Supplementary Tables and Figures

Questions	Label	Low (1)	High (10)
My thoughts were focused on an external task or activity:	Task	Not at all	Completely
My thoughts involved future events:	Future	Not at all	Completely
My thoughts involved past events:	Past	Not at all	Completely
My thoughts involved myself:	Self	Not at all	Completely
My thoughts involved other people:	People	Not at all	Completely
The emotion of my thoughts was:	Emotion	Negative	Positive
My thoughts involved images:	Images	Not at all	Completely
My thoughts were detailed and specific:	Detailed	Not at all	Completely
My thoughts were:	Deliberate	Spontaneous	Deliberate
I was thinking about solutions to problems (or goals):	Problem	Not at all	Completely
My thoughts were intrusive:	Intrusive	Not at all	Completely
My thoughts contained information I already knew (e.g., knowledge or memories):	Knowledge	Not at all	Completely
I was absorbed in the contents of my thoughts:	Absorbing	Not at all	Completely
My thoughts were distracting me from what I was doing:	Distracting	Not at all	Completely
My thoughts involved words:	Words	Not at all	Completely
My thoughts involved sounds:	Sounds	Not at all	Completely

Supplementary Table 1 | Multi-dimensional experience sampling (mDES) items used in the current study.

Note. Participants responded using a 1-10 continuous slider scale.

Supplementary	Table 2	Summary	of the	14 task	brain map	sources,	grouped i	nto pairs	based or	ı task
similarity.										

Task	Source	Description
Self-Reference	Murphy et al $(2019)^1$	Participant is shown an adjective and indicates whether the adjective applies to themselves or not.
Other-Reference	Murphy et al (2019) ¹	Participant is shown an adjective and indicates whether the adjective applies to another person or not.
Go/No-Go	Alam et al $(2018)^2$	Participant must respond with a button press ('go') or ignore ('no/go') presented stimuli.
Finger Tapping	Barch et al $(2013)^3$	Participant responds to a stimulus presentation with a button press (right-hand) as soon as it is presented.
Reading	Zhang et al $(2022)^4$	Participant reads sentences presented word by word in the centre of the screen.
Memory	Zhang et al $(2022)^4$	Participant is asked to recall a queued autobiographical memory.
0-Back	Turnbull et al (2019) ⁵	Participant must select whether a shape on the left or right side of the screen matches one in the centre.
1-Back	Turnbull et al (2019) ⁵	Participant must select whether a shape on the left or right side of the screen from the previous trial matches one in the centre.
Easy-Math	Wang et al (2020) ⁶	Participant must select the correct answer to single digit addition problems.
Hard-Math	Wang et al (2020) ⁶	Participant must select the correct answer to double digit addition problems.
Documentary	Van Essen et al (2013) ⁷	Participants watch a short documentary ("Welcome to Bridgeville") clip.
Sci-Fi	Van Essen et al (2013) ⁷	Participants must watch a Sci-Fi movie ("Inception") clip.
2-Back: Faces	Barch et al $(2013)^3$	Participant must determine whether a stimulus (face) has been shown 2 trials previously.
2-Back: Scenes	Barch et al (2013) ³	Participant must determine whether a stimulus (scene) has been shown 2 trials previously.

Task	Gradient 1	Gradient 2	Gradient 3	Gradient 4	Gradient 5
Easy Math	-0.02	0.14	0.08	-0.07	-0.06
Hard Math	-0.11	0.30	0.36	0.02	-0.23
Finger Tapping	-0.09	-0.20	0.22	0.02	0.16
Go/No-Go	-0.13	0.23	0.06	-0.14	-0.12
Friend-Reference	-0.03	-0.25	-0.09	0.15	0.10
Self-Reference	-0.11	-0.29	-0.10	0.18	0.09
Memory	-0.08	-0.31	-0.20	0.24	0.13
Reading	-0.14	-0.11	-0.22	0.09	0.01
Documentary	0.01	-0.02	-0.36	-0.02	0.24
Sci-Fi	-0.11	-0.02	-0.29	0.04	0.11
0-Back	-0.02	-0.22	0.11	-0.01	0.10
1-Back	-0.07	0.01	0.36	-0.03	-0.01
2-Back-Faces	0.01	0.21	0.33	-0.08	-0.16
2-Back-Scenes	-0.02	0.26	0.29	-0.06	-0.19

Supplementary Table 3 | Task map coordinates in 5-d 'brain space.'

