

## Supplementary Information

### **A multi-demand operating system underlying diverse cognitive tasks**

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## I. Supplementary Methods

### A. fMRI datasets

#### HCP datasets

**N-back working memory task** We used the high-load dynamic brain state from the HCP N-back task identified from our previous study <sup>1</sup>, as the reference state for all other cognitive tasks in the present study. The same sample from the previous study was used in the current study. We selected 122 individuals (ages: 22-36 years old, 79 female/43 male) from 500 subjects (HCP Q1-Q6 Data Release) based on the following criteria: (1) range of head motion in any translational and rotational direction less than 1 voxel; (2) average scan-to-scan head motion less than 0.25 mm; (3) performance accuracy greater than 50% in each task block and session; and (4) right handedness.

The HCP N-back working memory task combines the category specific representation task and the *n*-back working memory task in a single task across two sessions. Participants were presented with blocks of trials that consisted of pictures of faces, places, tools and body parts. Within each session, the 4 different stimulus types were presented in separate blocks. Furthermore, within each session, half of the blocks are 2-back working memory and half are 0-back working memory task. In the 2-back working memory task blocks, subjects were requested to determine whether the current stimulus matches the stimulus in two presentations of stimuli prior within the same block. In the 0-back working memory task blocks, subjects were requested to determine whether the current stimulus matches the target that was presented in the beginning of each block (cue). A 2.5 second cue indicated the task type (and target for 0-back task) at the beginning of each block. Each task session contained 8 task blocks (10 trials of 2.5 seconds each, for 25 seconds) and 4 fixation (“rest”) blocks (15 seconds). On each trial, the stimulus was presented for 2 seconds, followed by a 0.5 second inter-trial-interval (ITI).

**Relational processing (RP) task** We selected 90 individuals from the 122 who had also participated in the *n*-back study <sup>1</sup>. The following criteria were used: (1) complete behavioral and brain imaging data in two different acquisition sessions; (2) range of head motion in any translational and rotational direction less than 1 voxel; (3) average scan-to-scan head motion less than 0.25 mm.

The RP task involved a relational processing task and a control condition. In the relational processing condition, participants were presented two pairs of objects, with one pair at the top of the screen and the other pair at the bottom. Participants were required to determine whether the top pair of objects and the bottom pairs of objects are different in the same dimension or not. For example, the top pair differed in texture and the bottom pair differs in shape. In the control task, there were two objects presented at the top of the screen, one object at the bottom of the screen and a word in the middle to indicate dimension (e.g. “shape” or “texture”). Participants were told to judge whether the bottom object matches either of the top objects in that dimension. Each condition had 3 blocks and each block lasts 18 seconds. There were 4 trials in each relational processing block and 5 trials in each control matching block. In the relational condition, the stimuli were presented for 3500 ms, with a 500 ms ITI. In the matching condition, the stimuli were presented for 2800 ms, with a 400 ms ITI.

#### DMCC dataset

We used the Dual Mechanism of Cognitive Control (DMCC) dataset <sup>2</sup> which contains four different task paradigms for probing cognitive control: (1) AX continued performance task (AxCPT), (2) Cued task switching task (CuedTS), (3) Sternberg working memory task (Sternberg) and (4) Stroop interference task (Stroop). We used data from 50 individuals (19-42 years old, 31F/19M) out of a total of 89 participants in the DMCC dataset based on the following criteria: (1) complete behavioral and brain imaging data; (2) range of head motion in any translational and rotational direction was less than 1 voxel in all the tasks; (3) average scan-to-scan head motion was less than 0.25 mm in all the tasks.

**AxCPT** AxCPT is a continuous performance task which includes 4 different standard (Go) trial types: AX, AY, BX, and BY, and No-Go stimuli. Participants were presented with the letters A or B followed by letters X or Y (or not “X”), comprising AX, AY, BX, and BY pairs. They are asked to respond to the probe (“X”) only if it followed the contextual cue (“A”). Participants were to make another response to other cue–probe sequences (“A” then “Y,” “B” then “X,” or “B” then “Y”), each occurring with much lower probability than the target pair (“AX”). The proportions of trial types were set to ensure equal frequencies of A-cue and B-cue trials. There were 40% AX, 10% AY, 10% BX and 40% BY trials. No-Go stimuli occurred with low frequency (16.7%). Participants were instructed to withhold response on these trials. Presentation time of cues and probes was 500 msec. Probes were accompanied by a white rectangular border, presented 250 ms prior to probe onset. The cue-probe delay interval was 4 seconds, placing demand on goal (context) maintenance processes. The full condition includes 216 trials (72 AX, 18 AY, 18 BX, 72 BY, 18 A-No-Go, 18 B-No-Go).

**CuedTS** Participants performed a letter-digit task in which they were cued to respond to either the letter or number in target stimuli which consisted of a letter-digit pair (e.g., “D 3”, or “1 A”). Based on the cue, participants had to either categorize the letter as a vowel or consonant, or categorize the digit as even or odd depending on the cue. The Cued task switching task consists of sixteen different stimuli (1A, A1, 2A, A2, 1B, B1, 2B, B2, 3E, E3, 4D, D4, 5H, H5, 6I, and I6). Each trial began with a 300 ms fixation cue (“+”) in the center of the screen. Following the fixation is a 500 ms task cue (“attend number”/“attend letter”) presented in red. If the cue said “Attend Number”, participants decided if the number is odd or even. If the cue said “Attend Letter”, participants decided whether the letter was a consonant or vowel. A 4000 ms CTI followed. In incongruent trials, the two stimuli activated competing cue-dependent responses (e.g. “A 3”) whereas in congruent trials, the response was cue-independent (e.g. “A 2”). Within each scanning run, 3 task blocks alternated with 4 resting fixation blocks (30 sec duration); in each task block, the inter-trial interval was varied randomly (across 3 step sizes).

**Sternberg task** In this task participants determined whether a probe matches a list of stimuli presented previously. High and low load conditions differed in the number of stimuli that need to be maintained in working memory. The Sternberg working memory task included 4 different memory set list-lengths (5, 6, 7 and 8 items). The full condition included 90 trials. The proportions were 5-item: 40%, 6-item: 10%, 7-item: 20%, 8-item: 30%. The 5-item and 6-item trials denoted low load (LL) trials and the 7-item and 8-item trials denoted high load (HL) trials. The retention interval was 4 seconds after which a probe was presented. On half the trials the probe matched one of the stimuli presented during the encoding period.

**Stroop task** The Stroop Interference task is a color-word task, in which stimuli are words presented in different colored fonts and participants are asked to name the color of the font in which the words are presented. The task included congruent and incongruent trials. In congruent trials, the word name and font color were the same (e.g., the word RED presented in

red font). In incongruent trials, the word name and font color were different (e.g. the word RED presented in green). The full condition includes 72 congruent and 144 incongruent trials.

## Stanford dataset

**Stop-signal task (SST)** Forty-five children with ADHD or TD children (9-12 years old, 22F/23M) completed the SST task during MRI scanning. Each participant performed two runs of the SST with 96 trials per run. Participants were instructed to respond as quickly as possible to green arrows (Go Signal) with their right pointer or middle finger based on the direction of the arrow. In 33% of the trials, after a variable delay, the green arrow turned red (Stop Signal), indicating that the participant should cancel their (prepotent) response. The delay between the Go Signal and the Stop Signal, the SSD varied across trials in a step-wise fashion and was adjusted dynamically to individual performance: beginning at 165ms, it decreased by 33ms for a failed stop, and increased by 33ms for a successful stop.

## Task performance statistical test

The effect of cognitive control load was tested using paired t-test between AY and AX, BY and BX conditions in the AxCPT; between Incongruent and Congruent conditions in the CuedTS; between high and low load conditions in the Stern; between Incongruent and Congruent conditions in the Stroop; between relational and match conditions in the RP (Supplementary Table S2 and S6). Data met the assumptions of the statistical tests, including normality and equal variances.

## B. State space modeling using BSDS

### BSDS generative model

Here we briefly describe the BSDS model <sup>3</sup>. Let  $\mathbf{y}_t^s$  denote a  $D$ -dimensional vector of observed fMRI measurements in time  $t$  and for subject  $s$ . Further, let  $\mathbf{z}_t^s$  denote a 1-of- $K$  discrete vector of latent state variables of a hidden Markov model (HMM) with elements  $z_{kt}^s, \forall k = 1, \dots, K$ . Two consecutive time instances are dependent via a first-order Markov chain through an HMM. Specifically, probability distribution of  $\mathbf{z}_t^s$  depends on the state of the previous latent variable  $\mathbf{z}_{t-1}^s$  through a conditional distribution  $p(\mathbf{z}_t^s | \mathbf{z}_{t-1}^s, \mathbf{A}) = \prod_{k=1}^K \prod_{j=1}^K A_{jk}^{z_{t-1,j}^s z_{tk}^s}$  for all  $t > 1$  represented by the transition probabilities  $\mathbf{A}$ , where  $A_{jk} \equiv p(z_{tk}^s = 1 | z_{t-1,j}^s = 1)$ , and a marginal distribution  $p(\mathbf{z}_1^s | \boldsymbol{\pi}) = \prod_{k=1}^K \pi_k^{z_{1k}^s}$  represented by a vector of initial probabilities  $\boldsymbol{\pi}$  where  $\pi_k \equiv p(z_{1k}^s = 1)$  <sup>4</sup>. Next, we assume that at a given mode of the system given by the latent state  $z_{kt}^s = 1$ , observed vector  $\mathbf{y}_t^s$  is generated via a state space model in form of

Equations 1-2:

$$\mathbf{y}_t^s = \mathbf{U}_k \mathbf{x}_{kt}^s + \boldsymbol{\mu}_k + \mathbf{e}_{kt}, \quad \forall t | z_{kt}^s = 1, \quad (1)$$

$$\mathbf{x}_{kt}^s = \bar{\mathbf{X}}_{kt}^s \bar{\mathbf{V}}_k + \boldsymbol{\epsilon}_{kt}, \quad \forall t | z_{kt}^s = 1. \quad (2)$$

Line 1 of the model represents a probabilistic factor analysis model <sup>5,6</sup> where  $\mathbf{U}_k$  is a  $D \times P$  dimensional linear transformation matrix that transforms data to a subspace of lower dimensionality,  $P < D$ , described using a  $P$ -dimensional vector of latent space variables  $\mathbf{x}_{kt}^s$  mediated by an overall bias  $\boldsymbol{\mu}_k$  and a measurement noise  $\mathbf{e}_{kt} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Psi}_k)$ . Line 2 represents an autoregressive (AR) process of order  $R$  defined on the latent space variables of the factor

analysis model <sup>7</sup>.  $\vec{V}_k$  is a vector of AR coefficients.  $\bar{X}_{kt}^s = \text{diag}(\bar{x}_{kt}^s)$  is a block diagonal isotropic matrix with elements of  $\bar{x}_{kt}^s = (x_{k,t-1}^s, x_{k,t-2}^s, \dots, x_{k,t-R}^s)^T$  representing latent space variables from the previous  $R$  time frames where  $T$  indicates the transpose operator.  $\epsilon_{kt} \sim \mathcal{N}(\mathbf{m}_k, \Sigma_k)$  models the remaining error term in latent space. An AR process of a first order,  $R = 1$ , is defined on the representations of the observations in the latent subspace,  $x_{kt}^s$ . Variables  $(\Psi_k, \vec{V}_k, \mathbf{m}_k, \Sigma_k)$  are global latent variables which are not a function of time  $t$ . Detailed theoretical derivations are provided in our previous study <sup>3</sup>.

