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Hao-Ting Wang[1], Danilo Bzdok [2,3,4], Daniel Margulies[5], Cameron Craddock[6], Michael Milham[6], Elizabeth Jefferies [1] & Jonathan Smallwood[1] .

[1] Department of Psychology, The University of York, Heslington, York, England.

[2] Department of Psychiatry, Psychotherapy and Psychosomatics, RWTH Aachen University, Germany

[3]JARA-BRAIN, Jülich-Aachen Research Alliance, Germany

[4]Parietal team, INRIA, Neurospin, bat 145, CEA Saclay, 91191 Gif-sur-Yvette, France

[5] Neuroanatomy and Connectivity Group, Max Plank Institute for Cognition and Brain Sciences, Leipzig, Germany.

[6] Center for Biomedical Imaging and Neuromodulation, Nathan S. Kline Institute for Psychiatric Research, New York State Office of Mental Health

Address for correspondence:

Hao-Ting Wang, Department of Psychology, The University of York, Heslington, York, England, UK.

Email: haoting.wang@york.ac.uk

1 **Abstract**

2   Contemporary cognitive neuroscience recognises unconstrained processing varies

3 across individuals, describing variation in meaningful attributes, such as intelligence. It may

4 also have links to patterns of on-going experience. This study examined whether dimensions

5 of population variation in different modes of unconstrained processing can be described by the

6 associations between patterns of neural activity and self-reports of experience during the same

7 period. We selected 258 individuals from a publicly available data set who had measures of

8 resting-state functional magnetic resonance imaging, and self-reports of experience during the

9 scan. We used machine learning to determine patterns of association between the neural and

10 self-reported data, finding variation along four dimensions. 'Purposeful' experiences were

11 associated with lower connectivity - in particular default mode and limbic networks were less

12 correlated with attention and sensorimotor networks. 'Emotional' experiences were associated

13 with higher connectivity, especially between limbic and ventral attention networks.

14 Experiences focused on themes of 'personal importance' were associated with reduced

15 functional connectivity within attention and control systems. Finally, visual experiences were

16 associated with stronger connectivity between visual and other networks, in particular the

17 limbic system. Some of these patterns had contrasting links with cognitive function as assessed

18 in a separate laboratory session - purposeful thinking was linked to greater intelligence and

19 better abstract reasoning, while a focus on personal importance had the opposite relationship.

20 Together these findings are consistent with an emerging literature on unconstrained states and

21 also underlines that these states are heterogeneous, with distinct modes of population variation

22 reflecting the interplay of different large-scale networks.

23

1 Introduction

Unconstrained processing reflects important population level variation in measures of cognition, affect, and demographic / lifestyle factors. Psychological studies show that almost a third of on-going thought is unconstrained by events in the here-and-now (Killingsworth & Gilbert, 2010) with important links to cognitive and affective processing (Mooneyham & Schooler, 2013). In neuroscience, metrics defined from the brain during wakeful rest, describe the organisation of neural function at both the micro and macro scale (Glasser et al., 2016; Margulies et al., 2016). They also reflect individual differences in cognitive function (Finn et al., 2015), psychiatric conditions (Nooner et al., 2012) and demographic / lifestyle factors (Smith et al., 2015). These findings establish unconstrained neuro-cognitive processing as a core element of human cognition, highlighting the need to formally understand the underlying neural architecture, and the associated patterns of experience.

One perspective on unconstrained processing emphasises the role of memory, with contributions of conceptual and episodic representations to on-going thought (Binder, Desai, Graves, & Conant, 2009; Gusnard, Raichle, & Raichle, 2001). Psychological studies have shown patterns of unconstrained processing have links with memory retrieval, creativity and planning (Baird et al., 2012; Leszczynski et al., 2017; Medea et al., 2016; Poerio et al., 2017). Such evidence raises the possibility that episodic representations anchored in the medial temporal lobe (Moscovitch, Cabeza, Winocur, & Nadel, 2016) or conceptual representation anchored in anterior temporal lobe (Ralph, Jefferies, Patterson, & Rogers, 2017) contribute to on-going thought (Smallwood et al., 2016). It is hypothesised that these systems contribution to unconstrained states may be linked to the ability for these regions to become functionally decoupled from systems more directly involved in action and perception, allowing them to operate in an offline manner (Smallwood, 2013). This process of decoupling may also be important in neural systems closely allied to those involved in memory – the default mode network (Raichle et al., 2001). These regions of transmodal cortex are relatively distant in functional and structural space from systems involved in perception and action, potentially facilitating their role in stimulus independent aspects of cognition (Buckner & Krienen, 2013; Margulies et al., 2016; Mesulam, 1998). Together these 'representational' accounts of unconstrained processing highlight default mode and limbic networks as important candidate neural systems, especially when decoupled from systems directly involved in perception and action.

Alternative perspectives on unconstrained thought emerge from links between types of on-going experience and problems maintaining a task relevant goal in mind. This "executive-failure" view (Kane & McVay, 2012; McVay & Kane, 2010) takes as a starting point evidence that patterns of on-going thought, such as the experience of mind-wandering, are linked to problems on tasks including sustained attention (McVay & Kane, 2009) and measures of general aptitude and executive control (Mrazek et al., 2012). Task-based neuroimaging investigations highlight a network of regions that increase their activity across many different task situations - so called multiple demand regions (Duncan, 2010). These regions broadly correspond to three well described intrinsic networks: ventral attention, dorsal attention, and frontal-parietal networks. Since these systems are important for the effective performance of many different tasks then dysregulation within these systems could reflect the hypothesised 'executive-failure' contribution to aspects of on-going thought (McVay & Kane, 2010; Weissman, Roberts, Visscher, & Woldorff, 2006).

