{0,1,\dots,n}$ to average the Λ matrices) to estimate how informative the set of
 544 neural features containing up to n^{th} order correlations were.

545 We used a permutation-based procedure to form stable estimates of decoding accuracy for each set of
 546 neural features. In particular, we computed the decoding accuracy for each of 10 random group assignments
 547 of $\mathcal{G}_{\text{train}}$ and $\mathcal{G}_{\text{test}}$. We report the mean accuracy (along with 95% confidence intervals) for each set of neural
 548 features.

549 **Identifying robust decoding results**

550 The temporal decoding procedure we use to estimate which neural features support ongoing cognitive
551 processing is governed by several parameters. In particular, Equation 4 requires defining a kernel function,
552 which can take on different shapes and widths. For a fixed set of neural features, each of these parameters
553 can yield different decoding accuracies. Further, the best decoding accuracy for a given timepoint may be
554 reliably achieved by one set of parameters, whereas the best decoding accuracy for another timepoint might
555 be reliably achieved by a different set of parameters, and the best decoding accuracy across all timepoints
556 might be reliably achieved by still another different set of parameters. Rather than attempting to maximize
557 decoding accuracy, we sought to discover the trends in the data that were robust to classifier parameters
558 choices. Specifically, we sought to characterize how decoding accuracy varied (under different experimental
559 conditions) as a function of which neural features were considered.

560 To identify decoding results that were robust to specific classifier parameter choices, we repeated our
561 decoding analyses after substituting into Equation 4 each of a variety of kernel shapes and widths. We
562 examined Gaussian (Fig. 9c), Laplace (Fig. 9d), and Mexican Hat (Fig. 9e) kernels, each with widths of 5, 10,
563 20, and 50 samples. We then report the average decoding accuracies across all of these parameter choices.
564 This enabled us to (partially) factor out performance characteristics that were parameter-dependent, within
565 the set of parameters we examined.

566 **Reverse inference**

567 The dynamic patterns we examined comprise high-dimensional correlation patterns at each timepoint. To
568 help interpret the resulting patterns in the context of other studies, we created summary maps by computing
569 the across-timepoint average pairwise correlations at each order of analysis (first order, second order, etc.).
570 We selected the 10 strongest (absolute value) correlations at each order. Each correlation is between the
571 dynamic activity patterns (or patterns of dynamic high-order correlations) measured at two RBF nodes (see
572 Hierarchical Topographic Factor Analysis). Therefore, the 10 strongest correlations involved up to 20 RBF
573 nodes. Each RBF defines a spatial function whose activations range from 0 to 1. We constructed a map
574 of RBF components that denoted the endpoints of the 10 strongest correlations (we set each RBF to have a
575 maximum value of 1). We then carried out a meta analysis using Neurosynth³⁸ to identify the 10 terms most
576 commonly associated with the given map. This resulted in a set of 10 terms associated with the average
577 dynamic correlation patterns at each order.

⁵⁷⁸ **Data Availability**

⁵⁷⁹ The authors declare that the data supporting the findings of this study as well as the source data for
⁵⁸⁰ this paper are available at github.com/ContextLab/timecorr-paper/releases/tag/v0.4 and has been deposited
⁵⁸¹ in the Zenodo database under accession code <https://doi.org/10.5281/zenodo.5165253>. The source data
⁵⁸² underlying Figs. 2-6 and Supplementary Figs. S1-S9 are provided as a Source Data file. Source Data
⁵⁸³ are provided with the manuscript. The raw fMRI data are protected and are not available due to
⁵⁸⁴ data privacy laws. The processed fMRI dataset collected by³⁶ has been made publicly available⁹¹ at
⁵⁸⁵ arks.princeton.edu/ark:/88435/dsp015d86p269k.

⁵⁸⁶ **Code Availability**

⁵⁸⁷ All of our analysis code may be downloaded from github.com/ContextLab/timecorr-paper/releases/tag/v0.4.
⁵⁸⁸ We have also published a companion Python toolbox that may be downloaded from timecorr.readthedocs.io.