### Advantages of BSDS modelling

The BSDS model has the following key advantages over other approaches:

First, BSDS does not require arbitrary sliding windows, nor does it impose temporal boundaries associated with predefined task conditions – this is contrast to previous approaches for characterizing dynamic brain connectivity in fMRI data which rely on *ad hoc* procedures for determining critical parameters, such as the window length and number of brain states, which are known to greatly influence the estimation of dynamic brain states and connectivity <sup>8</sup>. In contrast, BSDS uses a Bayesian framework to automatically regulate model complexity and directly estimates the optimal number of latent states.

Second, BSDS applies HMM to state space variables of the observed fMRI data, resulting in a parsimonious model of generators underlying the observed data. BSDS applies HMM to latent space variables generated by an autoregressive process, resulting in greater robustness in state identification.

Third, BSDS allowed us to uncover brain states and their dynamic spatiotemporal properties, including probability and sequence of state transitions as well as inter-regional functional connectivity associated with each brain state, in an optimal subspace. In our previous study <sup>3</sup>, we demonstrated that BSDS is robust to noisy and abrupt local changes in fMRI, resulting in more accurately identifying brain states and their temporal dynamic properties than conventional data driven approaches.

Finally, a novel aspect of our study is its use a generative model of brain dynamics derived one task to identify similar states in other tasks. Our generative model allows us to investigate the correspondence between brain states across tasks and test the hypothesis that a latent brain state that is optimal for behavioral performance during working memory <sup>3</sup> also occurs in other cognitive tasks, and predicts behavior.

### C. Statistical significance in leave one ROI out analysis

To evaluate the statistical significance of leave one ROI out effect, we build a distribution of leave one ROI out effects from all brain states, from which the significance level ( $p$  value) for the effect of leave one ROI out in each ROI in the SH state (e.g. SH<sub>AxCPT</sub>) was obtained. An FDR correction ( $p < 0.05$ ) was applied to correct for multiple comparisons.

### D. General linear model analysis of task-related activation

A general linear model (GLM) analysis was used to determine task-related activation in each of seven cognitive control tasks <sup>9</sup>. Six motion parameters were entered as covariates of no interest, and both canonical hemodynamic response function (HRF) and its time-derivative were used to convolve the stimulus function to form task regressors.

*AxCPT* included seven task regressors: ANG, BNG, AX, AY, BX, BY and error. The contrast of interest is AY versus AX.

*CuedTS* included three task regressors: Congruent, Incongruent and error. The contrast of interest is Incongruent versus Congruent.

*Sternberg* included three task regressors: Low load, High load and error. The contrast of interest is HL versus LL.

*Stroop* included three task regressors: Congruent, Incongruent and error. The contrast of interest is Incongruent versus Congruent.

*SST* included four task regressors: Go Correct (Go), Go Error, Successful Stop (SuccStop), and Unsuccessful Stop (UnsuccStop). The contrast of interest is SuccStop versus Go.

*RP sessions 1 and 2* included three task regressors: Match, Relational Processing (Relation) and error. The contrast of interest is Relation versus Match.

Task-related activation for each contrast of interest was extracted in each ROI used in the BSDS analysis: bilateral AI, MFG, FEF, IPL and DMPFC, PCC and VMPFC.

## **E. gPPI analysis of task-related functional connectivity**

Seed-based generalized psychophysiological interaction (gPPI) was used to determine task-related functional connectivity<sup>10</sup>. Seeds were placed in the bilateral AI, MFG, FEF, IPL and DMPFC, the same ROIs used in the BSDS analysis. The gPPI model consisted of a physiological variable (the raw time series of a seed), multiple psychological variables (hemodynamic response function convolved main effect of condition of interest), and multiple interaction variables (deconvolved raw time series of the seed multiplied by main effect of condition of interest, and then convolved with the hemodynamic response function). Task-related connectivity was computed for each ROI and contrast of interest resulting in an 11x11 matrix with each column representing a seed and each row representing a target.

## **F. Comparison of state space models with conventional GLM and gPPI analyses**

In each of the seven cognitive tasks, we examined whether state-space models generated better model fits with the reference *n*-back working memory task than conventional GLM<sup>9</sup> and gPPI<sup>10</sup> analyses. For state-space models, we assessed the similarity in mean activity and covariance patterns between  $SH_{WM}$  and the best matched brain state  $SH_X$  in each task *X* using *Pearson's* correlation. Similarly, in the case of conventional GLM and gPPI analyses, the similarity in activation/deactivation and gPPI connectivity patterns between the *n*-back working memory task and each of the seven other cognitive control tasks was determined using *Pearson's* correlation.

## **G. Canonical correlation analysis and prediction model**

To characterize the relation between brain states and behavioral performance in different tasks, we first used canonical correlation analysis (CCA) to investigate multivariate relations between brain state and cognitive performance measures in each task<sup>11, 12</sup>. In each cognitive task, the occupancy rates of the latent brain states were the set of *X* variables and behavioral measures

were the set of Y variables. For the AxCPT, behavioral variables included RT in AX, AY, BX and BY trials. For the CuedTS, behavioral variables included accuracy and RT in congruent and incongruent trials. For the Sternberg, behavioral variables included accuracy and RT in high-load and low-load trials. For the Stroop, behavioral variables included accuracy and RT in congruent and incongruent trials. For the SST, behavioral variables included stop accuracy, unsuccessful stop RT, stop-signal delay and stop-signal reaction time. CCA was implemented using python scikit-learn package ([https://scikit-learn.org/stable/modules/generated/sklearn.cross\\_decomposition.CCA.html](https://scikit-learn.org/stable/modules/generated/sklearn.cross_decomposition.CCA.html)).

A prediction model based on the CCA was examined using leave-one-out cross validation procedure such that one subject's data was used as the test set and the rest of subjects' data were used as the training set. The training set was then used to train a canonical correlation model and weights from the trained model were applied on the test set to generate predicted canonical variables of X and Y in the test set. This procedure repeated N times (N is the sample size) such that each subject's data was used exactly once as a test set. The model performance was evaluated using correlation between predicted canonical variables of X and predicted canonical variables of Y across all the subjects.

## H. Univariate brain-behavior correlation analysis

We used *Pearson's* correlation to examine the association between the occupancy rate of brain state and task-specific measures of cognitive control abilities. Individual data points were excluded in the analyses if they were 3 standard deviations or more away from the means.

## I. Power analysis

We performed a power analysis based on the state-behavior relationship identified from our previous study<sup>3</sup>. If we set alpha at  $p=0.05$ , a sample size of 39 will provide power of 0.8 to detect the effect of interest.

## II. Supplementary Results

### Statistical significance of state matching

Space closeness was significant between  $SH_{WM}$  and  $SH_{AxCPT}$  ( $p=0.01$ ) in the AxCPT, between  $SH_{WM}$  and  $SH_{CuedTS}$  ( $p=0.01$ ) in the CuedTS, between  $SH_{WM}$  and  $SH_{Stern}$  ( $p=0.05$ ) in the Sternberg and between  $SH_{WM}$  and  $SH_{Stroop}$  ( $p=0.01$ ) in the Stroop. Space closeness was also significant between  $SH_{WM}$  and  $SH_{SST}$  ( $p=0.01$ ) in the SST. Space closeness was marginally significant between  $SH_{WM}$  and  $SH_{RP1}$  ( $p=0.1$ ) in RP Session 1 and significant between  $SH_{WM}$  and  $SH_{RP2}$  ( $p=0.04$ ) in RP Session 2 (**Supplementary Table S13**).

Temporal closeness was significant between  $SH_{WM}$  and  $SH_{AxCPT}$  ( $p=0.01$ ) in the AxCPT, between  $SH_{WM}$  and  $SH_{CuedTS}$  ( $p=0.01$ ) in the CuedTS, between  $SH_{WM}$  and  $SH_{Stern}$  ( $p=0.01$ ) in the Sternberg task and between  $SH_{WM}$  and  $SH_{Stroop}$  ( $p=0.01$ ) in the Stroop. Temporal closeness was also significant between  $SH_{WM}$  and  $SH_{SST}$  ( $p=0.05$ ) in the SST. Temporal closeness was significant between  $SH_{WM}$  and  $SH_{RP1}$  ( $p=0.01$ ) in RP Session 1 and significant between  $SH_{WM}$  and  $SH_{RP2}$  ( $p=0.01$ ) in the RP Session 2. (**Supplementary Table S13**).

### Statistical significance of MFG role in leave one ROI out analysis

In the AxCPT, CuedTS and Stroop tasks, the left and right middle frontal gyrus (MFG) had a significant impact on state similarity ( $p < 0.05$ , FDR corrected). In the Sternberg task, the left MFG had a significant impact on the state similarity ( $p < 0.05$ , FDR corrected). In the SST, the left MFG had marginally significant impact on state similarity ( $p = 0.065$ , FDR corrected). Taken together, across all the tasks, the MFG, encompassing the dorsolateral prefrontal cortex, had the highest impact on state similarity (**Supplementary Figure S5**), suggesting that this region is the most important and consistent brain region whose dynamic features contribute to a shared high-load brain state across cognitive tasks.

### **Robustness of state matching with respect to sample size of the N-back task**

To examine the robustness of our findings with respect to the sample size used in generating the reference optimal latent brain state  $SH_{WM}$ , we leveraged a larger sample (415 subjects) from the HCP 1200 n-back working memory task and repeated the same BDS analysis to identify the optimal latent brain state  $SH_{WM415}$ . Specifically, we applied similar data inclusion criteria as in our previous study with a more lenient behavioral criterion (accuracy > 50%) allowing more subjects to be included. The selection criteria were: (1) range of head motion in any translational and rotational direction less than 1 voxel; (2) average scan-to-scan head motion less than 0.25 mm; (3) performance accuracy per session > 50%; (4) criterion (1)–(3) met in both Sessions 1 and 2 separately; (5) right handed subjects, and (6) subjects are unrelated. This leads to the final sample size of 415 subjects (29±4 years old, 22-36 years old, 225 F/190 M).

We applied the same data analysis procedures as in our previous sample. We determined the optimal latent brain state in the n-back working memory task by its dominant occupancy rate in the 2-back working memory blocks and its positive correlation with 2-back task accuracy (**Supplementary Figure S10**). This optimal latent brain state was labeled as  $SH_{WM415}$ , to differentiate the optimal latent brain ( $SH_{WM}$ ) state reported previously<sup>3</sup>.

Next, we used two state-matching algorithms to determine the correspondence between states in each cognitive task and  $n$ -back tasks. Noteworthy, here the key question is whether the state matched to the optimal brain state in the n-back working memory task (from HCP 415 subjects) is the same state matched to the optimal brain state in the n-back working memory task reported in our previous study, which is generated using HCP 122 subjects. To facilitate a straightforward comparison, the new brain states from the n-back working memory task (from HCP 415 subjects) were labeled as  $SX_{WM415}$ , in particular the optimal brain state was labeled as  $SH_{WM415}$ , and the brain states from all the other cognitive control tasks remained the same labels, which are matched to the  $SH_{WM}$ . We found that  $SH_{AxCPT}$ ,  $SH_{CuedTS}$ ,  $SH_{Stern}$ ,  $SH_{Stroop}$ ,  $SH_{SST}$ ,  $SH_{RP1}$  and  $SH_{RP2}$  matches to  $SH_{WM415}$  in each corresponding cognitive task and results from two state-matching algorithm are converging (**Supplementary Figure S11-13**).