Note. Coordinates in 'brain space' represent Spearman rank correlation between each task map and the first five connectivity gradients described in Margulies et al.⁹

CC1	CC2	CC3	CC4
0.53	-0.28	-0.09	-2.56
1.34	0.39	-0.12	0.15
1.07	1.03	-2.07	-1.13
1.13	1.23	-1.62	-0.17
-0.31	-2.51	0.46	1.51
-0.20	-3.79	-2.10	1.15
0.87	0.44	-1.02	0.20
1.19	2.33	0.31	2.46
0.98	-0.88	0.86	-0.09
2.14	-0.69	1.66	-0.55
-2.36	0.41	-0.92	-0.47
-2.03	0.95	1.48	-0.13
-0.64	-0.34	1.73	-0.11
-3.15	0.39	-0.34	0.19
	CC1 0.53 1.34 1.07 1.13 -0.31 -0.20 0.87 1.19 0.98 2.14 -2.36 -2.03 -0.64 -3.15	CC1CC2 0.53 -0.28 1.34 0.39 1.07 1.03 1.13 1.23 -0.31 -2.51 -0.20 -3.79 0.87 0.44 1.19 2.33 0.98 -0.88 2.14 -0.69 -2.36 0.41 -2.03 0.95 -0.64 -0.34 -3.15 0.39	CC1CC2CC3 0.53 -0.28 -0.09 1.34 0.39 -0.12 1.07 1.03 -2.07 1.13 1.23 -1.62 -0.31 -2.51 0.46 -0.20 -3.79 -2.10 0.87 0.44 -1.02 1.19 2.33 0.31 0.98 -0.88 0.86 2.14 -0.69 1.66 -2.36 0.41 -0.92 -2.03 0.95 1.48 -0.64 -0.34 1.73 -3.15 0.39 -0.34

Supplementary Table 4 | Task-averaged Canonical Correlational Analysis (CCA) summed variates for each dimension of the 4-d 'state-space.'

Note. Most positive and negative scores for each dimension are emboldened.

mDES item	PC1	PC2	PC3	PC4	PC5
Absorbing	0.29	-0.06	0.20	-0.14	-0.11
People	0.30	0.09	-0.38	0.00	0.01
Problem	0.15	-0.08	0.59	0.14	-0.12
Words	0.25	-0.05	-0.03	0.03	0.62
Sounds	0.20	0.15	-0.17	0.58	0.37
Images	0.20	-0.04	-0.21	0.42	-0.56
Past	0.34	-0.10	-0.23	-0.30	-0.16
Distracting	0.21	0.49	0.10	-0.10	-0.01
Task	0.20	0.17	0.34	0.01	0.17
Intrusive	0.22	0.42	0.07	-0.05	-0.05
Deliberate	0.13	-0.42	0.24	0.13	0.14
Detailed	0.32	-0.32	0.13	0.04	-0.05
Future	0.26	0.20	0.16	0.27	-0.22
Emotion	0.17	-0.31	-0.27	0.20	0.04
Self	0.30	0.14	-0.16	-0.31	0.07
Knowledge	0.31	-0.27	0.01	-0.34	-0.02

Supplementary Table 5 | Component loadings of the first five components identified via the application of Principal Components Analysis (PCA) to the full 14-task battery mDES data (N observations = 7220, N = 190).

 $\overline{Note. \text{ Loadings} > 0.3 \text{ or } < -0.3 \text{ are emboldened.}}$

Task	PC1	PC2	PC3	PC4	PC5
Easy Math	-0.17	-0.46	0.83	-0.16	0.23
Hard Math	-0.36	-0.24	1.10	-0.28	0.24
Finger Tapping	-0.63	0.49	0.11	0.12	-0.06
Go/No-Go	-0.77	0.52	0.25	0.10	-0.25
Friend-Reference	1.07	-0.74	-0.82	-0.26	0.20
Self-Reference	0.74	-0.16	-0.26	-0.92	0.35
Memory	1.37	-0.57	-1.11	-0.32	-0.22
Reading	0.01	0.39	-0.06	0.06	0.30
Documentary	-0.50	0.32	-0.76	0.72	0.14
Sci-Fi	-0.25	0.37	-0.72	0.54	0.24
0-Back	-0.19	0.50	0.24	0.13	-0.22
1-Back	-0.23	-0.16	0.42	0.31	-0.03
2-Back-Faces	-0.16	0.00	0.08	0.32	-0.61
2-Back-Scenes	-0.33	-0.03	0.33	0.25	-0.57

Supplementary Table 6 | Task-averaged mDES coordinates in the 5-d 'thought-space.'