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⁵⁹⁶ **Author contributions**

⁵⁹⁷ 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. Writing:
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⁵⁹⁹ **Competing interests**

⁶⁰⁰ The authors declare no competing interests.

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780 **Figures**

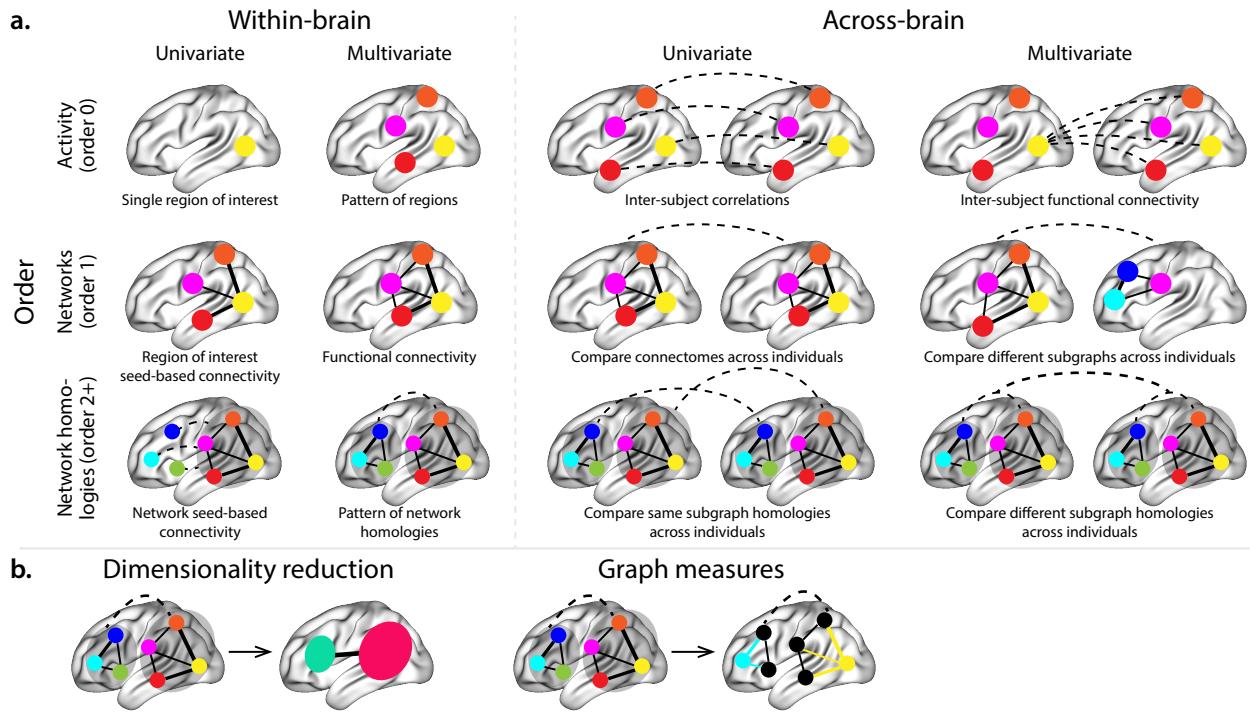


Figure 1: Neural patterns. a. A space of neural features. Within-brain analyses are carried out within a single brain, whereas across-brain analyses compare neural patterns across two or more individuals' brains. Univariate analyses characterize the activities of individual units (e.g., nodes, small networks, hierarchies of networks, etc.), whereas multivariate analyses characterize the patterns of activity 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 or non-linear transformations of the dimensions in the original space. Graph measures characterize each unit's participation in its associated network.