In summary, we replicated the key state matching results such that the state matched to  $SH_{WM415}$  is the same state matched to  $SH_{WM}$  in each cognitive task (**Supplementary Figures S11-S13**). Results further demonstrate the robustness and generalizability of our findings.

### **Robustness of state matching with respect to reference cognitive tasks**

To examine the robustness of our findings with respect to the choice of reference cognitive task, we tested state matching using alternative cognitive tasks as reference.

First, we used the HCP RP task as the reference task. The optimal latent brain state in the Relational Processing task was determined by the occupancy rate of the latent brain state and

relation to its cognitive control efficiency score (Accuracy/RT) (**Supplementary Table S9**). This optimal brain state in the RP task was the same state that best match with  $SH_{WM}$ , i.e.  $SH_{RP}$ . Next, using  $SH_{RP}$  as the reference state, we examined whether the state that matched to  $SH_{RP}$  was the same state matched to  $SH_{WM}$ . To simplify the comparison with original results, the same state labels were used in these analyses. **Supplementary Figure S14** shows the state matched to  $SH_{RP}$  in each DMCC task. **Supplementary Figure S15** shows the state matched to  $SH_{RP}$  in the SST. It turns out that, in each cognitive task, the state matched to  $SH_{RP}$  was the same state that matched  $SH_{WM}$ .

Second, we repeated the same analysis using the SST as the reference task. The optimal latent brain state in the SST was determined by the occupancy rate of the latent brain state and correlation with  $1/SSRT$ , the cognitive control performance index of the SST (**Supplementary Table S9**). The optimal brain state in the SST was the same state that best matched  $SH_{WM}$ , i.e.  $SH_{SST}$ . Next, using  $SH_{SST}$  as the reference state, we examined whether the state matched to  $SH_{SST}$  was the same state matched to  $SH_{WM}$ . To simplify the comparison with original results, the same state labels were used in these analyses. **Supplementary Figure S16** shows the state matched to  $SH_{SST}$  in each DMCC task. **Supplementary Figure S17** shows the state matched to  $SH_{SST}$  in the RP task. Again, it turns out that, in each cognitive task, the state matched to  $SH_{SST}$  was the same state that matched  $SH_{WM}$ .

In summary, we replicated the key state matching results such that the state matched to the optimal brain state in other reference cognitive tasks was the same state matched to the  $SH_{WM}$ . Results further demonstrate the robustness and generalizability of our findings.

### Robustness of the main findings with respect to ROI selection

To examine the robustness of the main findings with respect to ROI selection, we conducted additional analysis using ROIs from an independent meta-analysis. We used NeuroSynth with key term “working memory”, which produces a meta-analytic brain map of 1091 studies (<https://neurosynth.org/>). We selected 9 ROIs from the meta-analysis, including bilateral anterior insula, middle frontal gyrus, frontal eye field, intraparietal lobule and right dorsomedial prefrontal cortex, which match the ROIs used in the main analysis. Also, because the meta-analysis did not include deactivated regions, posterior cingulate cortex and ventromedial prefrontal cortex of the DMN in the main analysis were included in the new ROI set (**Supplementary Figure S18a**) in order to keep the same number of ROIs ( $N=11$ ) to match dimensionality and the same approximate cognitive systems. We then tested whether the optimal latent brain state in the n-back working memory task with ROI derived from the meta-analysis also plays behaviorally significant role in other cognitive tasks.

First, we applied BSDS to probe latent brain dynamics in the HCP n-back working memory task. Here the same sample of 122 subjects was used in the analysis. BSDS uncovered 4 distinct latent brain state (**Supplementary Figure S18b**). We determined the optimal latent brain state in the n-back working memory task by its dominant occupancy rate in the 2-back working memory blocks and its positive contribution to accuracy in the 2-back task condition ( $r=0.38$ ,  $p<0.001$ , **Supplementary Figure S18d**). Here, the optimal latent brain state is labeled as  $SH_{META}$ , to differentiate the optimal latent brain ( $SH_{WM}$ ) state reported in our previous study.

Next, we applied BSDS to probe latent brain dynamics in each of the four DMCC cognitive control tasks independently. BSDS uncovered 5 latent brain states in the AxCP, 6 latent brain states in the CuedTS, 5 latent brain states in the Sternberg and 6 latent brain states in the

Stroop. Two state-matching algorithms were used to determine the state that matches  $SH_{META}$ , which is labeled as  $SH_{AxCPT}$ ,  $SH_{CuedTS}$ ,  $SH_{Stern}$ ,  $SH_{Stroop}$  in each DMCC task, respectively (**Supplementary Figure S19**).

We then examined whether the latent brain state that matches  $SH_{META}$  plays an important role in cognitive control in each DMCC task. We conducted the same brain-behavior analyses, including multivariate CCA and univariate *Pearson's* correlation analysis. CCA revealed significant canonical correlations between occupancy rate (OR) of latent brain states and key behavioral measures in each DMCC task (**Supplementary Figure S20a-d**). Univariate analysis revealed that OR of  $SH_{AxCPT}$  is significantly and positively correlated with cognitive control index in the AxCPT ( $r=0.29$ ,  $p=0.04$ ); OR of  $SH_{CuedTS}$  is positively correlated with cognitive control index in the CuedTS with marginal significance ( $r=0.25$ ,  $p=0.08$ ); OR of  $SH_{Stern}$  is significantly and positively correlated with cognitive control index in the Sternberg ( $r=0.37$ ,  $p=0.007$ ); and OR of  $SH_{Stroop}$  is significantly and positively correlated with cognitive control index in the Stroop ( $r=0.28$ ,  $p=0.04$ ) (**Supplementary Figure S20e-h**).

Next, we applied BSDS to probe latent brain dynamics in the SST independently. BSDS uncovered 4 latent brain states in the SST. Two state-matching algorithms were used to determine the state that matches  $SH_{META}$ , which is labeled as  $SH_{SST}$  (**Supplementary Figure S21**).

We then examined whether the latent brain state that matches  $SH_{META}$  plays an important role in the SST. We conducted the same brain-behavior analyses, including multivariate CCA and univariate *Pearson's* correlation analysis. CCA revealed significant canonical correlations between OR of latent brain states and key behavioral measures in the SST (**Supplementary Figure S22**). Univariate analysis revealed that OR of  $SH_{SST}$  is significantly and positively correlated with cognitive control index in the SST ( $r=0.32$ ,  $p=0.03$ ) (**Supplementary Figure S22**).

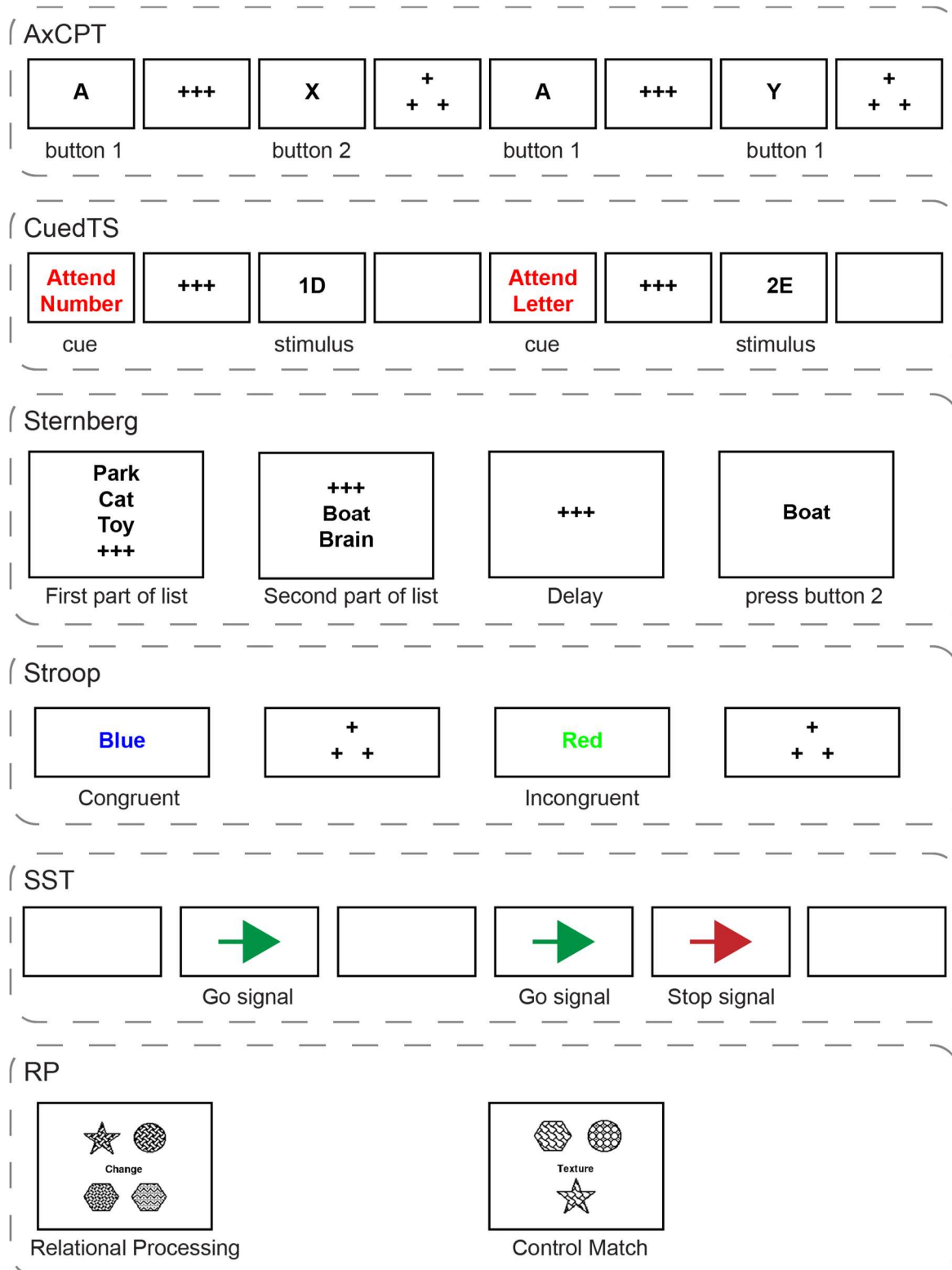
Finally, we applied BSDS on the RP task. In both sessions of the RP task, BSDS uncovered 4 latent brain states. Two state-matching algorithms were used to determine the states that match  $SH_{META}$ , which are labeled as  $SH_{RP1}$  and  $SH_{RP2}$  in session 1 and 2, respectively (**Supplementary Figure S23**).

We examined whether the latent brain state that matches  $SH_{META}$  plays an important role in each session of the RP task. We conducted the same brain-behavior analyses, including multivariate CCA and univariate *Pearson's* correlation analysis. CCA revealed significant canonical correlations between OR of latent brain states and key behavioral measures in each session of the RP task (**Supplementary Figure S24a**). Univariate analysis revealed that OR of  $SH_{RP1}$  is significantly and positively correlated with cognitive control index in the session 1 ( $r=0.25$ ,  $p=0.02$ ) and OR of  $SH_{RP2}$  is significantly and positively correlated with cognitive control index in the session 2 ( $r=0.28$ ,  $p=0.01$ ) (**Supplementary Figure S24b**).