Note. Coordinates in 'thought-space' represent the dot product between each components' component loadings and each original mDES observation (i.e., PCA scores). Shown here are the task-averaged PCA scores

Supplementary Table 7 | Results of a series of spin tests to ascertain the relationship between the task maps and gradients. In these tests the correlation between the real task maps and the gradients are compared to 1000 synthetic distributions of brain data that preserve the spatial distribution of the original brain data. Note these correlations only involve the cortex and so may differ from the correlations in Supplementary Table 3 which include the sub cortex and the cerebellum.

Task		Gradient 1	Gradient 2	Gradient 3	Gradient 4	Gradient 5
Documentary	r	0.10	0.26	-0.48	0.07	0.34
	р	0.47	0.14	0.01	0.66	0.01
SciFi	r	-0.04	0.32	-0.38	0.1	0.22
	р	0.78	0.08	0.01	0.53	0.09
Friend	r	0.13	-0.02	-0.24	0.15	0.24
	р	0.27	0.91	0.01	0.16	0.02
2 Back Scene	r	0.1	0.59	0.41	-0.38	-0.14
	р	0.48	0.01	0.01	0.01	0.19
2 Back Faces	r	0.18	0.5	0.4	-0.41	-0.06
	р	0.18	0.01	0.01	0.01	0.55
Easy Maths	r	0.04	0.3	0	-0.23	-0.02
	р	0.77	0.01	1	0.06	0.84
Memory	r	0.07	0.06	-0.29	0.42	0.09
	р	0.57	0.67	0.01	0.01	0.37
Hard Maths	r	-0.09	0.46	0.36	-0.37	-0.14
	р	0.53	0.01	0.01	0.01	0.19
1 Back	r	0.05	0.21	0.56	-0.36	0.06
	р	0.74	0.12	0	0.01	0.61
Reading	r	-0.17	-0.11	-0.43	0.2	0.08
	р	0.26	0.53	0.01	0.16	0.55
Finger Tapping	r	-0.05	-0.12	0.18	-0.2	0.27
	р	0.66	0.43	0.02	0.07	0.01
0 Back	r	0.13	0.2	0.43	-0.19	0.13
	р	0.28	0.04	0.01	0.1	0.14
Go No Go	r	-0.35	0	0.04	-0.39	-0.16
	р	0	0.99	0.69	0	0.15
Self	r	0.02	-0.02	-0.17	0.22	0.27
	р	0.83	0.82	0.05	0.03	0.01

Term	CCA 1	Term	CCA 2	Term	CCA 3	Term	CCA 4
Tasks	0.281	Motor	0.145	Pain	0.259	Visual	0.204
Spatial	0.248	Task	0.123	Speech	0.231	Motor	0.165
Working Memory	0.227	Working Memory	0.119	Auditory	0.225	Pain	0.148
Action	0.213	Anticipation	0.114	Listening	0.218	Movement	0.118
Attention	0.212	Monetary	0.107	Acoustic	0.198	Objects	0.1
Object	0.195	Reward	0.102	Sounds	0.194	Motion	0.1
Visual	0.182	Incentive	0.1	Vocal	0.192	Vision	0.098
Visuospatial	0.181	Gain	0.099	Speech Production	0.182	Nociceptive	0.089
Calculation	0.178	Incentive delay	0.092	Sound	0.178	Stimulation	0.088
Load	0.169	Losses	0.088	Music	0.176	Finger	0.086
RestingState	-0.209	Social	-0.243	Working Memory	-0.155	Autobiographical	-0.257
Reward	-0.16	Autobiographical	-0.221	Visual	-0.153	Theory Of Mind	-0.225
Autobiographical	-0.135	Comprehension	-0.218	Memory	-0.15	Social	-0.214
Anticipation	-0.12	Sentences	-0.216	Retrieval	-0.122	Retrieval	-0.21
Monetary	-0.115	Emotional	-0.198	Task	-0.121	Memories	-0.185
Motivation	-0.107	Linguistic	-0.196	Calculation	-0.119	Mental States	-0.183
Incentive	-0.106	Theory Of Mind	-0.193	Objects	-0.105	Memory Retrieval	-0.177
Emotional	-0.103	Listening	-0.189	Load	-0.101	Semantic	-0.175
Reward Anticipation	-0.102	Memories	-0.188	Spatial	-0.1	Mentalizing	-0.173
Incentive Delay	-0.098	Spoken	-0.184	Arithmetic	-0.099	Memory	-0.172

Supplementary Table 8 | The top ten positive and top ten negative correlations with each of the CCA maps as generated using Neurosynth (<u>https://neurosynth.org/decode/</u>).