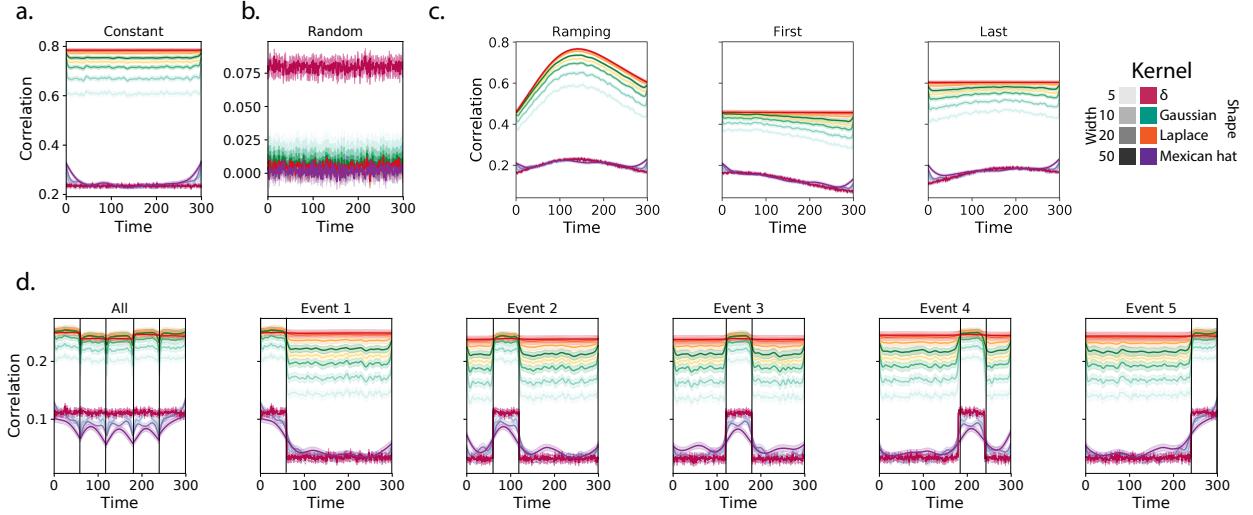


Figure 2: Recovering known dynamic first-order correlations from synthetic data. Each panel displays the average correlations between the vectorized upper triangles of the recovered correlation matrix at each timepoint and either the true underlying correlation at each timepoint or a reference correlation matrix. (The averages are taken across 100 different randomly generated synthetic datasets of each given category, each with $K = 50$ features and $T = 300$ timepoints.) Error ribbons denote 95% confidence intervals of the mean (taken across datasets). Different colors denote different kernel shapes, and the shading within each color family denotes the kernel width parameter. For a complete description of each synthetic dataset, see Synthetic data: simulating dynamic first-order correlations. **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 the 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. The vertical lines denote event boundaries. Source data are provided as a Source Data file.