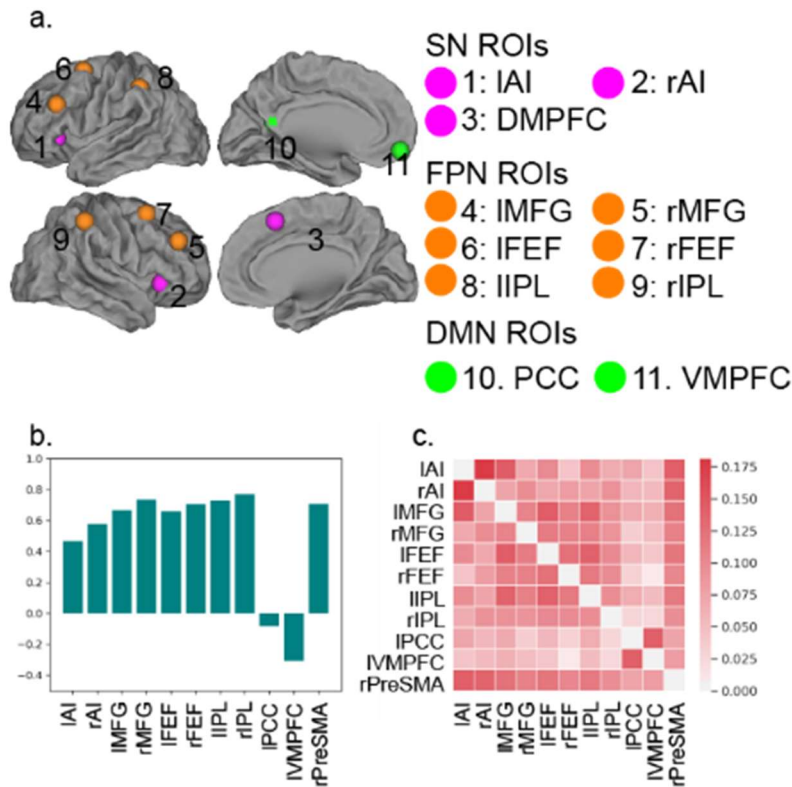
In summary, we replicated the key results in the main analysis using ROIs derived from the meta-analysis, demonstrating the robustness of our findings with respect to the selection of ROIs.

### III. Supplementary Figures

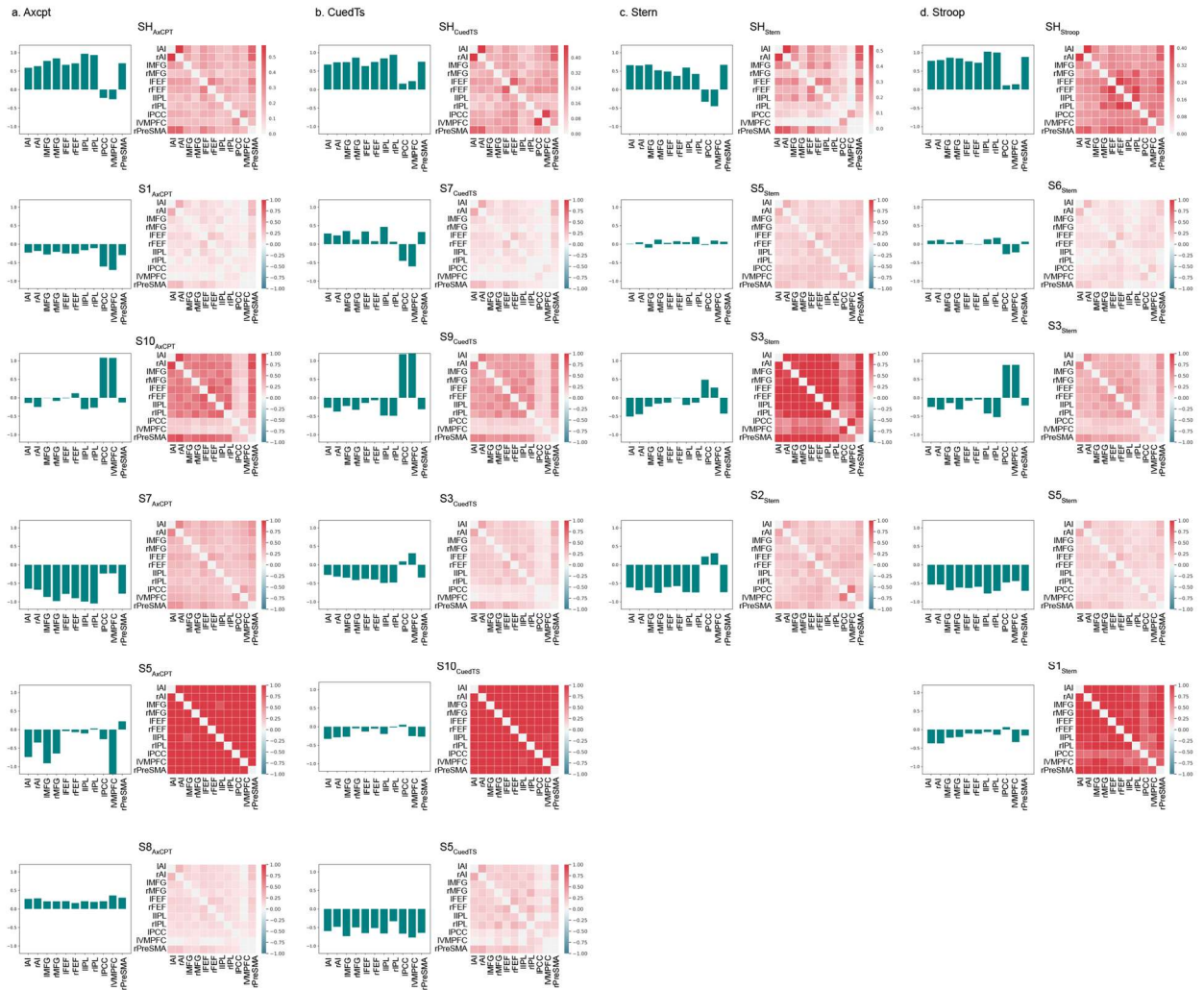
**Supplementary Figure S1.** Schematic overview of AxCPT, CuedTS, Sternberg, Stroop, SST and RP tasks.



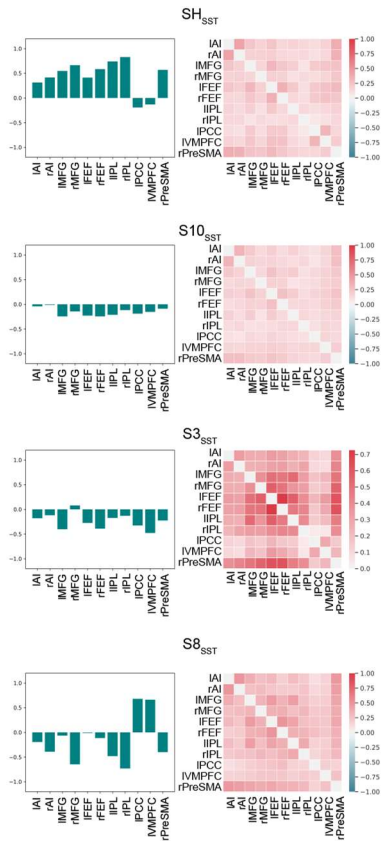
**Supplementary Figure S2.** Brain network model with nodes in the Saliency Network (SN), Frontal-Parietal Network (FPN) and Default Mode network (DMN) (a): 1, left anterior insula (IAI); 2, right anterior insula (rAI); 3, dorsomedial prefrontal cortex (DMPFC); 4, left middle frontal gyrus (IMFG); 5, right middle frontal gyrus (rMFG); 6, left frontal eye field (IFEF); 7, right frontal eye field (rFEF); 8, left intraparietal lobule (IIPL); 9, right intraparietal lobule (rIPL); 10, posterior cingulate cortex (PCC) and 11, ventromedial prefrontal cortex (VMPFC). Multivariate features associated with  $SH_{WM}$ , the task-optimal reference  $n$ -back working memory task. **(b)** Mean and **(c)** Covariance. Source data are provided as a Source data file.



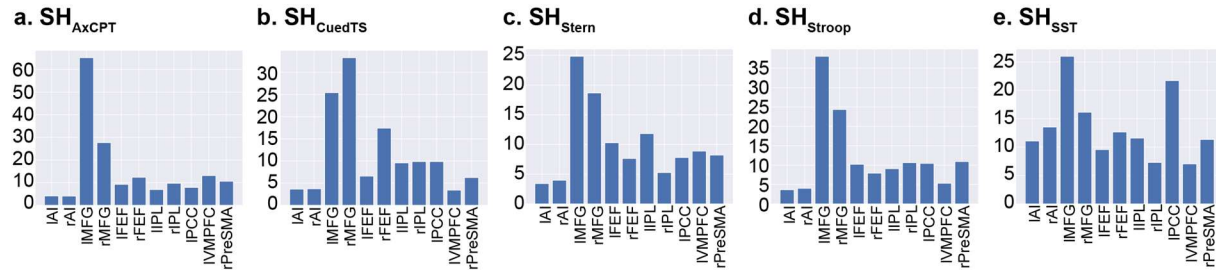
**Supplementary Figure S3.** Brain states in each of the four dual models of cognitive control (DMCC) tasks and their relation to the reference state  $SH_{WM}$ . Each state is characterized by a unique activation/deactivation and connectivity pattern ( $N=50$ ). (a) In the AxCPT,  $SH_{AxCPT}$  is the brain state that matches  $SH_{WM}$ ; the other states  $S1_{AxCPT}$ ,  $S10_{AxCPT}$ ,  $S7_{AxCPT}$ ,  $S5_{AxCPT}$ ,  $S8_{AxCPT}$  do not match  $SH_{WM}$ . (b) In the CuedTS,  $SH_{CuedTS}$  is the brain state that matches  $SH_{WM}$ ; the other states  $S7_{CuedTS}$ ,  $S9_{CuedTS}$ ,  $S3_{CuedTS}$ ,  $S10_{CuedTS}$ , and  $S5_{CuedTS}$  do not match  $SH_{WM}$ . (c) In the Sternberg,  $SH_{Stern}$  is the brain state that matches  $SH_{WM}$  whereas  $S5_{Stern}$ ,  $S4_{Stern}$ , and  $S2_{Stern}$  are the other states. (d) In the Stroop,  $SH_{Stroop}$  is the brain state that matches  $SH_{WM}$ ; the other states  $S6_{Stroop}$ ,  $S3_{Stroop}$ ,  $S5_{Stroop}$ , and  $S1_{Stroop}$  do not match  $SH_{WM}$ . Source data are provided as a Source data file.