	Γ	Deliberate Probl	em-Solvi	ng		Detailed Know	wledge			Intrusive Dist	raction			Positive Enga	igement	<u> </u>
Parameters	b	95% CI	t	р	b	95% CI	t	р	b	95% CI	t	р	b	95% CI	t	р
(Intercept)	-0.12	-0.94 - 0.70	-0.29	0.772	0.31	-0.74 - 1.37	0.58	0.560	-0.43	-1.59 - 0.73	-0.73	0.466	0.29	-0.69 - 1.26	0.58	0.565
Easy Math	0.92	0.86 - 0.98	31.13	<0.001	0.14	0.08 - 0.21	4.49	<0.001	-0.71	-0.780.64	-20.63	<0.001	-0.12	-0.190.05	-3.23	0.001
Hard Math	0.62	0.57 - 0.68	21.05	<0.001	2.19	2.12 - 2.25	67.70	<0.001	-0.98	-1.050.91	-28.44	<0.001	3.63	3.56 - 3.70	101.23	<0.001
Finger tapping	0.87	0.82 - 0.93	29.51	<0.001	-0.80	-0.860.74	-24.80	<0.001	1.18	1.12 - 1.25	34.42	<0.001	0.89	0.82 - 0.96	24.79	<0.001
Go/No-Go	3.29	3.23 - 3.35	110.90	< 0.001	-0.98	-1.040.92	-30.40	<0.001	3.07	3.00 - 3.14	89.30	<0.001	-0.78	-0.850.71	-21.85	<0.001
Friend	-2.39	-2.442.33	-80.50	<0.001	0.50	0.43 - 0.56	15.34	<0.001	-1.00	-1.070.93	-29.11	<0.001	-0.96	-1.030.89	-26.70	<0.001
You	-1.94	-1.991.88	-65.31	<0.001	0.88	0.82 - 0.95	27.42	< 0.001	2.28	2.21 - 2.35	66.36	<0.001	0.01	-0.06 - 0.08	0.30	0.762
Documentary	-0.57	-0.640.50	-15.96	<0.001	-3.53	-3.613.45	-90.59	< 0.001	-5.34	-5.425.26	-128.75	<0.001	2.95	2.86 - 3.03	68.21	<0.001
SciFi	-0.21	-0.280.14	-5.98	<0.001	-2.42	-2.492.34	-62.02	<0.001	1.40	1.32 - 1.48	33.82	<0.001	1.75	1.66 - 1.83	40.38	<0.001
1B	1.56	1.50 - 1.62	52.60	<0.001	0.53	0.47 - 0.60	16.49	<0.001	0.57	0.50 - 0.64	16.53	<0.001	-0.48	-0.550.41	-13.33	<0.001
0B	0.11	0.05 - 0.17	3.66	< 0.001	-0.17	-0.230.10	-5.17	<0.001	-0.27	-0.330.20	-7.76	<0.001	-3.74	-3.813.67	-104.34	<0.001
Read	-0.96	-1.020.90	-32.45	<0.001	0.01	-0.05 - 0.08	0.42	0.673	2.40	2.34 - 2.47	69.90	<0.001	-0.60	-0.670.53	-16.70	<0.001
Memory	-3.60	-3.663.54	-121.38	<0.001	0.72	0.66 - 0.78	22.33	<0.001	-0.04	-0.11 - 0.03	-1.20	0.229	0.11	0.04 - 0.18	3.15	0.002
2B-Face	1.19	1.12 - 1.26	33.19	<0.001	1.42	1.35 - 1.50	36.53	<0.001	-1.29	-1.371.21	-31.06	<0.001	-1.97	-2.061.89	-45.58	<0.001
Age	0.00	-0.04 - 0.05	0.10	0.919	-0.01	-0.07 - 0.05	-0.35	0.730	0.01	-0.06 - 0.07	0.20	0.846	-0.01	-0.06 - 0.04	-0.29	0.772
Man	0.02	-0.16 - 0.20	0.19	0.853	-0.19	-0.42 - 0.04	-1.63	0.106	-0.22	-0.48 - 0.03	-1.74	0.083	0.16	-0.05 - 0.37	1.48	0.141
Non-binary	-0.06	-0.37 - 0.25	-0.36	0.717	0.37	-0.03 - 0.77	1.84	0.067	0.31	-0.13 - 0.75	1.40	0.163	-0.37	-0.740.00	-1.98	0.050