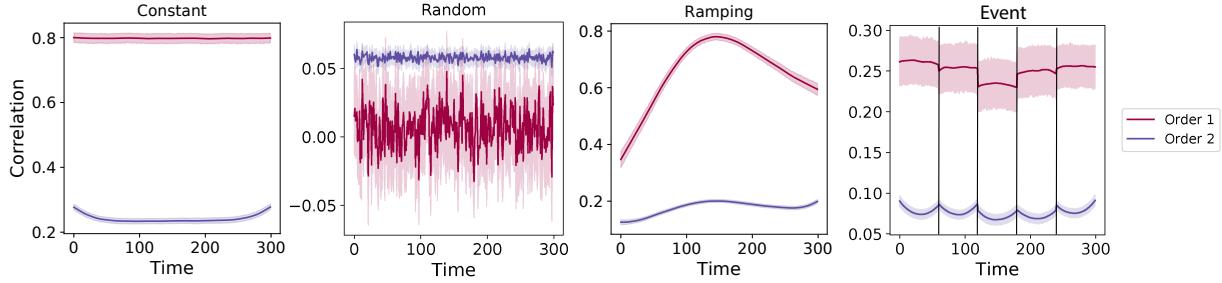


Figure 3: Recovery of simulated first-order and second-order dynamic correlations. Each panel displays the average correlations between the vectorized upper triangles of the recovered first-order and second-order correlation matrices and the true (simulated) first-order and second order correlation matrices at each timepoint and for each synthetic dataset. (The averages are taken across 100 different randomly generated synthetic datasets of each given category, each with $K = 10$ features and $T = 300$ timepoints.) Error ribbons denote 95% confidence intervals of the mean (taken across datasets). For a complete description of each synthetic dataset, see Synthetic data: simulating dynamic higher-order correlations. All estimates represented in this figure were computed using a Laplace kernel (width = 20). **Constant.** These datasets have stable (unchanging) underlying second-order correlation matrices. **Random.** These datasets are generated using a new independently drawn second-order correlation matrix at each timepoint. **Ramping.** These datasets are generated by smoothly varying the underlying second-order correlations between the randomly drawn correlation matrices at the first and last timepoints. **Event.** These datasets are each generated using five randomly drawn second-order correlation matrices that each remain stable for a fifth of the total timecourse. The vertical lines denote event boundaries. Note that the “dips” and “ramps” at the boundaries of sharp transitions (e.g., the beginning and ends of the “constant” and “ramping” datasets, and at the event boundaries of the “event” datasets) are finite-sample effects that reflect the reduced numbers of samples that may be used to accurately estimate correlations at sharp boundaries. Source data are provided as a Source Data file.

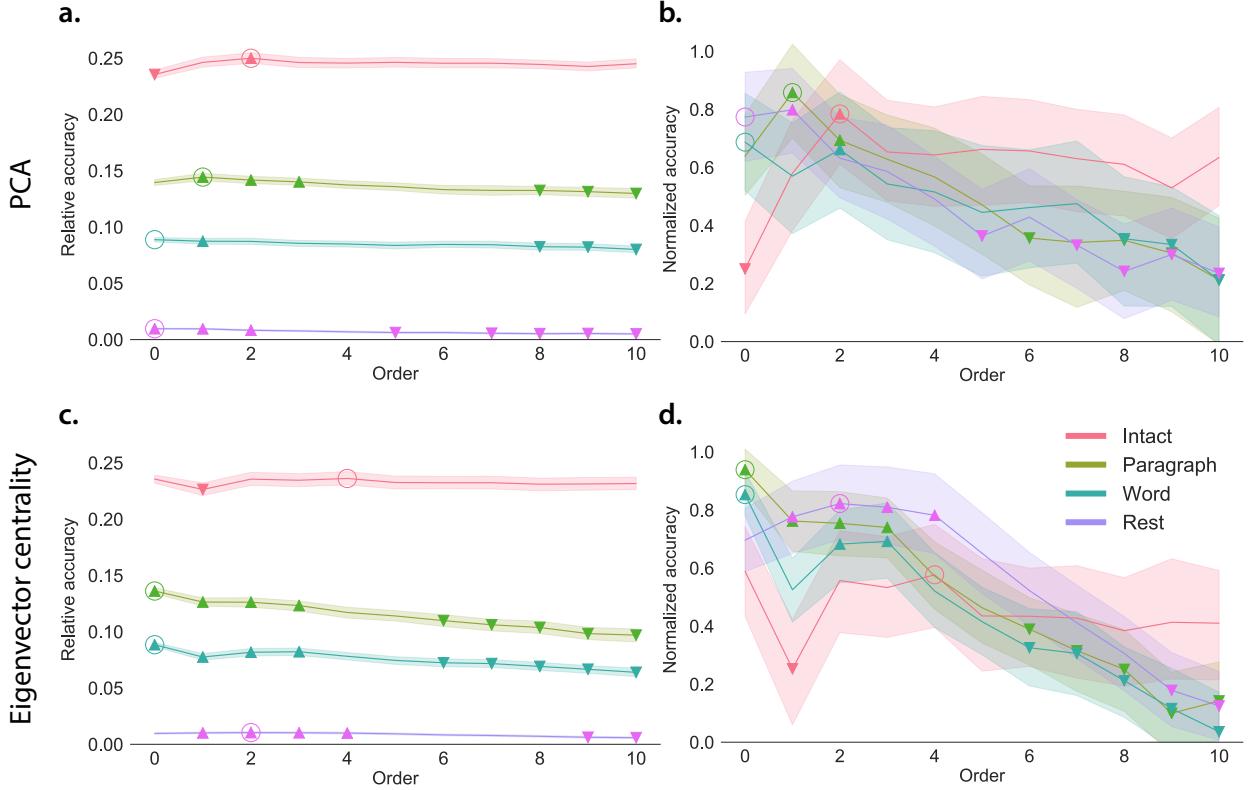


Figure 4: Across-participant timepoint decoding accuracy varies with correlation order and cognitive engagement.