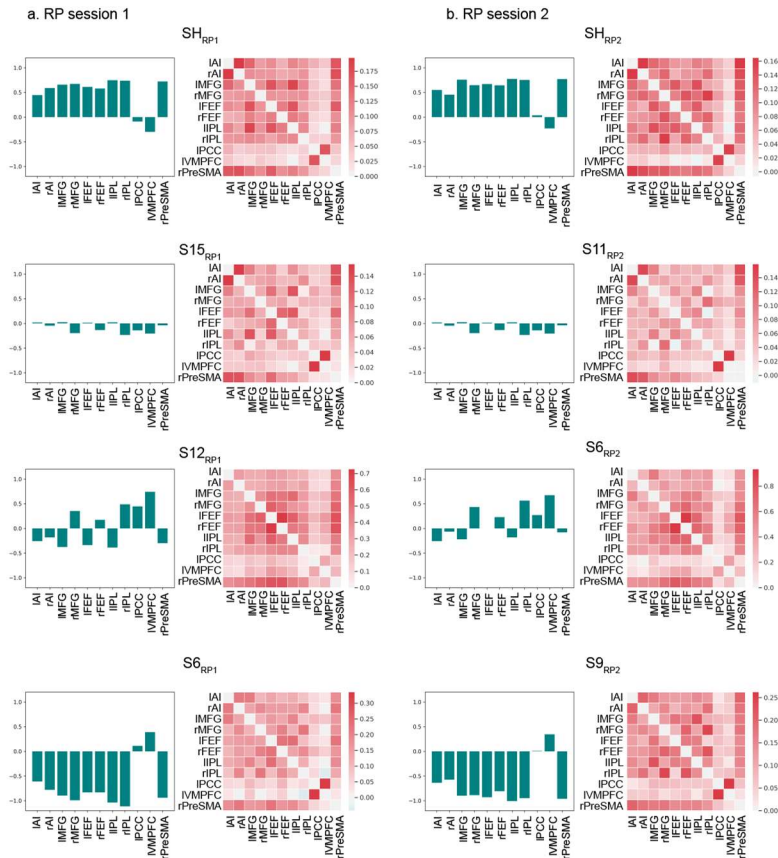
**Supplementary Figure S4.** Brain states in SST and their relation to the reference state  $SH_{WM}$  (N=45). Each state is characterized by a unique activation/deactivation and connectivity patterns.  $SH_{SST}$  is the brain state that matches  $SH_{WM}$ ; the other states  $S10_{SST}$ ,  $S3_{SST}$ , and  $S8_{SST}$  do not match  $SH_{WM}$ . Source data are provided as a Source data file.



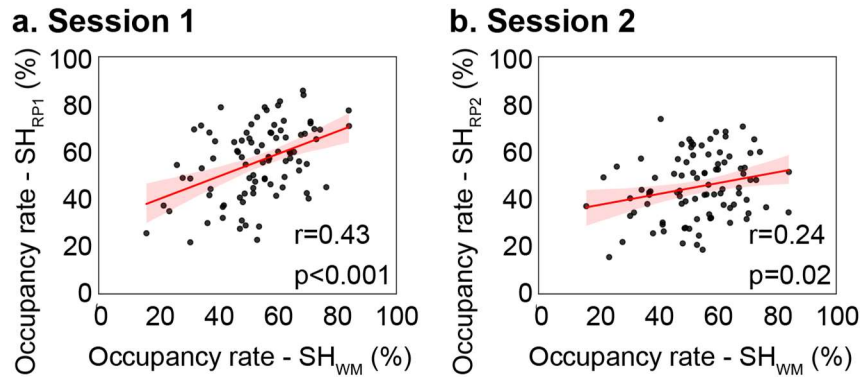
**Supplementary Figure S5. Leave one ROI out analysis reveals critical role of middle frontal gyrus (MFG).** The MFG was the single most important brain region whose dynamic features contribute to shared latent brain states across cognitive tasks. **(a)**  $SH_{AxCPT}$ , **(b)**  $SH_{CuedTS}$ , **(c)**  $SH_{Stern}$ , **(d)**  $SH_{Stroop}$ , and **(e)**  $SH_{SST}$ . Source data are provided as a Source data file.



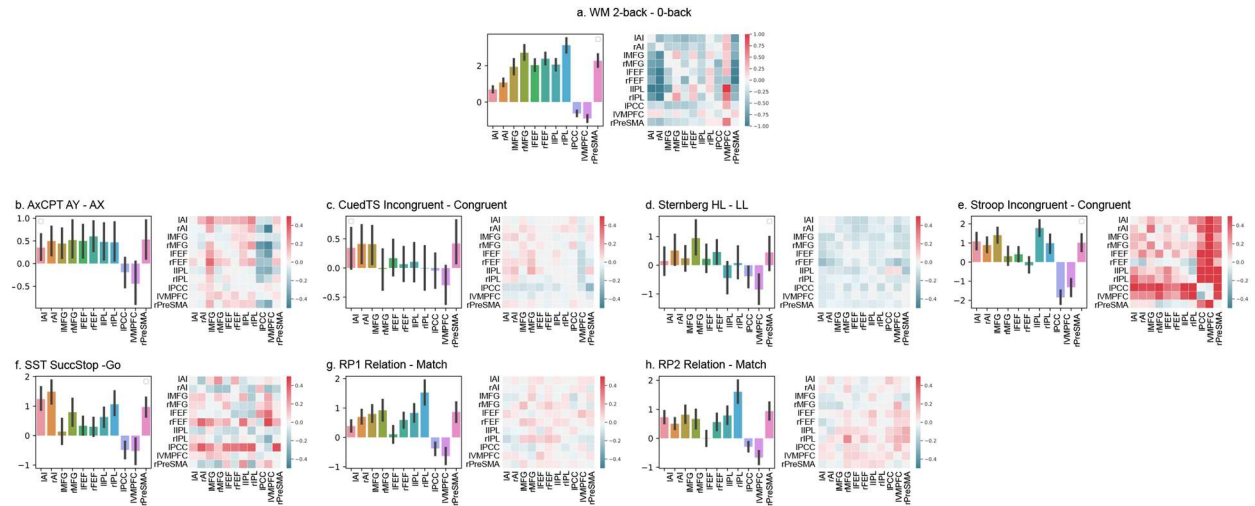
**Supplementary Figure S6.** Brain states in the RP task and their relation to the reference state  $SH_{WM}$  (N=90). Each state is characterized by a unique activation/deactivation and connectivity patterns. **(a)** In Session 1,  $SH_{RP1}$  is the brain state that matches  $SH_{WM}$ ,  $S15_{RP1}$ ,  $S12_{RP1}$ , and  $S6_{RP1}$  are the other states. **(b)** In Session 2,  $SH_{RP2}$  is the brain state that matches  $SH_{WM}$ ; the other states  $S11_{RP2}$ ,  $S6_{RP2}$ , and  $S9_{RP2}$  do not match  $SH_{WM}$ . Source data are provided as a Source data file.



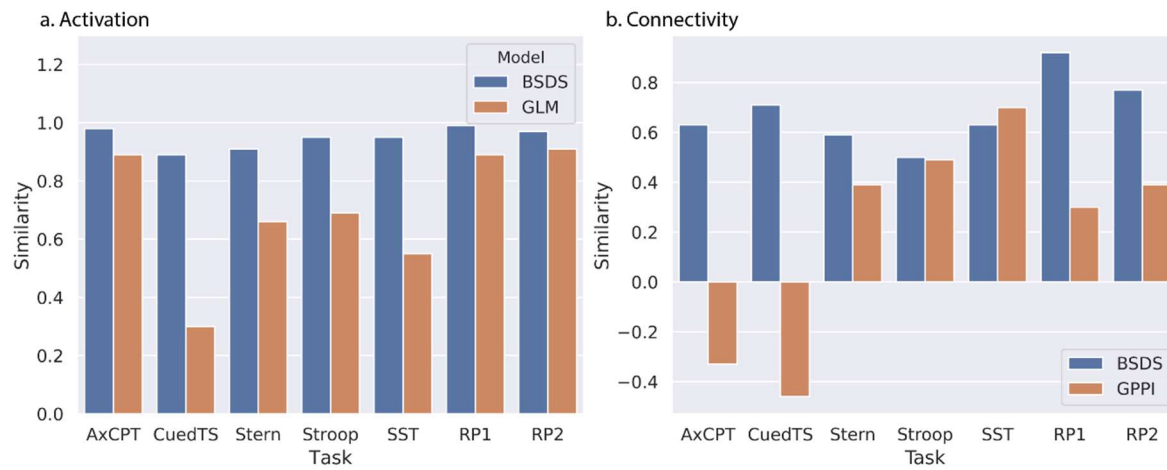
**Supplementary Figure S7. Shared latent brain states within individuals across sessions during the relation processing task.** (a) Individuals (N=90) who have the higher occupancy rates of the  $SH_{WM}$  during the n-back working memory task also have the higher occupancy rates  $SH_{RP1}$  in Session 1 ( $r=0.43$ ,  $p<0.001$ , *Pearson's correlation*). (b) Findings were replicated in Session 2 with  $SH_{RP2}$  ( $r=0.24$ ,  $p=0.02$ , *Pearson's correlation*). The regression estimate is presented with 95% confidence interval (shaded area). P values were not adjusted for multiple comparisons. Source data are provided as a Source data file.



**Supplementary Figure S8.** Activation and connectivity patterns in each of the four dual models of cognitive control (DMCC) tasks (N=50). Contrasts of interest include (a) 2back *minus* 0-back in the *n*-back working memory task; (b) AY *minus* AX in the AxCPT task; (c) Incongruent *minus* Congruent in the CuedTS task; (d) High load (HL) *minus* Low load (LL) in the Sternberg task; (e) Incongruent *minus* Congruent conditions in the Stroop; (f) SuccStop *minus* Go in the SST task, (g) Relation Processing *minus* Match Control in the RP task sessions 1 and 2. Data are presented as mean values  $\pm$  SEM. Source data are provided as a Source data file.

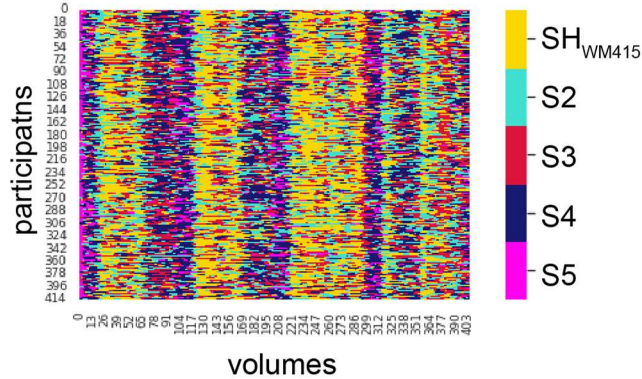


**Supplementary Figure S9.** (a) Similarity of activation/deactivation measures between the reference  $n$ -back working memory task and each of the other seven cognitive tasks using BSDS state-space models (blue) and conventional GLM (orange). (b) Similarity of connectivity measures between the reference  $n$ -back working memory task and each of the other seven cognitive tasks using BSDS state-space models (blue) and conventional GLM (orange). Across all seven cognitive tasks BSDS-derived models generated better model fits with the reference  $n$ -back working memory task than conventional GLM and gPPI analyses. AxCPT: AY-AX; CuedTS: Incongruent-Congruent; Stern: HL-LL; Stroop: Incongruent-Congruent; SST: SuccStop-Go; RP1: Relation Processing session 1; RP2: Relation Processing session 2. Source data are provided as a Source data file.

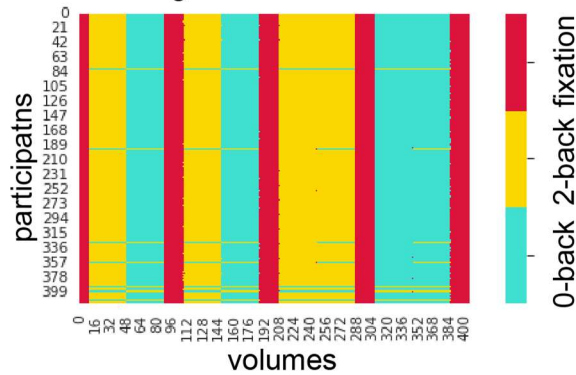


**Supplementary Figure S10. Latent brain states uncovered from the HCP n-back working memory task with 415 subjects.** (a) Temporal evolution of the five latent brain state identified in each of the 415 subjects. (b) Corresponding task waveforms of the three task conditions in the n-back WM task-0-back, 2-back and fixation blocks-are shown in the same layout. (c) OR of the optimal latent brain state for the 2-back condition ( $SH_{WM415}$ ) was significantly correlated with performance accuracy in the 2-back condition ( $r=0.27$ ,  $p<0.001$ , *Pearson's correlation*). The regression estimate is presented with 95% confidence interval (shaded area). Source data are provided as a Source data file.