Other aspects of unconstrained processing could reflect the importance of affective processes, or different modalities of processing. On-going thought is linked to mood state: Experimental inductions of mood (Smallwood, Fitzgerald, Miles, & Phillips, 2009; Smallwood & O'Connor, 2011), as well as natural fluctuations (Poerio, Totterdell, & Miles, 2013; Ruby, Smallwood, Engen, & Singer, 2013) impact on on-going thought. Contemporary accounts of emotional processing emphasise the role of limbic regions including the amygdala (Bzdok, Laird, Zilles, Fox, & Eickhoff, 2013; Lindquist, Wager, Kober, Bliss-Moreau, & Barrett, 2012) and anterior aspects the insula (Touroutoglou, Hollenbeck, Dickerson, & Barrett, 2012), suggesting these regions may be important in determining affective aspects of on-going thought. Psychological studies of on-going thought also suggest that another important dimension of unconstrained processing may reflect the different modalities of processing (Konishi, Brown, Battaglini, & Smallwood, 2017; Smallwood et al., 2016). It has been shown, for example, that the visual system plays an important role in the expression of visual imagery (Ganis, Thompson, & Kosslyn, 2004; Kosslyn, Ganis, & Thompson, 2001). Recent work has extended this evidence to shown patterns of activity with visual regions are linked to the emergence of visual, non-verbal, elements of on-going thought (Raij & Riekki, 2017). It is also possible that sensorimotor processes may be implicated in language processing during unconstrained processing, given that a role for these regions in langauge processing extends beyond production (Bzdok et al., 2016; Pulvermuller, 2010; Pulvermuller & Fadiga, 2010).

2 Current study

Our study aimed to identify patterns of intrinsic connectivity associated with different patterns of unconstrained states and examines their neuro-cognitive features from the perspectives outlined above. We used a large publicly available dataset, containing measures of resting-state functional magnetic resonance imaging (fMRI), and an accompanying self-report instrument describing cognition experienced during the resting-state (Gorgolewski et al., 2014; Nooner et al., 2012). We previously explored the relationships between patterns of on-going thought and measures of neural activity, such as the fractional amplitude of low frequency oscillations, as well as the regional homogeneity of neural activity, in a sub sample of this data set (Gorgolewski et al., 2014). In this study we focused on connectivity, we applied sparse canonical correlation analysis (SCCA) to obtain a conjoined decomposition of self-reports of experience with matrices of whole brain connectivity data. This analysis produces multivariate patterns that reflect dimensions of variation that are mutually constrained by both brain and experience. In this way we capitalize on the fact that self-reports of experience during scanning and descriptions of on-going neural processing provide complementary descriptions of unconstrained cognition. Our analysis, therefore, helps define, at a population level, the shared links between brain patterns and different types of experience. It is important to note that this approach necessarily conflates state and trait related aspects of any brain-experience associations that are identified in this manner, and this aspect of our design should be borne in mind when interpreting our results. As our analytic approach respects the multivariate nature of brain and behaviour space, it can accommodate complex many-to-many relationships between patterns of connectivity and self-reports, and therefore is sensitive to the possibility of complex relationships in the underlying data. We took two steps to explore the robustness of the components that our study identifies. First, we use permutation testing to examine the extent to which our components are different from those that would be achieved based on a null distribution. Second we established whether these neuro-cognitive dimensions are associated with performance on a battery of available cognitive tasks, including measures of executive control and intelligence. When interpreting the results produced through our analysis it is important to give greater weight to components that show evidence of robustness in both comparisons.

We use the dimensions our analysis produces, and their links with cognitive function to evaluate the perspectives on unconstrained thought outlined earlier. 'Representational' accounts emphasise links with neural systems involved in memory, such as the limbic system,

121 and regions of transmodal cortex, such as the default mode network. They highlight states with

122 lower levels of functional communication between these regions and those more directly

123 involved in external action. In contrast, 'executive-failure' accounts emphasise dysregulation

124 in attention and control networks as contributing to patterns of on-going thought that are linked

125 to problems in domain general task performance. Affective accounts highlight limbic regions

126 as important hubs in aspects of on-going thoughts linked to emotion. Finally, modality specific

127 influences on unconstrained thought may depend on information codes represented in regions

128 that specialise in that particular types of information, such as a role of visual cortex in

129 experiences dominated by images. Notably, some views lead to dissociable predictions with

130 respect to cognitive performance. For example, executive-failure accounts predict patterns of

131 thoughts linked to worse performance on measures of cognitive function, while

132 representational accounts makes the alternative prediction.

133 3 Materials and Methods

134 3.1 Participant

135 We analysed 258 participants (females = 162; age range *18 – 55*, *M* = 34.97, *SD* =

136 12.24) obtained from the enhanced Nathan Kline Institute-Rockland sample (NKI-RS;

137 http://fcon_1000.projects.nitrc.org/indi/enhanced/). Full details of the acquisition of this

138 sample can be found in Nooner et al., 2012. We selected participants between 18 and 55

139 years old as our sample, this choice allowed us to maximise the cohesive nature of our

140 sample. All the participants have the MRI data and less than 5 missing data points among the

141 selected assessments.

142 3.2 Cognitive measures and Questionnaires

143 Based on prior studies examining the links between spontaneous thought and cognitive

144 performance (see Mooneyham & Schooler, 2013) we selected established neuropsychological

145 measures linked to executive control, abstract reasoning and intelligence. The meaures

146 included the Delis-Kaplan Executive Function System (D-KEFS; Swanson, 2005), Wechsler

147 Abbreviated Scale of Intelligence (WASI-II; Wechsler, 1999), and Wechsler Individual

148 Achievement Test – Second Edition Abbreviated (WIAT-IIA; Wechsler, 2005). In D-KEFS

149 we selected the tower test (move accuracy ratio), colour-word interference test (errors

150 inhibition/switching), verbal fluency test (letter fluency - category fluency), design fluency

test (design accuracy), trail making test (sequencing errors score + set-loss errors score + time-discontinue errors score), and the proverb test (a measure of abstract semantic reasoning). We used the rescaled score ($M = 10$, $SD = 3$) in our analysis. Tasks measures that reflected error rates (i.e. the colour-word interference test and trail making test) were reversed, so that high rescaled scores indicated better task performance. All the scores were transformed to z-scores.

3.3   On-going cognition measure

The New York Cognition Questionnaire (NYC-Q) is a self-report tool used to assess the thoughts experienced at rest (Gorgolewski et al., 2014; Sanders, Wang, Schooler, & Smallwood, 2017). It assesses thoughts and feelings experienced during the resting-state period. The first section contains 23 questions about the content of thought. These questions covers the temporal, social, emotional aspects of spontaneous thoughts that have been shown to be important by prior studies (e.g. Ruby et al., 2013). Participants rated each question on a scale of 1 (Completely did not describe my thoughts) to 9 (Completely did describe my thoughts). The second section contains 8 questions about the forms thoughts take, capturing aspects of experience such as modality and detail associated with experience that prior studies suggest as important for spontaneous thoughts (Smallwood et al., 2016). Participants rated each question on a scale of 1 (Completely did not characterise my experience) to 9 (Completely did characterise my experience). In the current study we analysed the two sections together to provide single solutions that combined information on both the content form of experience. The full list of questions and the corresponding labels are presented in Table 1. The questionnaire was administrated once after the resting-state scan in order to assess experiences during the scanning session. For the full details of the NYC-Q, please refer to Gorgolewski et al., 2014. We have placed the questionnaire measure used in this study along with an example self-report collection task on GitHub at the following address: https://github.com/htwangtw/restingstate_thoughtreports.