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: $\frac{1}{400}$; these chance accuracies were subtracted from the observed accuracies to obtain the relative accuracies reported on the y-axis). The error ribbons denote 95% confidence intervals of the means 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 (upward facing) or lower (downward facing) decoding accuracy than the mean of all other features (via a two-tailed *t*-test, thresholded at $p < 0.05$). Figure 5 displays additional comparisons between the decoding accuracies achieved using different sets of neural features. The circled values represent the maximum decoding accuracy within each experimental condition.

b. Normalized timepoint 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 of the mean).

c. Timepoint 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 timepoint 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. See Figures S1 and S2 for decoding results broken down by kernel shape and width, respectively. Source data are provided as a Source Data file.

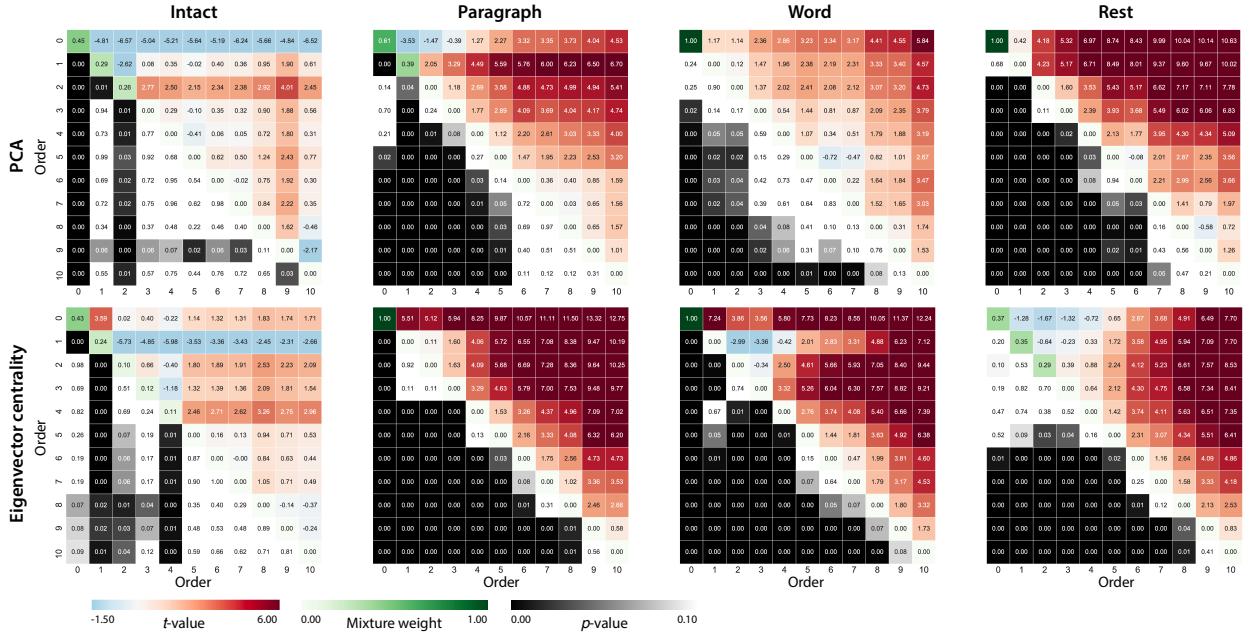


Figure 5: Statistical summary of decoding accuracies for different neural features. Each column of matrices displays decoding results for one experimental condition (intact, paragraph, word, and rest). We considered dynamic activity patterns (order 0) and dynamic correlations at different orders (order > 0). We used two-tailed t -tests to compare the distributions of decoding accuracies obtained using each pair of features. The distributions for each feature reflect the set of average decoding accuracies (across all kernel parameters), obtained for each random assignment of training and test groups. In the upper triangles of each matrix, warmer colors (positive t -values) indicate that the neural feature indicated in the given row yielded higher accuracy than the feature indicated in the given column. Cooler colors (negative t -values) indicate that the feature in the given row yielded lower decoding accuracy than the feature in the given column. The lower triangles of each map denote the corresponding p -values for the t -tests. The diagonal entries display the relative average optimized weight given to each type of feature in a decoder that included all feature types (see Feature weighting and testing). Source data are provided as a Source Data file.