Supplementary Table 9 | Unstandardised parameter estimates for the linear mixed models comparing summed CCA variates between tasks.



Supplementary Figure 1. Spatial brain maps and network configuration of each connectivity gradient making up the 5-d 'brain-space'. a-e) spatial maps for gradients 1-5 (top = left hemisphere, bottom = right). Red = Positive, Blue = Negative. **f)** Radar plot of network configuration of each dimension. Points represent average gradient value in each of the Yeo-7 brain networks¹¹. Network-averaged values were z-scored within each gradient prior to plotting. The maximum value ('High') is 3 and the minimum value ('Low') is -3. Each color represents a different dimension, as shown in the legend at the bottom of the plot (Dim = dimension, DAN = dorsal attention network, VAN = ventral attention network, FPN = fronto-parietal network, DMN = default mode network). Figure adapted from Mckeown et al¹².



Supplementary Figure 2. Scree plot showing the eigenvalues corresponding to each of the PCA components generated by our analysis.



Supplementary Figure 3. Box plots showing distribution of PCA 'thought-space' dimensions grouped by task. a) Word clouds representing the five thought patterns identified via PCA applied to mDES data from all 14 tasks in the task battery (each word = mDES item; the size of word = magnitude of item loading on that pattern; colour = direction of loading, red = positive, blue = negative). b) Box plots showing the distribution of each PCA thought pattern (x-axis; corresponding word clouds shown above), grouped by each of the 14 tasks (y-axis). Centre line shows the median. Lower and upper hinges correspond to 1^{st} and 3^{rd} quartiles. Upper whisker extends from the hinge to the largest value (up to 1.5 * Inter-quartile range [IQR] from the hinge) and lower whisker extends from hinge to smallest value (up to 1.5 * IQR). Data beyond end of whiskers plotted individually as points.⁹ N = 190, N observations = 7220.



Supplementary Figure 4. Association between task performance metrics and 'Intrusive Distraction' dimension of 'thought-space.' a) Word cloud representing the 'Intrusive Distraction' dimension (each word = experiential feature as assessed via experience sampling, size of word = importance of experiential feature to dimension, color = polarity; red = positive, blue = negative). **b**) Line plot (of predicted values) showing main effect of 'Intrusive Distraction' (x-axis) for task accuracy (z-scored within each task separately; y-axis). Error bar = 95% CIs for each predicted value interval. Data included in model is plotted in each plot as black points (N observations = 1520). c) Line plots (of predicted values) showing significant interaction between 'Intrusive Distraction' (x-axis) and 'Task' (facets) for task accuracy (z-scored within each task separately; y-axis). Error bars = 95% CIs for each predicted value interval (unadjusted). Red asterisks indicate which simple slopes are significant when adjusting for 8 estimates (8 tasks). Data included in model is plotted in each plot as black points (N observations = 1520). d) Line plots (of predicted values) showing significant interaction between 'Intrusive Distraction' (x-axis) and 'Task' (facets) for task response time (z-scored within each task separately; y-axis). Error bars = 95% CIs for each predicted value interval (unadjusted). Data included in model is plotted in each plot as black points (N observations = 1512). Note: Predicted value range of line plot spans beyond raw data in some facets of the interaction plots as the predicted value range is set uniformly across all task levels when using the emmip() function of the emmeans¹⁰ R package; greater uncertainty in prediction at these ranges is highlighted by wider confidence intervals. Across all plots, N = 190.



Supplementary Figure 5. Unthresholded group-level task brain maps used in the current study. Each row represents one of the seven pairs, grouped together in terms of task similarity. In each cell, the top row is the left hemisphere (left-hand-side = medial; right-hand-side = lateral), and the bottom row is the right hemisphere (left-hand-side = medial). All task maps are z-stat contrast maps (task > baseline).