Table 1 The New York Cognition Questionnaire (NYC-Q)

#	Questions	Labels
Q01	I thought about things I am currently worried about	Concerns
Q02	I thought about people I have just recently met	People
Q03	I thought of people I have known for a long time (friends)	Friend

Q04	I thought about members of my family	Family
Q05	I thought about an event that took place earlier today	Today - Past
Q06	I thought about an interaction I may possibly have in the future	Social - Future
Q07	I thought about an interaction with somebody that took place in the past	Social - Past
Q08	I thought about something that happened at a place very close to me	Near Location
Q09	I thought about something that made me feel guilty	Guilt
Q10	I thought about an event that may take place later today	Today - Plan
Q11	I thought about something that happened in the recent past (last couple of days but not today)	Recent Past
Q12	I thought about something that happened a long time ago in the past	Distant Past
Q13	I thought about something that made me angry	Anger
Q14	I thought about something that made me happy	Happiness
Q15	I thought about something that made me cheerful	Cheerfulness
Q16	I thought about something that made me calm	Calm
Q17	I thought about something that made me sad	Sadness
Q18	I thought about something that is important to me	Importance
Q19	I thought about something that could still happen today	Today - Future
Q20	I thought about something that may take place in the distant future	Distant Future
Q21	I thought about something that could take place in the near future (days or weeks but not today)	Near Future
Q22	I thought about personal worries	Worries
Q23	I thought about something that happened in a place far away from where I am now	Distant Location
Q24	In the form of images:	Image
Q25	In the form of words:	Words
Q26	Like an inner monologue or audiobook:	Monologue
Q27	Like a television program or film:	Film
Q28	Had a strong and consistent personal narrative:	Narrative
Q29	Had a clear sense of purpose:	Purpose
Q30	Vague and non-specific:	Vague
Q31	Fragmented and disjointed:	Fragment

3.4 MR data processing

3.4.1 Resting-state fMRI.

We used resting-state fMRI to describe the general functional organisation of the brain. We selected resting-state multiband functional magnetic resonance imaging (R-mfMRI; TR = 1400msec; voxel size = 2mm isotropic; duration = 10 minutes) for our analysis. Functional and structural data were pre-processed using Configurable Pipeline for the Analysis of Connectomes (C-PAC; https://fcp-indi.github.io/) to interface with FMRIB's Software Library (FSL version 5.0, www.fmrib.ox.ac.uk/fsl). Individual FLAIR and T1 weighted structural brain images were extracted using Brain Extraction Tool (BET). Structural images were linearly registered to the MNI-152 template using FMRIB's Linear Image Registration Tool (FLIRT). The resting-state functional data were pre-processed and analysed using the FMRI Expert Analysis Tool (FEAT). X, Y, Z displacement and the three axis rotations were used to calculate the mean frame displacement (FD), characterising movement of each participant during the scanning session (Power et al., 2014). Mean of the absolute values for FD were later used to account for subject specific head motion. No global signal regression was applied. The individual subject analysis involved: motion correction using MCFLIRT; slice-timing correction using Fourier space time series phase-shifting; spatial smoothing using a Gaussian kernel of FWHM 6 mm; bandpass filtering (0.1 Hz < f < 0.009 Hz); six motion parameters (as estimated by MCFLIRT) regressed out; cerebrospinal fluid and white matter signal regressed out (top five PCA components, CompCor method).

3.4.2 Connectivity matrices

To describe the functional architecture of the whole brain, we transformed the resting-state BOLD time series into connection strength values of the different networks for each participant. The whole brain parcellation was obtained from connectivity-based functional parcellation created by Yeo and collegues (Yeo et al., 2011). The 7 network parcellation was used in the current study. We split the networks into two hemispheres and extracted clusters. Two voxels are considered connected only if they are adjacent within the same x, y, or z direction. This yielded 57 clusters from the Yeo 7 networks parcellation. The implementation of spatial clusters extraction was retrieved from python library Nilearn (Abraham et al., 2014; http://nilearn.github.io/, version 0.3.1). Next, we extracted and then averaged the time series of all voxels within each cluster to create a cluster specific time series. We used these time series to create region-to-region symmetrical correlation matrices representing the

210   correlations of the network signal that was computed for all the individual subjects. The off-
211   diagonal of each correlation matrix contained 1596 unique region-region connection strengths
212   (i.e., the upper or lower trinagle of the network covariance matrix). This approach provided a
213   measure of connection strength of the whole brain for each participant. Finally, Fisher's r-to-
214   z transformation was applied to each network covariance matrix.