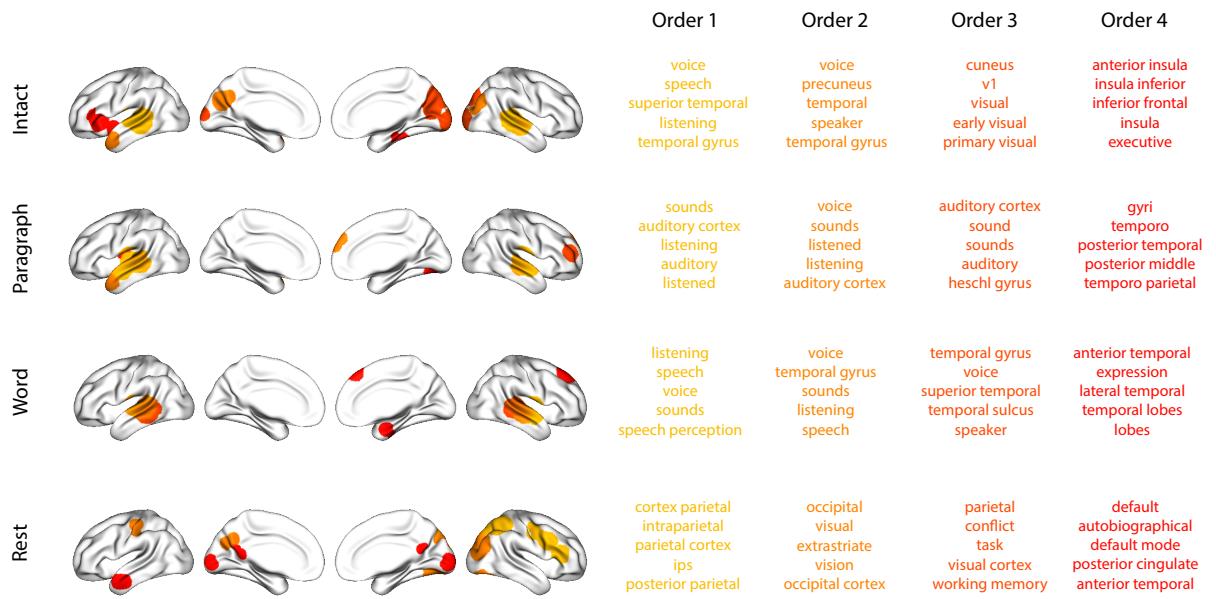


Figure 6: Top terms associated with the most strongly correlated nodes at each order. Each color corresponds to one order of inter-subject functional correlations. To calculate the dynamic correlations, eigenvector centrality has been used to project the high-dimensional patterns of dynamic correlations onto a lower-dimensional space at each previous order, which allows us to map the brain regions at each order by retaining the features of the original space. The inflated brain plots display the locations of the endpoints of the 10 strongest (absolute value) correlations at each order, thresholded at 0.999, and projected onto the cortical surface⁹⁰. The lists of terms on the right display the top five Neurosynth terms³⁸ 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: Fig. S5; paragraph: Fig. S6; word: Fig. S7; rest: Fig. S8). Source data are provided as a Source Data file.