Supplementary Figure 6. Radar plot of network configuration of each significant CCA dimension. Points represent average CCA-weighted gradient value in each of the Yeo-17 brain networks¹¹. Each color represents a different dimension, as shown in the legend at the bottom of the plot (Dim = dimension, DAN = dorsal attention network, VAN = ventral attention network, FPN = fronto-parietal network, DMN = default mode network).



Supplementary Figure 7. Box plots showing distribution of CCA 'state-space' dimensions grouped by task. a) Word clouds representing how each CCA dimension organizes thought patterns identified via PCA applied to mDES data (each word = mDES item, size = magnitude of the summed weighted loading (see Methods), and colour = direction [red = positive, blue = negative]). b) Spatial brain maps representing how each CCA dimension organizes whole-brain neural patterns identified by correlating task brain maps with dimensions of brain function variation (gradients; see Methods). In each map, positive values are red and negative values are blue. c) Box plots showing the distribution of each CCA summed variate (x-axis; corresponding to above word clouds and brain maps), grouped by each of the 14 tasks (y-axis). Centre line shows the median. Lower and upper hinges correspond to 1st and 3rd quartiles. Upper whisker extends from the hinge to the largest value (up to 1.5 * Inter-quartile range [IQR] from the hinge) and lower whisker extends from hinge to smallest value (up to 1.5 * IQR). Data beyond end of whiskers plotted individually as points.⁹ N = 190, N observations = 7220.



Supplementary Figure 8. Association between task performance metrics and dimensions of CCA 'statespace.' a) Line plots (of predicted values) showing significant main effects for task accuracy (predictors: 'Deliberate Problem-solving,' 'Intrusive Distraction,' and 'Positive Engagement'). Y-axis = z-scored (within each task separately) accuracy, X-axis = CCA dimension (summed variates; see Methods). Word clouds in bottom corners of each plot represent the X variates of each CCA dimension (size of word = importance of experiential feature to dimension, color = polarity; red = positive, blue = negative). Error bars = 95% CIs for each predicted value interval. Data included in model is plotted in each plot as black points (N observations = 1520). b) Faceted line plot (of predicted values) showing the significant interaction between 'Intrusive Distraction' (x-axis) and 'Task' for task accuracy (y-axis; z-scored within each task), with the word cloud representing 'Intrusive Distraction'. Error bars = 95% CIs for each predicted value interval (unadjusted). Red asterisks indicate which task slopes are significant when adjusting for 8 estimates (8 tasks). Data included in model is plotted in each plot as black points (N observations = 1520). c) Faceted line plot (of predicted values) showing the significant interaction between 'Inner Speech' (x-axis) and 'Task' for task response time (y-axis; zscored with each task), with the word cloud representing 'Inner Speech'. Error bars = 95% CIs for each predicted value interval (unadjusted). Red asterisks indicate which task slopes are significant when adjusting for 8 estimates. Data included in model is plotted in each plot as black points (N = observations 1512). Note: Predicted value range of line plot spans beyond raw data in some facets of the interaction plots as the predicted value range is set uniformly across all task levels when using the emmip() function of the emmeans¹⁰ R package; greater uncertainty in prediction at these ranges is highlighted by wider confidence intervals. Across all plots, N = 190.



Supplementary Figure 9. Histograms showing the distributions of distances (i.e., error) for the 14-task CCA 'state-space' prediction of 'brain-space' coordinates using unseen experience sampling data. Each plot shows the 1) distribution of distances between the true and predicted coordinates for each task (emboldened title indicates which task), and 2) the three distributions of distances between the true coordinates for that task and the predicted coordinates for the other three tasks (see Methods). Distances are shown on x-axis and count is shown on y-axis. The mean of each distribution is plotted as a dotted line in the same colour as the distribution, as coded in the legend at the bottom of all plots. N = 95.



Supplementary Figure 10. Using the 10-task CCA 'state-space' to make predictions of brain coordinates in 'brain-space' using new experience sampling data in 4 tasks. a) A 3-d scatter plot showing 1) the true locations of the subset of 4 tasks (in black) and 2) the predicted locations (in red) of the subset of 4 tasks in 'brain-space.' b) Bar graphs showing the 1) mean of the distribution of distances between the true and predicted coordinates for each task (emboldened title indicates which task), and 2) the mean of the three distributions of distances between the true coordinates for that task and the predicted coordinates for the other three tasks (see Methods). Error bars = Standard Error, unadjusted. c) Heatmap highlighting that the mean distance between each task's true brain coordinates (the diagonal) is smaller than the mean distance between each task's true brain coordinates and the other three tasks' predicted brain coordinates. N = 95.