3.5   Conjoint decomposition of functional connectomes and mind-wandering measures

3.5.1   Decomposition method

218   We performed a sparse canonical correlation analysis (SCCA; see Hastie, Tibshirani, &
219   Wainwright, 2015) on the functional connectomes and the NYC-Q reports, to yield latent
220   components that reflect multivariate patterns across neural organisation and experience (For
221   similar application, see Wang et al., 2017). SCCA maximised the linear correlation between
222   the low-rank projections of two sets of multivatiate data sets with sparse model to regularise
223   the decomposition solutions a process that helps maximise the interpretability of the results.
224   The regularisation function of choice is L_1 penalty, which produces 'sparse' coefficients,
225   meaning that the canonical vectors (i.e., translating from full variables to a data matrix's low-
226   rank components of variation) will contain a number of exactly zero elements. L_1
227   regularisation conducted (i) feature selection (i.e., select only relevant components) and (ii)
228   model estimation (i.e., determine what combination of components best disentangles the
229   neuro-cognitive relationship) in an identical process. This way we handle adverse behaviours
230   of classical linear models in high-dimensional data. A reliable and robust open-source
231   implementation of the SCCA method was retrieved as R package from CRAN (PMA,
232   penalized multivariate analysis, version 1.0.9, Witten, Tibshirani, & Hastie, 2009). The
233   amount of L_1 penalty for the functional connectomes and the NYC-Q reports were chosed by
234   cross-validation. The procedure is described below.
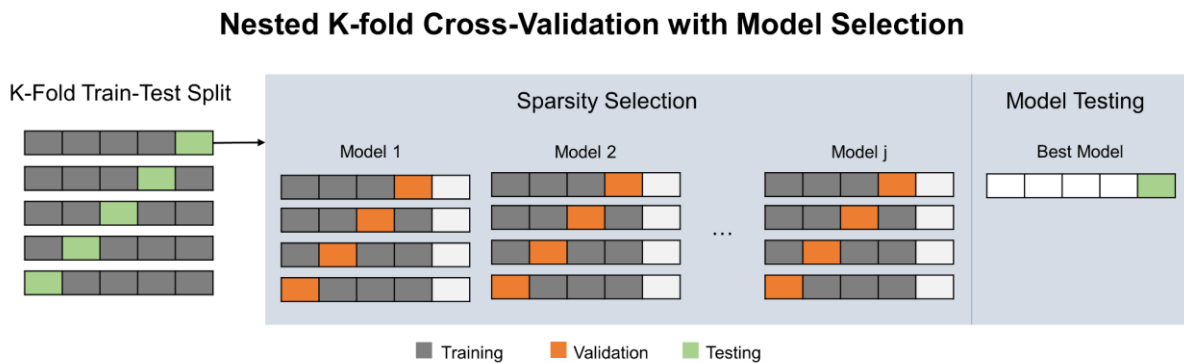
3.5.2   Model selection

236   We employed cross-validation (CV) to select the most useful model across population
237   samples and avoid overfitting (Bzdok & Yeo, 2017). The amount of the two L_1 penalty terms
238   for the functional connectomes and the NYC-Q reports, respectively, were chosen by a nested
239   K-fold CV, where the coefficient for the penalty were chosen using a grid search to maximise
240   the quality of CV objective metric. The objective metric of choice cumulative explained

variances. The explained variance of each latent compoent was calculated using the squared canonical correlation. High explained variance suggests a high pattern recovery rate between the two data set. The sparse assumption is fundamentally in conflict with the statistical goal of finding compontents with high explained variance. Therefore we decided the number of components in the model before searching for the best parameter.

We performed confound removal on functional connectomes and the NYC-Q reports as suggested by prior studies (Smith et al., 2015). We removed the effects of nuisance variables from the dataset. These confound variables were sex, age, and head motion indicated by Jenkinson's mean FD (Jenkinson, Bannister, Brady, & Smith, 2002). The removal steps was performed on the training set in each CV fold. We standardized the confound by calculating the z-score, and also squared the three confound measures to account for potentially nonlinear effects of these confounds. The 6 resulting confounds were regressed out of both data matrices. The implementation of the confound removal method (Friston et al., 1994) was retrieved from python library Nilearn (Abraham et al., 2014; http://nilearn.github.io/, version 0.3.1).

The number of latent components was determined by a preliminary analysis with no sparsity and calculated the explained variances for the two datasets (i.e., brain network correlations and questionnaire ratings). The explained variance increased with the number of components and growth stablised at 10 components. We selected the number of components based on the point where the tangent stablised. This led to a model of 4 components, and it accounted for a total of 78% of the variance in connection strength and 29% of the variance in the self-report data. Next, we determind the two coefficients for the L_1 penalty terms that was associated with the best model performance with 4 latent components. We searched for the best L_1 penalty values between 0.1 and 0.9 in 0.1 increments, which resulted in 81 set of paramters. For the nested K-Fold CV, we first separate the data into 5 consecutive folds after shuffling the data and retained one fold as the evaluation set (N $\sim= 50$); the other four folds were used as the development set. The development set was further separated into 5 folds for parameter selection and each fold (N $\sim=40$) was used as the validation set once. The model was estimated on the training folds with all parameter sets, and after completion, we trained the model with the winning parameter on the whole develpment set and the finally tested the performance on the independent, unseen evaluation set. We selected the final parameters according to the best performance on the evaluation set across all folds of the outer CV loop (**Figure 1**). This parameter set is used to train on the full development set and tested on the

274 evaluation set. The parameter grid search and k-fold CV was conducted by the

275 implementation in a Python library scikit-learn (Pedregosa et al., 2011; http://scikit-

276 learn.org/stable/, version 0.18.2). The detailed algorithm for selecting the penalty values are

277 presented in **Appendix: Nested K-Fold CV**.

278

Figure 1. A diagram of the nested k-fold cross-validation with model selection.

280 The model with the best test performance was selected as the final model. The final

281 model's sparsity coefficient are 0.8 (functional connectivity) and 0.5 (self-reports), and the

282 out-of-sample explained variance was 48%. We used the ensuing canonical vectors of the

283 winning SCCA model to compute the latent component scores. There are two sets of

284 canonical scores in a latent compoent, a weighted sum of variables forms the canonical

285 vectors. For each latent compoennt, we averaged the z-score of the canonical scores of the

286 connection strength and NYC-Q as the combined scores. These scores described the

287 summary of the experience with both the neural basis and the content reports.

3.6 Test of component robustness

289 After identifying the well performed components in compressing the brain-experience data,

290 we examined the robustness of the four components in two different ways. The permutation

291 test is a purely data-driven strategy that access the chance of discovering components in null

292 samples. We also leveraged the brain-experience components to explain the cognitive

293 functions, so that we can identify meaningful patterns by well-established cognitive

294 measurements.

3.6.1 Permutation test

296 We used permutation testing to assess the robustness of the components identified through

297 our analysis. We constructed a null distribution for each canonical component by holding the

298 functional connectivity data in place and randomising the row order of self-reports data. This
299 permutation scheme broke the link of individual differences in the dataset, therefore testing
300 the robustness of the components in the hypothetical population. By calculating the false-
301 discovery rate in the null distribution, we can conclude the possibility of discovering our
302 components by chance with the given penalty coefficients. Hypotheses that are accepted with
303 a 5% level of significance. In the current analyses we adopt the permutation test with the
304 FWE-corrected p-value by Smith and colleagues (2015) with data argumentation to increase
305 the size of the resampling datasets to 1000. The four components were compared to the first
306 sparse canonical correlation of the permuted sample. The low-rank components are more
307 relevant that the rest, therefore we yield more conservative p-value by comparing to the first
308 canonical correlation only. We performed 5000 permutation tests to get enough estimates for
309 4 decimal places.