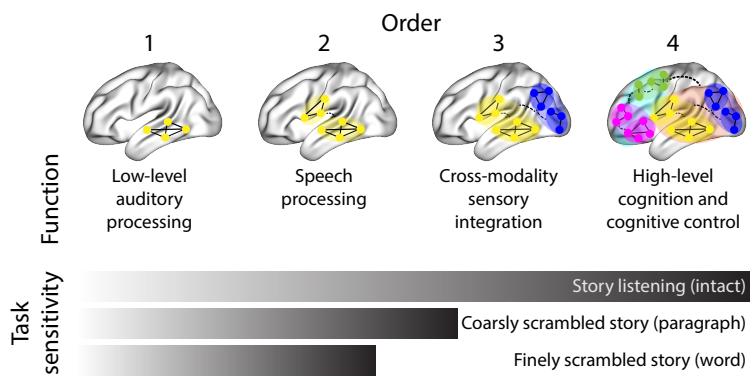


Figure 7: Proposed high-order network dynamics underlying high-level cognition during story listening. Schematic depicts higher orders of network interactions supporting higher-level aspects of cognitive processing. When tasks evoke richer, deeper, and/or higher-level processing, this is reflected in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

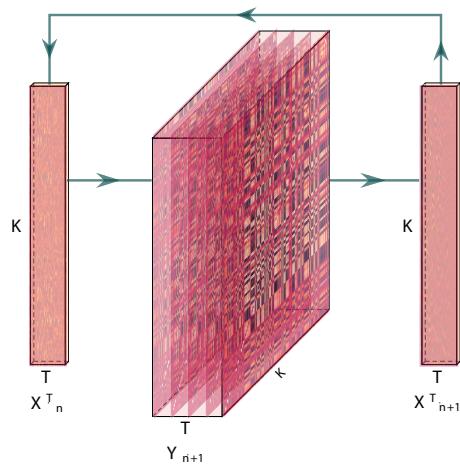


Figure 8: Estimating dynamic high-order correlations. Given a T by K matrix of multivariate timeseries data, \mathbf{X}_n (where $n \in \mathbb{N}, n \geq 0$), we use Equation 4 to compute a timeseries of K by K correlation matrices, \mathbf{Y}_{n+1} . We then approximate \mathbf{Y}_{n+1} with the T 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{X}_n and \mathbf{X}_{n+1} are displayed in the figure for compactness.

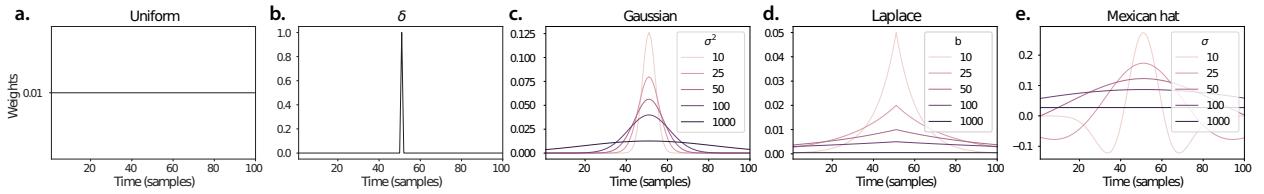


Figure 9: Examples of kernel functions. Each panel displays per-timepoint weights for a kernel centered at $t = 50$, evaluated at 100 timepoints ($\tau \in [1, \dots, 100]$). **a. Uniform kernel.** The weights are timepoint-invariant; observations at all timepoints are weighted equally, and do not change as a function of τ . This is a special case kernel 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.