Supplementary Methods

Predicting Task Performance Metrics using Task Locations in PCA 'Thought-Space'

To examine the associations between the dimensions of the 'thought-space' and task performance, we ran two linear mixed models in which the outcome variable was either mean accuracy or mean response time, with 'Task' and the task-average of each of the PCA components (1-5) as the explanatory variables. Two-way interactions between 'Task' and each of the PCA components (1-5) were also included. The outcome variables (mean accuracy and mean response time) were z-scored, within each task separately, to adjust for differences in task demands across different tasks. Accordingly, in these models, the main effect of 'Task' can be ignored. Age and gender were included as nuisance covariates. Participant number was included as a random intercept (see Main Methods for mixed model implementation details).

Mean response time was calculated over correct trials only. In these task performance models, cases exhibiting a z-scored accuracy less than -2.5 and cases exhibiting a z-scored response time more than 2.5 were considered outliers, and the z-scores of these outliers were set to zero to mitigate their influence on the results. The Bonferroni-adjusted alpha level was 0.025 for the two models (reported p-values unadjusted unless otherwise stated). Diagnostic plots confirmed there was homoscedasticity and normality of residuals for the response time analysis, however, the QQ plot and histogram indicated the normality assumption was violated (left-skew) for the accuracy analysis. Therefore, the results from this model should be evaluated with caution.

In total, data from 8 tasks was included in these models as the other 6 tasks did not record response time or accuracy. There were 8 missing values for response time due to technical errors in data collection and no missing values for accuracy (accuracy N observations = 1520, response time N observations = 1512).

Accuracy model formula: lmer(Z-scored (within-task) Mean Accuracy ~ Task + Task-Mean PC1 + Task-Mean PC2 + Task-Mean PC3 + Task-Mean PC4 + Task-Mean PC5 + Task: Task-Mean PC1 + Task: Task-Mean PC3 + Task: Task-Mean PC4 + Task: Task-Mean PC5 + Age + Gender + (1|Participant))

Response time model formula: lmer(Z-scored (within-task) Mean Response Time ~ Task + Task-Mean PC1 + Task-Mean PC2 + Task-Mean PC3 + Task-Mean PC4 + Task-Mean PC5 + Task: Task-Mean PC1 + Task: Task-Mean PC2 + Task: Task-Mean PC3 + Task: Task-Mean PC4 + Task: Task-Mean PC5 + Age + Gender + (1|Participant))

The task accuracy analysis revealed a significant main effect of 'Intrusive Distraction' [F(1, 1392) = 60.98, P < 0.001], indicating that this pattern of thought was linked to worse accuracy [b = -0.13, 95% CI [-0.16, -0.10]] across all tasks where performance was possible to assess (see Supplementary Figure 4a and 4b). In addition, the task accuracy analysis revealed a significant interaction between 'Task' and 'Intrusive Distraction' [F(7, 1387) = 4.26, P < 0.001], indicating that the negative association between 'Intrusive Distraction' and accuracy was strongest in the Hard-Math [b = -0.31, adjusted 95% CI [-0.42, -0.20], t(1424) = -7.48, adjusted P < 0.001], Go/No-Go [b = -0.20, adjusted 95% CI [-0.34, -0.05], t(1425) = -3.66, adjusted P = 0.002], and 1-Back tasks [b = -0.15, adjusted 95% CI [-0.26, -0.03], t(1433) = -3.54, adjusted P = 0.003] (P-values and CIs for simple slopes Bonferroni-adjusted for 8 estimates; see Supplementary Figure 4c).

The task response time analysis revealed a significant interaction between 'Task' and 'Intrusive Distraction' [F(7, 1371) = 2.65, P = 0.010]. Examination of the simple slopes of each level of 'Task', Bonferroni-adjusted for 8 estimates, revealed no significant simple slopes and examination of the contrasts of the simple slopes, Tukey-adjusted for comparing a family of 8 estimates, revealed no significant comparisons. For completeness, the largest positive simple slope was for the Hard-Math task [b = 0.11, adjusted 95% CI [-0.04, 0.25], t(1404) = 1.94, adjusted P = 0.422] and the largest negative estimate was for the 2-Back-Scenes task [b = -0.10, adjusted 95% CI [-0.21, 0.07], t(1407) = -2.09, adjusted P = 0.295] (P-value and CI Bonferroni-adjusted for 8 tasks; see Supplementary Figure 4d).