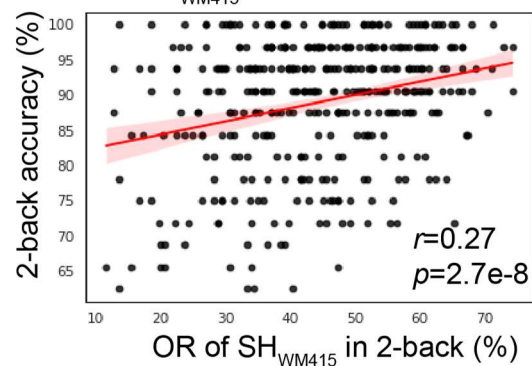
a. Temporal evolution of brain states



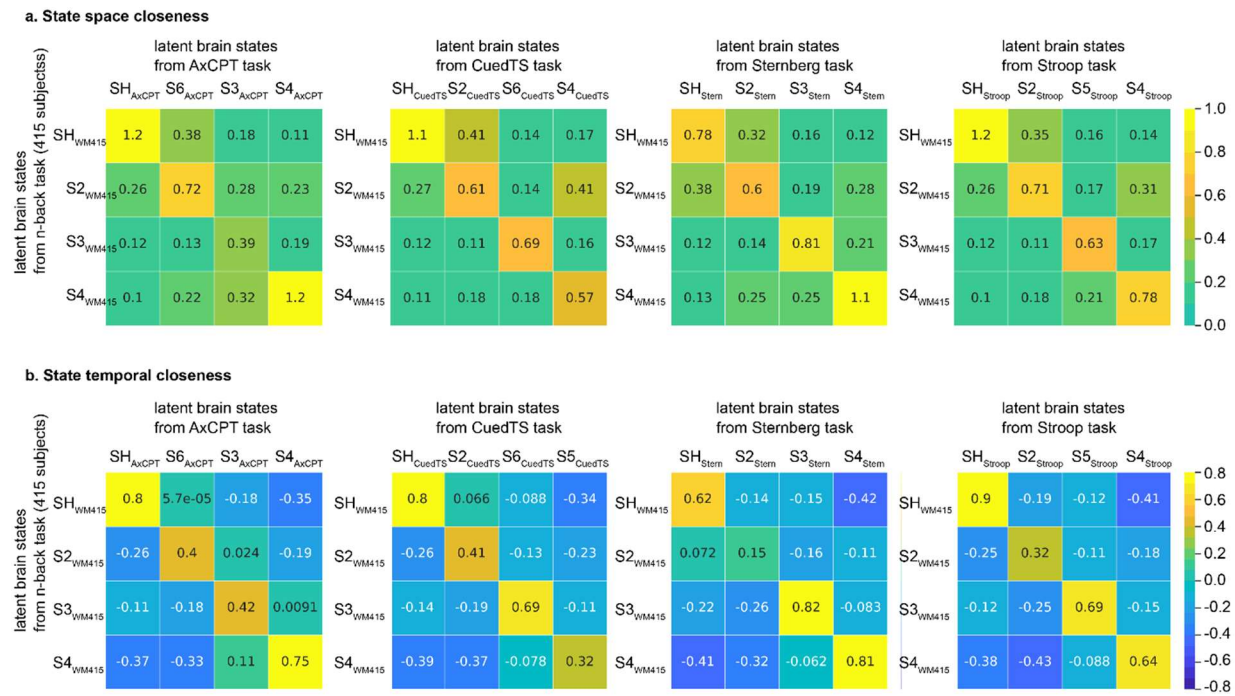
b. Task design of three conditions in n-back



c. OR of  $SH_{WM415}$  in relation to 2-back ACC

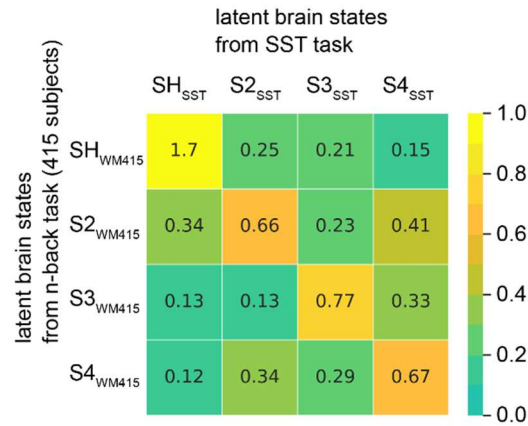


**Supplementary Figure S11. Shared latent brain state across four different dual mode of cognitive control (DMCC) tasks using reference  $SH_{WM415}$  reference states. (a,b)** BSDS uncovered 6 dynamic brain states in the AxCPT (N=50).  $SH_{AxCPT}$  showed the highest state space closeness ( $c=1.2$ ) and highest state temporal closeness ( $r=0.8$ ) with  $SH_{WM415}$ . BSDS uncovered 6 dynamic brain states in the CuedTS task.  $SH_{CuedTS}$  showed the highest state space closeness ( $c=1.1$ ) and the highest state temporal closeness ( $r=0.8$ ) with  $SH_{WM415}$ . BSDS uncovered 4 dynamic brain states in the Sternberg working memory task.  $SH_{Stern}$  showed the highest state space closeness ( $c=0.78$ ) and highest state temporal closeness ( $r=0.62$ ) with  $SH_{WM415}$ . BSDS uncovered 5 dynamic brain state in the Stroop task.  $SH_{Stroop}$  showed the highest state space closeness ( $c=1.2$ ) and the highest state temporal closeness ( $r=0.9$ ) with  $SH_{WM415}$ .  $SH_{WM415}$  refers to the high-load dynamic brain state in the n-back working memory task from a HCP cohort of 415 subjects. In each task, four best matched latent states are illustrated here. Color bars are the scales for state space closeness and state temporal closeness.

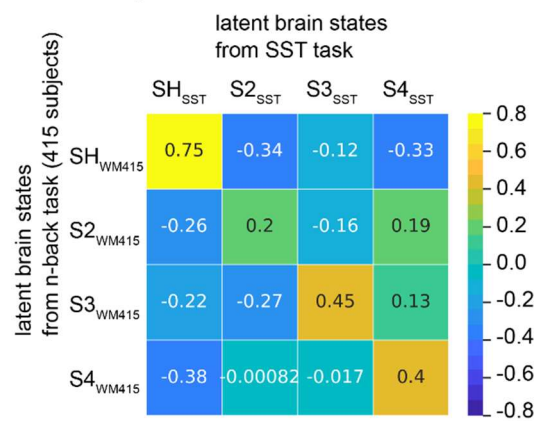


**Supplementary Figure S12. Shared latent brain states in the SST using the  $SH_{WM415}$  reference state.** (a) BSDS uncovered 4 dynamic brain states ( $N=45$ ).  $SH_{SST}$  showed the highest state space closeness ( $r=1.7$ ). (b)  $SH_{SST}$  also showed the highest state temporal closeness ( $c=0.75$ ) with  $SH_{WM415}$ .  $SH_{WM415}$  refers to the high-load dynamic brain state in the n-back working memory task from a HCP 1200 cohort of 415 subjects. Color bars are the scales for state space closeness and state temporal closeness.

**a. State space closeness**

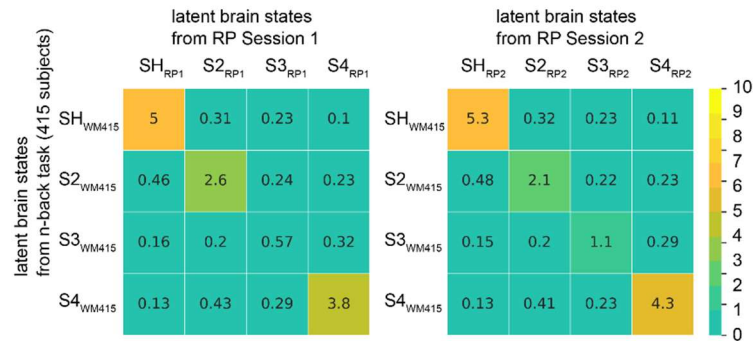


**b. State temporal closeness**

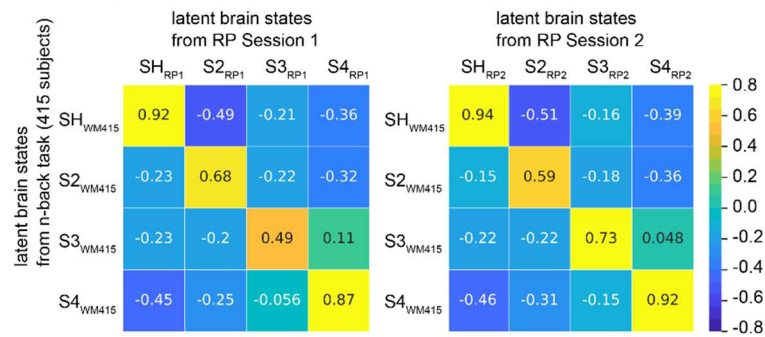


**Supplementary Figure S13. Shared latent brain states in the RP task using  $SH_{WM415}$  reference states. (a, b)** BSDS uncovered 4 dynamic brain states in both Sessions 1 and 2 (N=90).  $SH_{RP1}$  has the highest state space closeness ( $c=5$ ) and the highest state temporal closeness ( $r=0.92$ ) with  $SH_{WM415}$  in Session 1.  $SH_{RP2}$  has the highest state space closeness ( $c=5.3$ ) and the highest state temporal closeness ( $r=0.94$ ) with  $SH_{RP}$  in Session 2.  $SH_{WM415}$  refers to the high-load dynamic brain state in the n-back working memory task from a HCP 1200 cohort of 415 subjects. Color bars are the scales for state space closeness and state temporal closeness.