310 **3.6.2   Group analysis**
311 To determine how patterns of unconstrained neuro-cognitive activity related to performance
312 on the battery of cognitive tests, we conducted an independent statistical analysis on the
313 identical subjects. A Type III multivariate multiple regression with Pillai's trace test was
314 applied to 4 individual scores for each of the latent components describing experience from
315 the SCCA were the independent variables, and the original 8 measures of cognitive
316 performance were the dependent variables that we hoped to described by the linear
317 combination of the latent components. Pillai's trace test is considered to be the most powerful
318 and robust statistic for general use (Huberty & Olejnik, 2006). The p-values reported were
319 based on Bonferroni correction. We also performed a principal components analysis (PCA) to
320 identify the patterns of covariance among the 8 measures of cognitive performance and
321 compressed the data. The relation between the principle score and the 4 brain-expereince
322 diemsnons identified through SCCA was examined in a linear regression model with Pillai's
323 trace test. The analysis was conducted in R (version 3.3.1). The multivariate multiple
324 regression was conducted in R (version 3.3.1) using function 'Manova' in R package 'car'
325 (companion to applied regression, version 2.1-5).

326 ## 3.7   Code availbility
327 The full analysis pipeline is freely avalible at https://github.com/htwangtw/patterns-of-
328 thought.

329

4 Results

4.1 Determining constituent categories of experience

We used Sparse Canonical Correlation Analysis (SCCA) to determine connectome-wide dimensions that describe common variance shared by descriptions of brain and experience. This took as input individual scores for the connections between each of the regions extracted from Yeo's 7 networks parcellation and the scores of each item of the New York Cognition Questionnaire (NYC-Q).

We applied SCCA with nested 5-fold CV as the model selection strategy. We obtained a model of 4 canonical components with penalty levels of 0.8 on the functional connectivity and 0.5 on the NYC-Q that indicated the best out-of-sample prediction on our data (see **3.5.2 Model Selection**). The canonical correlations of the 4 latent components were 0.28, 0.19, 0.16, and 0.07. The latent components yielded by the best model are presented in **Figure 2**. For the ease of presentation and interpretation, we summarized the components as network-network connectivity instead of 57-by-57 connectivity matrices. The heat maps describe the network-to-network correlations while the word clouds describe the loadings on the self-report items. The components in full and the heat map for the self-report items can be found in **Supplementary Materials.**

Component 1, describes patterns of reduced within network connectivity within all of the networks studied, with this pattern most prominent in the dorsal attention network. Between network connections are generally reduced, with the exception of visual to limbic. Sensorimotor was decoupled from all the other systems, and, in addition, the default and limbic were most decoupled from the attention networks. Experiential themes in Component 1 are dominated by themes related to deliberate planning with a verbal component (high loadings on "words", "monologue", "today-plan", "social-future", "purpose" and "deliberate"). We refer to this pattern of reports as reflecting thoughts with "purpose".

Component 2 is dominated by relatively higher within and between network connections. Connectivity within each network was strong with the exception of the limbic network. Between network connections were stronger, with this pattern most apparent in the connections between limbic and ventral attention. In addition, the visual network was strongly correlated with the other networks. This component is dominated by emotional responses (high loadings on "anger", "guilt", "cheerfulness" and "happiness") and social

content ("friends" and "people"). We refer to this pattern of reports as reflecting "emotional" experience.

Component 3 emphasises reduced connections both between and within networks. Within network connectivity is weakest for the dorsal and ventral attention networks. Edge-to-edge connections are low, with the ventral and dorsal attention and fronto-parietal networks showing reduced correlations with each other as well as the visual and sensorimotor systems. This component was characterised by themes linked to personal "importance" with social temporal contents ("distant future", "near future", "social past", "family" and "recent past"). We refer to this pattern of reports as reflecting "personal importance".

Component 4 has the most heterogeneous pattern of within and between network connectivity. It is associated with stronger connections within networks with the exception of the limbic system. In addition, the visual system was strongly connected to all other networks, with this pattern most apparent for the limbic network. In contrast, lower network-to-network connectivity was observed between the default mode and sensori-motor and attention networks. This component is characterised by experiential patterns reflecting a modality difference in experience, with the highest loadings on "images" and lowest on "inner monologue". We refer to this pattern of reports as describing "modality".
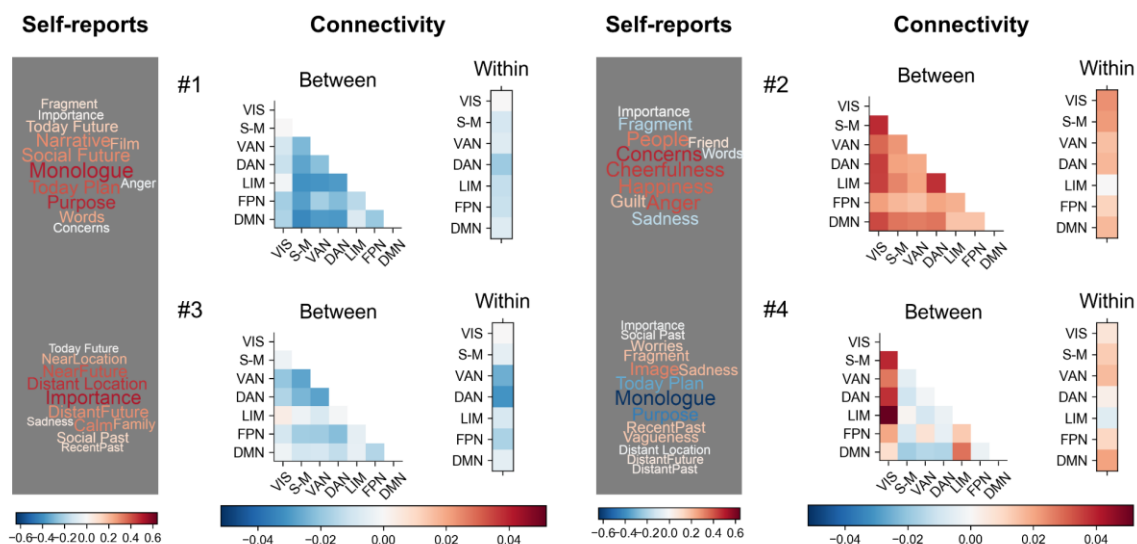
Figure 2. Unique neuro-cognitive dimensions of population variation revealed by sparse canonical correlation analysis of measures of whole brain connectivity and self-reported

381 **descriptions of on-going experience.** The heat map describes the canonical variate of the

382 network-to-network connectivity between different Yeo networks. The connectivity matrices

383 desribes the coeffiecents from the model, seperated into within and between network

384 relationships. The word clouds reflect the coeffiencts on the relevant self-report items. In

385 both cases the colour bars indicate the magnitudes of the coefficients. A detailed version of

386 the canonical variates and alternative presentation of the self-report coefficients can be found

387 in **Supplimentary Material Figure S1- S5**.