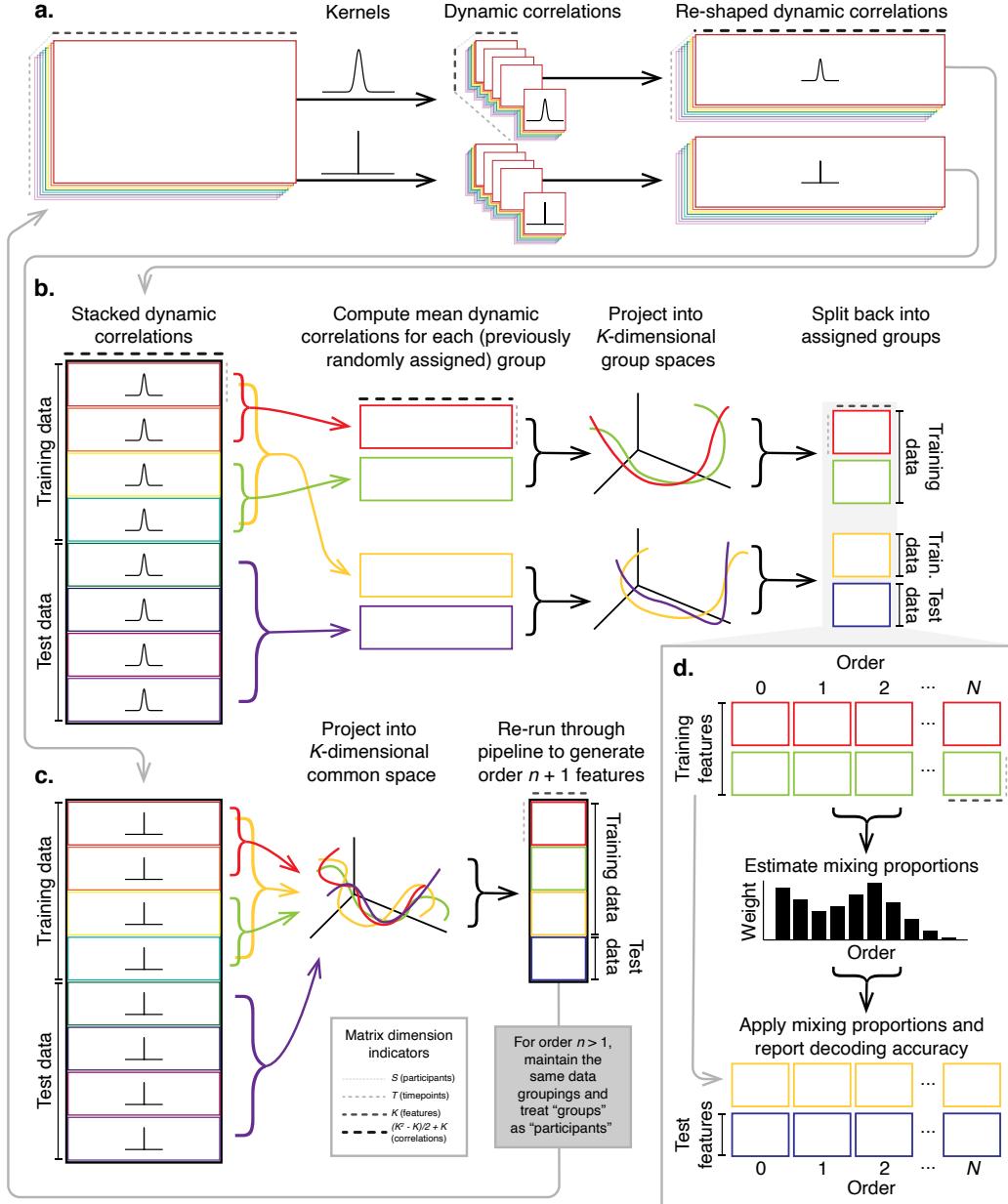


Figure 10: Decoding analysis pipeline. **a. Computing dynamic correlations from timeseries data.** Given a timeseries of observations as a $T \times K$ matrix (or a set of S such matrices), we use Equation 4 to compute each participant's DISFC (relative to other participants in the training or test sub-group, as appropriate). We repeat this process twice—once using the analysis kernel (shown here as a Gaussian in the upper row of the panel), and once using a δ function kernel (lower row of the panel). **b. Projecting dynamic correlations into a lower-dimensional space.** We project the training and test data into K -dimensional spaces to create compact representations of dynamic correlations at the given order (estimated using the analysis kernel). **c. Kernel trick.** We project the dynamic correlations computed using a δ function kernel into a common K -dimensional space. These low-dimensional embeddings are fed back through the analysis pipeline in order to compute features at the next-highest order. **d. Decoding analysis.** We split the training data into two equal groups, and optimize the feature weights (i.e., dynamic correlations at each order) to maximize decoding accuracy. We then apply the trained classifier to the (held-out) test data.