**a. State space closeness**

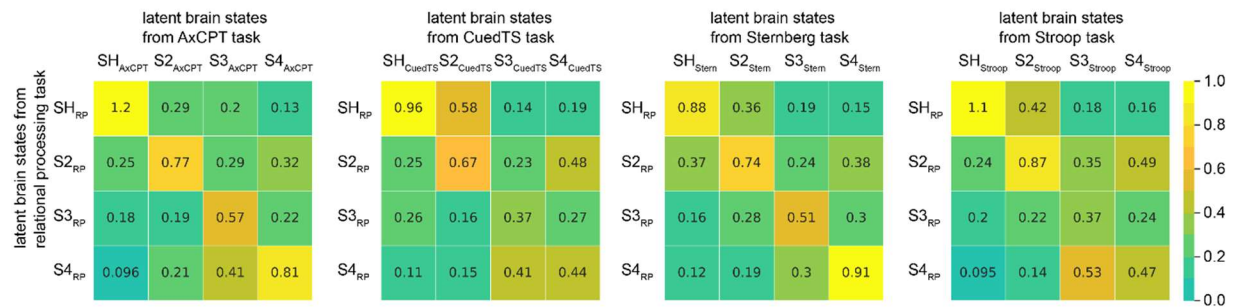


**b. State temporal closeness**

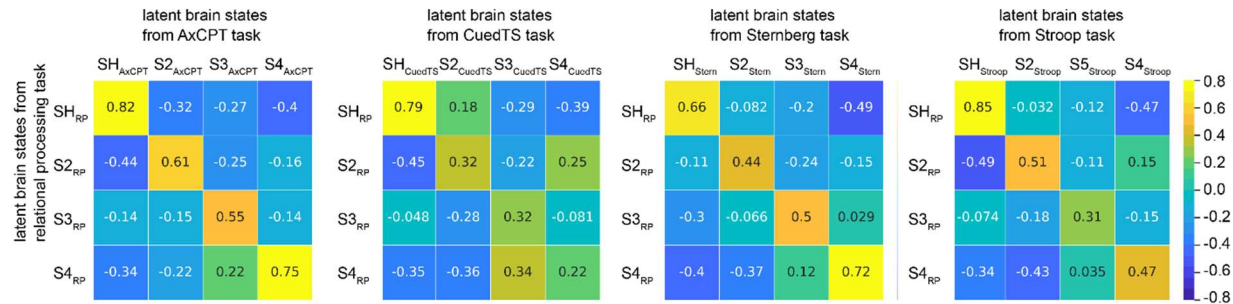


**Supplementary Figure S14. Shared latent brain state across four different dual mode of cognitive control (DMCC) tasks using reference states  $SH_{RP}$  from the RP task. (a,b)** BSDS uncovered 6 dynamic brain states in the AxCPT (N=50).  $SH_{AxCPT}$  showed the highest state space closeness ( $c=1.2$ ) and highest state temporal closeness ( $r=0.82$ ) with  $SH_{RP}$ . BSDS uncovered 6 dynamic brain states in the CuedTS task.  $SH_{CuedTS}$  showed the highest state space closeness ( $c=0.96$ ) and the highest state temporal closeness ( $r=0.79$ ) with  $SH_{RP}$ . BSDS uncovered 4 dynamic brain states in the Sternberg working memory task.  $SH_{Stern}$  showed the highest state space closeness ( $c=0.88$ ) and highest state temporal closeness ( $r=0.66$ ) with  $SH_{RP}$ . BSDS uncovered 5 dynamic brain state in the Stroop task.  $SH_{Stroop}$  showed the highest state space closeness ( $c=1.1$ ) and the highest state temporal closeness ( $r=0.85$ ) with  $SH_{RP}$ .  $SH_{RP}$  refers to the high-load dynamic brain state in the RP task. In each task, the best matched four latent states are illustrated here. Color bars are the scales for state space closeness and state temporal closeness.

**a. State space closeness**

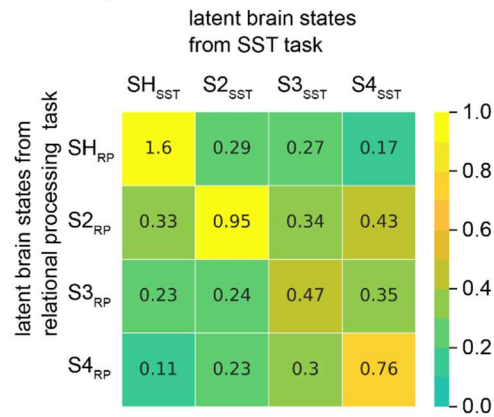


**b. State temporal closeness**

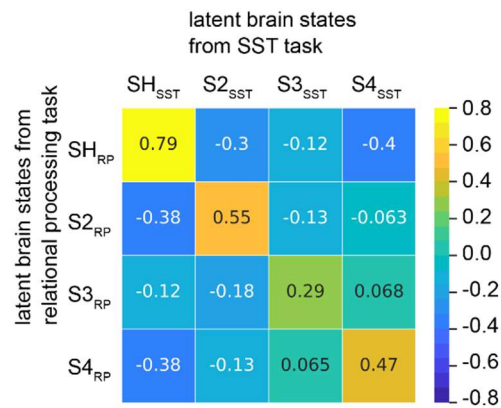


**Supplementary Figure S15. Shared latent brain states in the SST using reference states  $SH_{RP}$  from the RP task.** (a) BSDS uncovered 4 dynamic brain states ( $N=45$ ).  $SH_{SST}$  showed the highest state space closeness ( $r=1.6$ ). (b)  $SH_{SST}$  also showed the highest state temporal closeness ( $c=0.79$ ) with  $SH_{RP}$ .  $SH_{RP}$  refers to the high-load dynamic brain state in the RP task. Color bars are the scales for state space closeness and state temporal closeness.

**a. State space closeness**

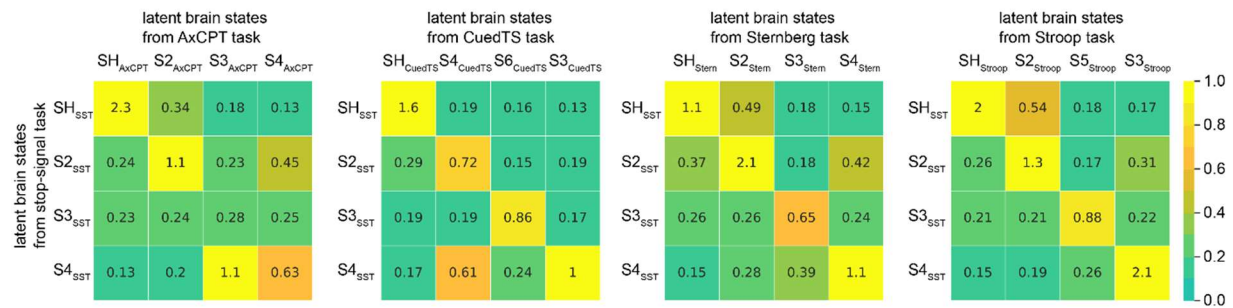


**b. State temporal closeness**

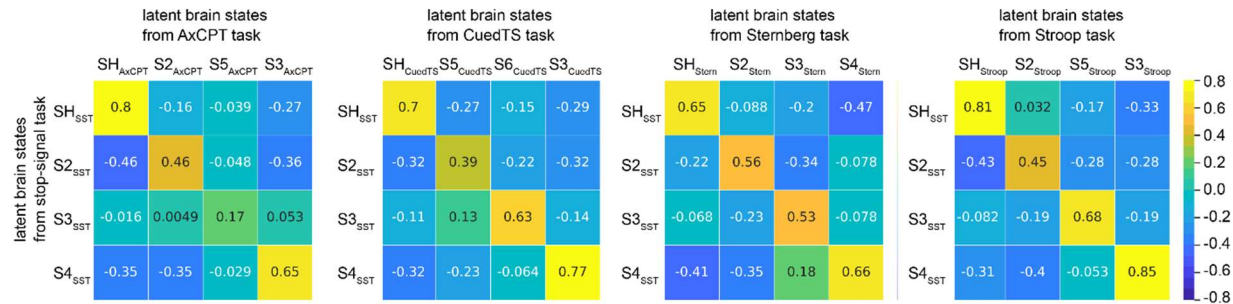


**Supplementary Figure S16. Shared latent brain state across four different dual mode of cognitive control (DMCC) tasks using reference states  $SH_{SST}$  from the SST. (a,b) BDS** uncovered 6 dynamic brain states in the AxCPT (N=50).  $SH_{AxCPT}$  showed the highest state space closeness ( $c=2.3$ ) and highest state temporal closeness ( $r=0.8$ ) with  $SH_{SST}$ . BDS uncovered 6 dynamic brain states in the CuedTS task.  $SH_{CuedTS}$  showed the highest state space closeness ( $c=1.6$ ) and the highest state temporal closeness ( $r=0.7$ ) with  $SH_{SST}$ . BDS uncovered 4 dynamic brain states in the Sternberg working memory task.  $SH_{Stern}$  showed the highest state space closeness ( $c=1.1$ ) and highest state temporal closeness ( $r=0.65$ ) with  $SH_{SST}$ . BDS uncovered 5 dynamic brain state in the Stroop task.  $SH_{Stroop}$  showed the highest state space closeness ( $c=2$ ) and the highest state temporal closeness ( $r=0.81$ ) with  $SH_{SST}$ .  $SH_{SST}$  refers to the high-load dynamic brain state in the stop-signal task. In each task, the best matched four latent states are illustrated here. Color bars are the scales for state space closeness and state temporal closeness.

**a. State space closeness**

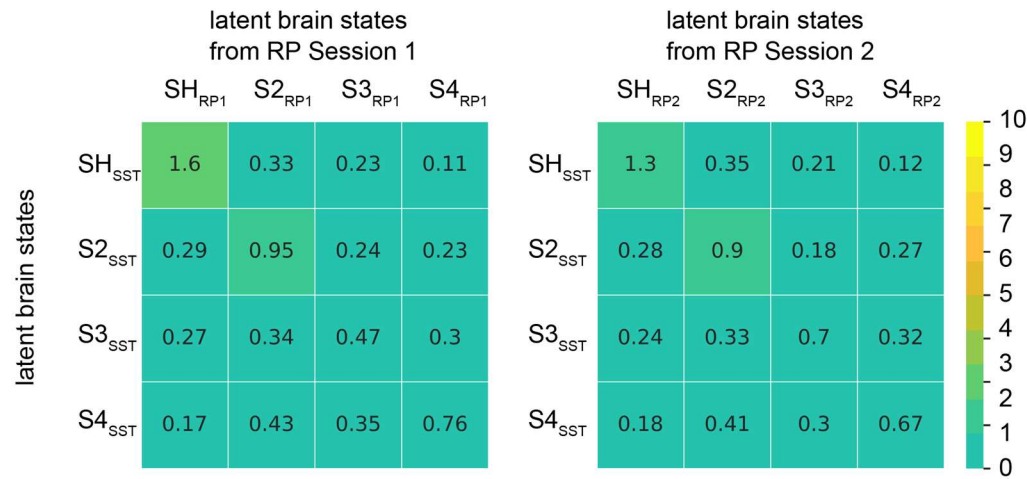


**b. State temporal closeness**

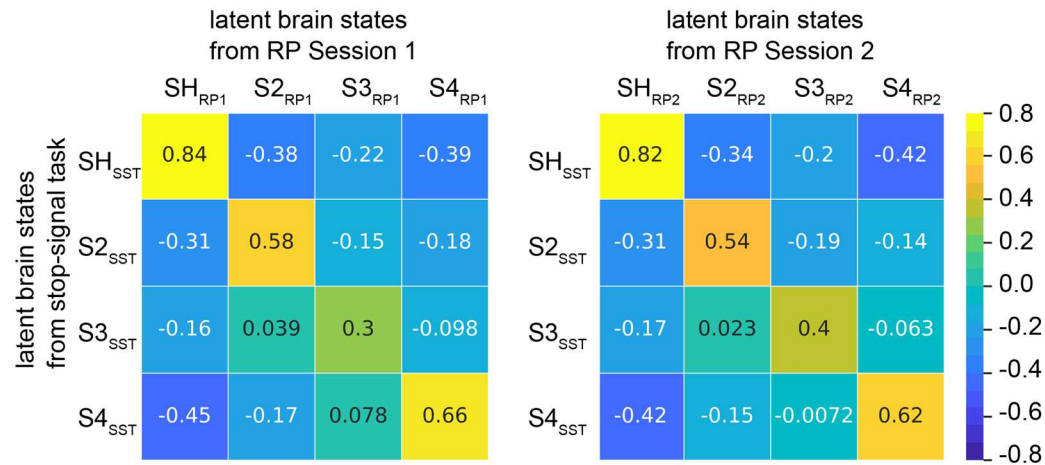


**Supplementary Figure S17. Shared latent brain states in the RP task using reference states  $SH_{SST}$  from the SST.** (a, b) BSDS uncovered 4 dynamic brain states in both Sessions 1 and 2 (N=90).  $SH_{RP1}$  has the highest state space closeness ( $c=1.6$ ) and the highest state temporal closeness ( $r=0.84$ ) with  $SH_{SST}$  in Session 1.  $SH_{RP2}$  has the highest state space closeness ( $c=1.3$ ) and the highest state temporal closeness ( $r=0.82$ ) with  $SH_{RP}$  in Session 2.  $SH_{SST}$  refers to the high-load dynamic brain state in the SST. Color bars are the scales for state space closeness and state temporal closeness.