388 ## 4.2   The relationship between neuro-cognitive components and cognitive

389 ## function assessed in the laboratory

390 Having documented four neuro-cognitive dimensions, we next examined the robustness of

391 the components using two complementary approaches. We first used a permutation test to

392 identify the chance of discovering components in a null samples as employed by Smith and

393 colleagues (2015). The top three components passed the permutation test and the 4th

394 component showed variance that was similar to that produced in a null sample (Component 1

395 $p = 0.0002$; Component 2 $p = 0.0010$; Component 3 $p = 0.0204$, Component 4 $p = 0.998$, $\alpha =$

396 0.05). This analysis suggests that Components 1 – 3 are unlikely to have occurred by chance.

397 Component 4 may be a Type II error and so we discuss this component in only a limited

398 manner moving forward.

399 Our next test of the robustness of our components is whether they explained unique

400 patterns of expertise in our battery of cognitive tasks. We used multiple multivariate

401 regression model in which performance on the battery of selected tasks was the dependent

402 variables and the individual scores for each of the canonical components describing

403 experience from the SCCA were the independent variables. In this analysis two of the four

404 canonical components described significant variance in our battery of tasks at multivariate

405 level: Component 1 ($F(8, 246) = 2.21$, $p = .027$, $\eta^2_p = .067$) and Component 3 ($F(8, 246) =$

406 2.56, $p = .024$, $\eta^2_p = .068$).

407 In the univariate results of the significant component, Component 1 was linked to

408 good performance in proverb test ($\beta = 0.48$, $t(251) = 3.27$, $p = .006$, 95% CI [0.191 0.766])

409 and both fluid intelligent tests WASI ($\beta = 0.39$, $t(251) = 2.74$, $p = .033$, 95% CI [0.111

410 0.677]) and WIAT ($\beta = 0.45$, $t(251) = 3.15$, $p = .009$, 95% CI [0.167 0.724]). Component 3

411 showed a reversed pattern of the cognitive functions related to Component 1: proverb test (β

412 $= -0.45$, $t(251) = -0.14$, $p = .007$, 95% CI [-0.176 -0.727]); WASI ($\beta = -0.42$, $t(251) = -3.10$,

413 *p* = . 012, 95% CI [-0.151 -0.693]) and WIAT (*β* = -0.41, *t*(251) = -3.06, *p* = . 012, 95% CI [-
414 0.148 -0.682]). The relationships between the neuro-cognitive dimensions and the pattern of
415 relationships on the full cognitive battery and the adjusted variable scatter plots of the
416 significant results are summarized in the form of a heat map in **Figure 3**.
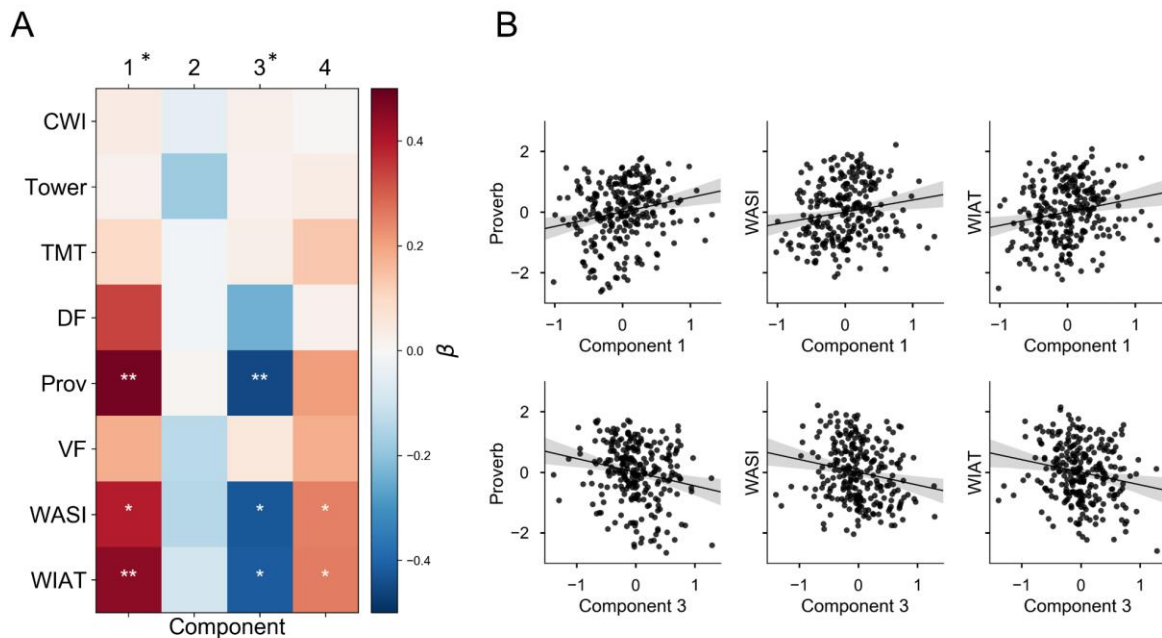
417

418 **Figure 3. The relationship between the different neural-cognitive components and the**
419 **measures assessed in the cognitive battery.** The components 1 and 3 were significant at the
420 multivariate level determined by multiple multivariate regression, indicated by the asterisk
421 outside of the heat map. The cells with asterisk(s) indicates the significant resluts from the
422 univariate test (bonferroni corrected) and the parameter estimates for each variable. CWI –
423 Colour-word interference, DF – Design fluency, Pro- Proverbs, TOW – Tower of London,
424 TMT – Trail making task, VF- Verbal Fluency, WASI – Wechseler Adult Intelligence Test,
425 WIAT – Weschler Individual Attainment Test. P-value significant codes: 0 "***" 0.001 "**"
426 0.01 "*".