Predicting Task Performance Metrics using Task Locations in CCA 'State-Space'

To examine the associations between the dimensions of the 'state-space' and task performance, we ran two linear mixed models in which the outcome variable was either mean accuracy or mean response time with 'Task' and the task-averages for each of the significant CCA dimension's summed variates (1-4) as the explanatory variables. Two-way interactions between 'Task' and each of the CCA dimensions (1-4) were also included. The outcome variables (mean accuracy and response time) were z-scored, within each task separately, to adjust for differences in task demands across different tasks. Accordingly, in these models, the main effect of 'Task' can be ignored. Age and gender were included as nuisance covariates. Participant number was included as a random intercept (see Methods for mixed model implementation details).

Mean response time was calculated over correct trials only. In these task performance models, cases exhibiting a z-scored accuracy less than -2.5 and cases exhibiting a z-scored response time more than 2.5 were considered outliers, and the z-scores of these outliers were set to zero to mitigate their influence on the results. The Bonferroni-adjusted alpha level was 0.025 for the two models (reported p-values unadjusted unless otherwise stated). Diagnostic plots confirmed there was homoscedasticity and normality of residuals for the response time analysis, however, the QQ plot and histogram indicated the normality assumption was violated (left skew) for the accuracy analysis. Therefore, the results from this model should be evaluated with caution.

In total, data from 8 tasks was included in these models as the other 6 tasks did not record response time or accuracy. There were 8 missing values for response time due to technical errors in data collection and no missing values for accuracy (accuracy N observations = 1520, response time N observations = 1512).

Accuracy model formula: lmer(Z-scored (within-task) Mean Accuracy ~ Task + Task-Mean CC1 + Task-Mean CC2 + Task-Mean CC3 + Task-Mean CC4 + Task: Task-Mean CC1 + Task: Task-Mean CC2 + Task: Task-Mean CC3 + Task: Task-Mean CC4 + Age + Gender + (1|Participant))

Response Time model formula: lmer(Z-scored (within-task) Mean Response Time ~ Task + Task-Mean CC1 + Task-Mean CC2 + Task-Mean CC3 + Task-Mean CC4 + Task: Task-Mean CC1 + Task: Task-Mean CC2 + Task: Task-Mean CC3 + Task: Task-Mean CC4 + Age + Gender + (1|Participant))

The task accuracy analysis revealed a significant main effect of 'Deliberate Problem-solving' [F(1, 1401) = 12.66, P < 0.001], indicating that 'Deliberate Problem-Solving' was associated with lower accuracy across all tasks in which accuracy could be assessed [b = -0.10, 95% CI [-0.15, -0.05]]. In addition, the task accuracy analysis revealed a significant main effect of 'Intrusive Distraction' [F(1, 1273) = 20.79, P < 0.001], indicating

that 'Intrusive Distraction' was associated with lower accuracy [b = 0.10, 95% CI [-0.14, -0.6]]. There was also a significant main effect of 'Positive Engagement' [F(1, 1433) = 11.76, P < 0.001], indicating that 'Positive Engagement' was associated with higher accuracy [b = 0.07, 95% CI [0.03, 0.11]]. All significant main effects are presented in Supplementary Figure 8a. Finally, there was a significant interaction between 'Intrusive Distraction' and 'Task' [F(7, 1381) = 3.90, P < 0.001], indicating that 'Intrusive Distraction' was associated with the strongest negative influence on lower accuracy in the Hard-Math task [b = -0.34, adjusted 95% CI [-0.50, -0.19], t(1436) = -6.04, adjusted P < 0.001] (P-value and CI adjusted for 8 tasks; see Supplementary Figure 8b).

The response time analysis revealed a significant interaction between 'Positive Engagement' and 'Task' [F(7, 1384) = 2.37, P = 0.021], indicating that 'Positive Engagement' was associated with slower response time in the 2-Back-Scenes task [b = 0.25, adjusted 95% CI [0.06, 0.45], t(1414) = 3.87, adjusted P = 0.003] (P-value and CI adjusted for 8 tasks; see Supplementary Figure 8c).

Supplementary References

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