427   Finally, we performed a simple principle commponent analysis on the eight task
428 measures to explore the associations between experience and the structure of the laboratory
429 data. The aim of this analysis was to see if the pattern retrieved from the univariate level in
430 the previous multiple multivariate regression was related to the internal structure of the data.
431 Component selection was determined based on the scree plot, and we accepted one
432 component explaining 39% of the variance. The principle component loaded on the
433 intelligence measures and the proverb test. We fitted a linear model to this data to understand

434   the relationship to the four canonical components. The results are reported in **Figure 4**. The

435   overall linear model was significant ($F(4, 253) = 5.43$, $p = .0003$). In the linear regression

436   model, Component 1 ($\beta = 0.82$, $t(253) = 3.5$, $p = .001$, 95% CI [0.36 1.29]) showed

437   significant contribution to explaining the task principle component. Component 3 showed a

438   negative correlation to the task components ($\beta = -0.69$, $t(253) = -3.04$, $p = .003$, 95% CI [-

439   1.13 -0.24]). The relationships between tasks and the neuro-cognitive components here were

440   similar to the ones uncovered by the multiple multivariate regression. In this analysis

441   Component 4 ($\beta = 0.442$, $t(253) = 3.09$, $p = .002$, 95% CI [0.16 0.72]) showed a significant

442   contribution in the regression model, but it did not pass the permutation test of robustness (p

443   = 0.998). The related results should be treated cautiously. Together with our prior analysis,

444   these results suggest that Components 1 and 3 are the most robust components identified in

445   our study.
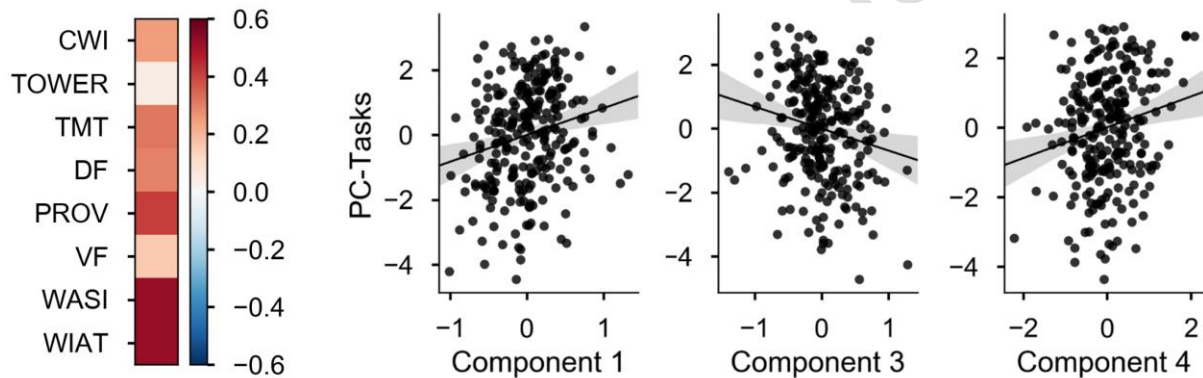
446

447   **Figure 4. The principle component and its relationship to the different neural-cognitive**

448   **components.** The heat map describes the principle component of the task battery, and the

449   scatter plots describe the association with the components identified in our study. Component

450   1 and 3 passed the permutation test for component robustness significantly contributed in

451   explaining the principle component of the task. Component 4 showed a significant

452   contribution in the regression model, but it did not pass the permutation test. The related

453   results should be treated cautiously.

454

5 Discussion

We set out to describe different modes of neuro-cognitive patterns derived through the simultaneous decomposition of whole brain connectivity data with self-reports of on-going experience. We used a whole brain parcellation that describes cortical function in seven independent networks (Yeo et al., 2011). We combined this data with self-reports of the experience of our participants at rest, using a multivariate approach that allows for the possibility of many-to-many mappings between neural patterns and on-going cognition. Our analyses identified four stable canonical components, describing unique dimensions of neural-experiential variation. Permutation testing demonstrated the statistical robustness of Components 1-3. Furthermore, two components (1 and 3) described independent patterns of performance in a battery of commonly used cognitive measures. This association with cognitive performance that establishes a source of independent validity for these neuro-cognitive components since they are related to independent measures of cognitive performance. We next consider the fit between the dimensions produced by our analysis and theoretical views of unconstrained neuro-cognitive processing.

We found evidence broadly consistent with contemporary representational accounts of unconstrained processing. The neural patterns described by Component One reflect a pattern of reduced correlation between regions with links to memory and representation (e.g. limbic, default mode) from those with links to external behaviour (e.g. visual and sensorimotor cortex and attention networks). This pattern was associated with experiences characterised by a sense of purposefulness, and with verbally mediated content that was social and temporal in nature. Participants high on this dimension were proficient at generating abstract semantic links and performed well on measures of reasoning and intelligence. Together the features of Component One support the hypothesis that the functional decoupling of systems important for memory and representation are important for aspects of unconstrained cognition (Smallwood, 2013). This capacity may arise from the topographical organisation of the cortex, in which neural systems that can take on more transmodal properties tend to be located in regions that are more distant in functional and structural terms (Buckner & Krienen, 2013; Margulies et al., 2016; Mesulam, 1998). This spatial location may allow neural signals in these regions to take on properties that are discrepant from the neural signal more closely tethered to inputs describing the external world (Buckner & Krienen, 2013; Friston, 2013). The pattern identified by Component One, therefore, may reflect a pattern of population variation describing the hypothesised role of functional decoupling of memory and representational systems plays in

the generation of more abstract aspects of human cognition (Margulies et al., 2016; Mesulam, 1998). Importantly, in our prior work, limbic and default mode networks were the most distant in functional connectivity terms from unimodal systems (Margulies et al., 2016).

Our data also highlights neural patterns that capture the hypothesised influence of attention and control on on-going thought (McVay & Kane, 2010). Component 3 highlights links between reduced connectivity within attention and control systems and patterns of thought that emphasise personal importance. This is associated with worse performance on measures of intelligence and reasoning. The combination of a focus on personally important themes linked to poor performance on measures of general aptitude, captures the hallmark psychological features of the current concerns X executive-failure accounts of on-going thought (McVay & Kane, 2010). This view suggests that failures in attentional control lead to highly personally relevant cognition to intrude into ongoing thought, leading to lapses in task performance. Importantly, the neural pattern described by this component emphasises dysregulated connectivity both within and between networks implicated in attention and control by task-based studies (Duncan, 2010). Our prior work established that spontaneous mind-wandering is linked to cortical thinning within regions linked to attention and control, such as the intra-parietal sulcus (Golchert et al., 2017). Spontaneous mind-wandering has been linked to worse cognitive control (Robison & Unsworth, 2018), as well as showing stronger links with attention related problems, including ADHD (Seli, Smallwood, Cheyne, & Smilek, 2015). Together with these prior studies, our data suggests that population variation in the intrinsic neural functioning within networks with an established role in external task performance captures the hypothesised contribution of executive-failure to patterns of on-going thought.

The method of decomposition used in the current study also highlighted patterns related to affective processing and the modality of the experience that are similar to those seen in our prior work that applied principal components analysis (PCA) to self-reported data only. Component Four places experiences with visual features ("images") in opposition to experiences with verbal features ("monologue"), capturing dissociations between visual and verbal thinking observed in our prior studies (Konishi et al., 2017; Medea et al., 2016; Smallwood et al., 2016). The accompanying neural pattern were associated with higher connectivity between the visual network with other networks, in particular the limbic system. It is important to note that our permutation analysis failed to validate this component, so despite its association with task performance using the PCA analysis it should be treated with relative

caution. Component Two loads on emotional experiences ("cheerfulness", "anger", "guilt" and "happiness") with the exception of those that are unhappy ("sad"). In neural terms this component was characterised by high levels of connectivity, however, unlike Component Four, this was highest between limbic and ventral attention networks. This pattern of coupling is consistent with accounts that emphasise interactions between saliency and limbic systems in affective processing (Touroutoglou et al., 2012). In the case of Component Two permutation testing indicated this component was likely to be robust in statistical terms, however, we did not observe associations with task performance. As with Component Four, interpretations of Component Two should be made with caution in lieu of more empirical work.

Before closing it is worth considering several important limiting factors of our study. We focused on patterns of population variance in unconstrained neuro-cognitive processing that were measured once in each individual. Our study, therefore, cannot separate the influences state and traits on our observed components. Treating patterns of unconstrained processing as a trait is common in both the psychological (McVay & Kane, 2009; Smallwood, Ruby, & Singer, 2013) and neural domains (Smith et al., 2015). Nonetheless, it remains an open question how consistent these components will be across individuals over time, as well as which aspects may be better described as traits. Importantly, by its very nature there are dimensions of experience that our study cannot adequately address. We cannot, for example, identify brain-experience associations that are highly dynamic in nature and in particular those that change rapidly within an individual. Insight into this issue could be achieved by a focus on dynamic rather than static connectivity (Kucyi, 2017). For example, the application of techniques such as sliding window analysis (Chang & Glover, 2010) or Hidden Markov models (Vidaurre, Smith, & Woolrich, 2017) to fMRI could provide information that would complement our analyses. However, it may also be more important to examine these across multiple sessions within the same individuals, as this would also make it most possible to dissociate state from trait related influences on neural activity (Mueller et al., 2013). There are also types of experience that may be difficult to assess using the measure of retrospective experience sampling we have employed (Smallwood & Schooler, 2015). For important features of experience, such as whether it has evolving features (Mills, Raffaelli, Irving, Stan, & Christoff, 2017), or when the participant is unaware of the content of their experience (Schooler, 2002), these experiential features may be best assessed using experience sampling techniques that capture momentary elements of experience (Smallwood, 2013).

554   There are a number of methodological improvements that could enhance future studies of
555   brain-experience association. A recent benchmark study by Ciric and colleagues (Ciric et al.,
556   2017) shows that scrubbing can improve the performance of resting state analyses. Regarding
557   to the analysis pipeline, we gained hyper-parameters and best model with nested-CV an
558   approach that can help prevent overfitting (Bzdok & Yeo, 2017). There are also alternative
559   ways that could provide better tests of the robustness of the components we identified. We
560   assessed the validity of the components in three different ways; 1) with a data-driven, non-
561   parametric permutation test (Smith et al., 2015) that establishes the statistical validity of the
562   identified components and 2) by establishing the relationship between the laboratory
563   cognitive measures and 3) by consideration of their links with contemporary theoretical
564   accounts of ongoing cognition. In our study, Components 1 and 3 were statistically
565   significant in both cases and fitted well with contemporary accounts of ongoing cognition.
566   Accordingly we place encourage readers to focus on these patterns from our data. There are
567   alternative strategies that could help validate the robustness of patterns of brain-experience
568   association. One approach could be to compare the relationship between multiple sessions
569   within the same individual (Poldrack et al., 2015) and to have a larger sample that would
570   allow the reproducibility of these results through a formal split-half validation procedure. To
571   achieve this latter aim for future studies, we have placed the questionnaire measure used in
572   this study along with an example self-report collection task on GitHub at the following
573   address: https://github.com/htwangtw/restingstate_thoughtreports. We encourage interested
574   investigators to apply these measures in their resting-state investigation and to also upload the
575   resultant data onto open fMRI. These studies could be used in conjunction with the openly
576   access data used in this study to enable future investigations the opportunity to cross validate
577   experiential analyses in a more sophisticated manner than we have been able to achieve in
578   this study. The analysis pipeline of the current study can be further unified into one frame
579   work that benefits from both validation strategies. We can include the number of components
580   along with penalty coefficients in the hyper-parameters determined in the CV process, or
581   determine the best penalty terms with the first component. The permutation test will then
582   identify the reliable components occurring above chance level. After all the data-driven
583   component selection, we can examine the survived components through their relations with
584   well-documented cognitive measures and conclude the meaningful patterns. Finally, it is
585   likely that our measure of on-going thought lacks important questions regarding the content
586   of experience. It will be important, therefore, in the future to examine the relationships of the
587   type described in this study with a more exhaustive description of on-going experience. We

588 hope that by publishing our questionnaire collection task in a GitHub repository we will be
589 able to harness the power of the broader community to help generate and test plausible
590 questions for use in future studies.

591

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8 Competing Interests

607 The authors have declared that no competing interests exist.

9 Appendix: Nested K-Fold CV

608

609 1. Separate the model into 5 folds. In every iteration, 1 fold is the test set and the rest are
610 the development set.

611 2. For each outer fold:

612   a. For each parameter set to be considered:

613   i. Separate the development set into 5 folds. . In every iteration, 1 fold is
614   the validation set and the rest are the training set.

615   ii. For each inner fold:

616   1. Train the model on the training set

617   2. Calculate test error in the validation set

618   iii. Compute the average inner CV test error.

619   b. Choose the best parameter set with minimum average test error.

620   c. Use this parameter set to train on the development set.

621   d. Calculate test error in the test set

622 3. Determine the optimal model based on the outer fold test error

623 4. Train the full dataset on the optimal model

624

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