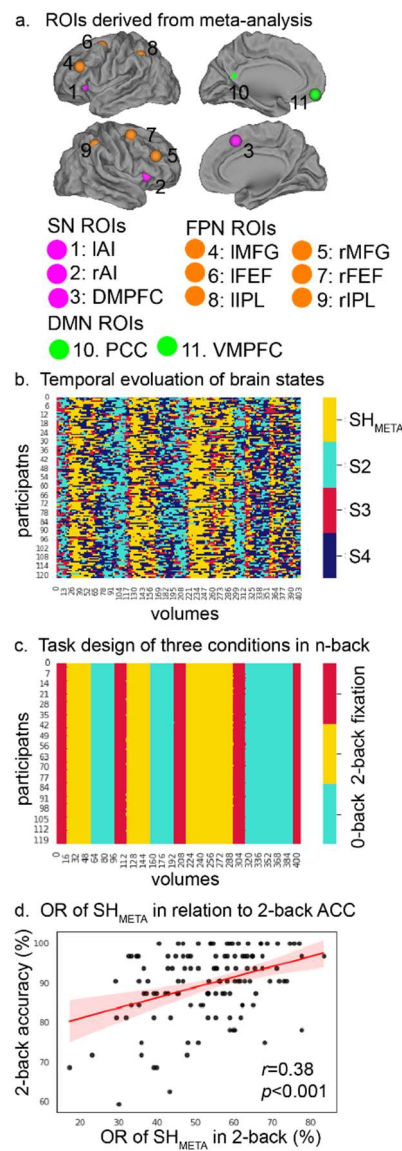
**a. State space closeness**



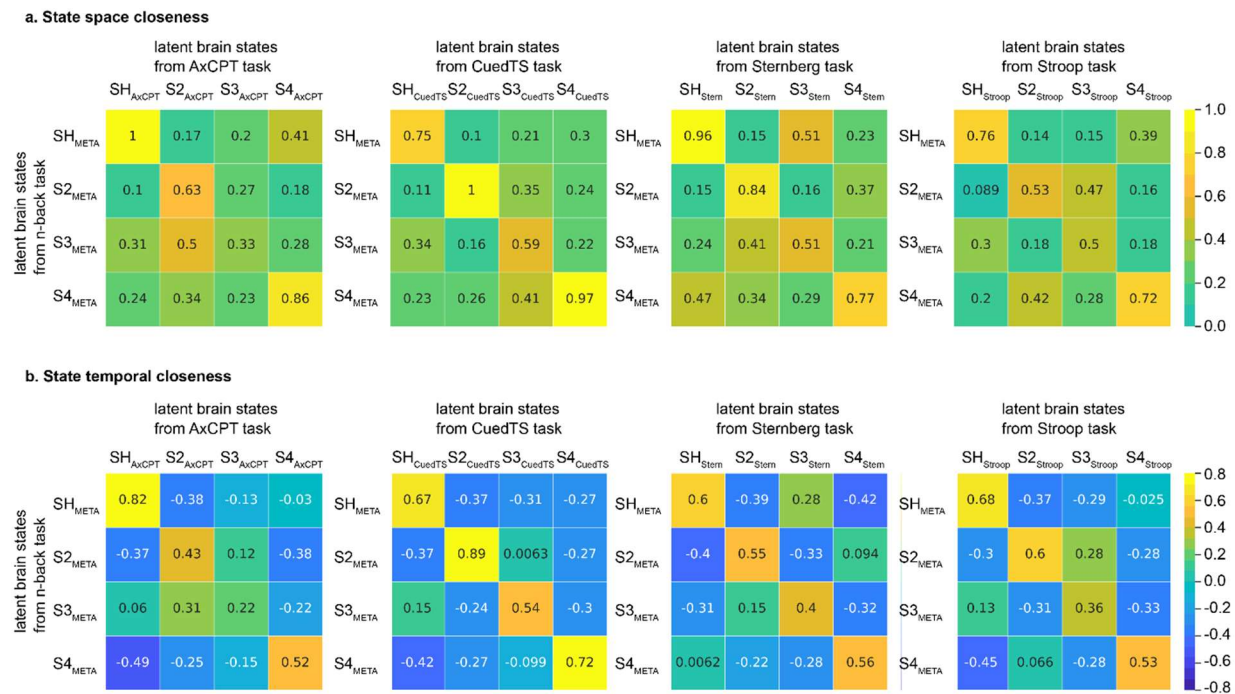
**b. State temporal closeness**



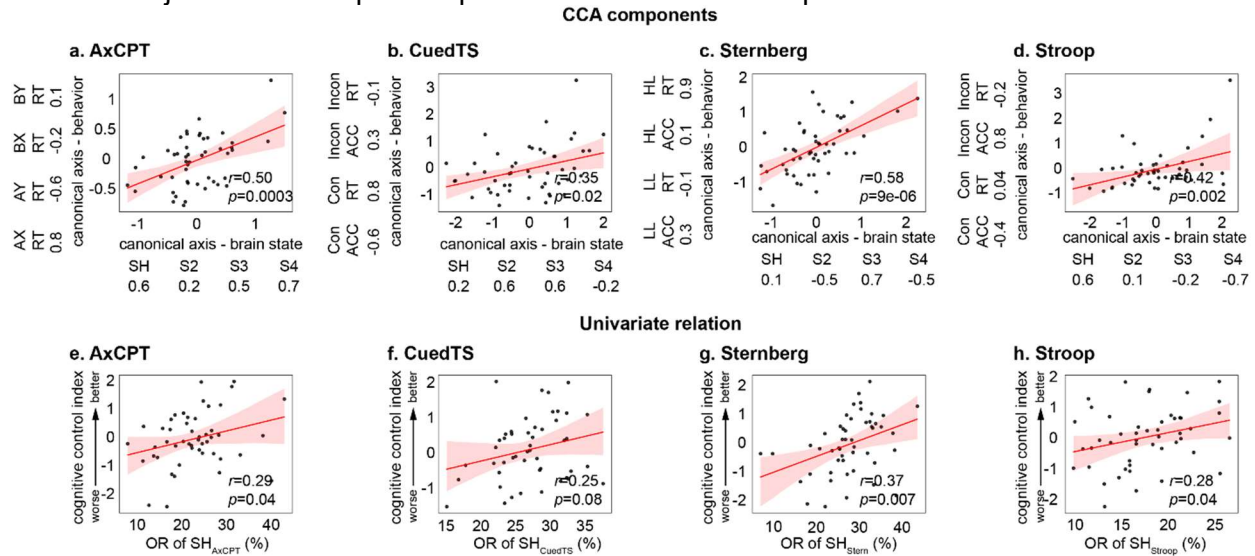
**Supplementary Figure S18. Latent brain states uncovered from the HCP n-back working memory task with ROIs from an independent meta-analysis. (a)** ROIs derived from meta-analysis of working memory in NeuroSynth. 1, left anterior insula (lAI); 2, right anterior insula (rAI); 3, dorsomedial prefrontal cortex (DMPFC); 4, left middle frontal gyrus (lMFG); 5, right middle frontal gyrus (rMFG); 6, left frontal eye field (lFEF); 7, right frontal eye field (rFEF); 8, left intraparietal lobule (lIPL); 9, right intraparietal lobule (rIPL); 10, posterior cingulate cortex (PCC) and 11, ventromedial prefrontal cortex (VMPFC). SN: salience network; FPN: frontoparietal network; DMN: default mode network. **(b)** Temporal evolution of the 4 latent brain state identified in each of the 122 subjects. **(c)** Corresponding task waveforms of the three task conditions in the n-back WM task-0-back, 2-back and fixation blocks-are shown in the same layout. **(d)** OR of the optimal latent brain state for the 2-back condition ( $SH_{META}$ ) was significantly correlated with performance accuracy in the 2-back condition ( $r=0.27$ ,  $p<0.001$ , *Pearson's* correlation). The regression estimate is presented with 95% confidence interval (shaded area). Source data are provided as a Source data file.



**Supplementary Figure S19. Shared latent brain state across four different dual mode of cognitive control (DMCC) tasks (reference is SH<sub>META</sub>) with ROIs derived from an independent meta-analysis. (a,b) BSDS uncovered 5 dynamic brain states in the AxCPPT (N=50). SH<sub>AXCPPT</sub> showed the highest state space closeness (c=1) and highest state temporal closeness (r=0.82) with SH<sub>META</sub>. BSDS uncovered 6 dynamic brain states in the CuedTS task. SH<sub>CuedTS</sub> showed the moderate state space closeness (c=0.75) and the moderate state temporal closeness (r=0.67) with SH<sub>META</sub>. BSDS uncovered 5 dynamic brain states in the Sternberg working memory task. SH<sub>Stern</sub> showed the highest state space closeness (c=0.96) and the highest state temporal closeness (r=0.6) with SH<sub>META</sub>. BSDS uncovered 6 dynamic brain state in the Stroop task. SH<sub>Stroop</sub> showed the highest state space closeness (c=0.76) and the highest state temporal closeness (r=0.68) with SH<sub>META</sub>. SH<sub>META</sub> refers to the high-load dynamic brain state in the n-back working memory task with ROIs derived from an independent meta-analysis. In each task, the best matched four latent states are illustrated here. Color bars are the scales for state space closeness and state temporal closeness.**

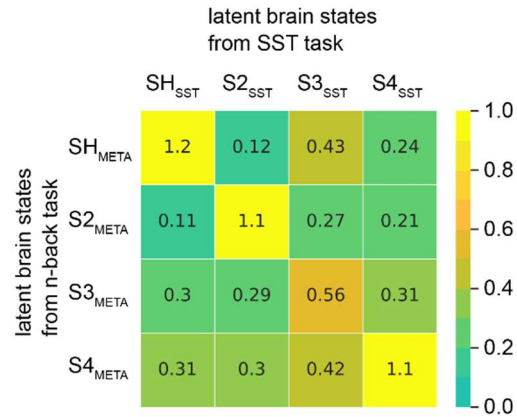


**Supplementary Figure S20. Latent brain states are associated with task performance in all four dual mode of cognitive control (DMCC) tasks with ROIs derived from an independent meta-analysis.** Multivariate CCA revealed significant correlations between occupancy rates of latent brain states and behavioral variables in all the DMCC tasks, including (a) AxCPT, (b) CuedTS, (c) Sternberg and (d) Stroop (N=50). In each task, the component in which linear combination of behavioral variables that best represents general cognitive control was selected to investigate the relationship between latent brain state and behavioral performance. Univariate *Pearson's* correlation revealed significant correlation between occupancy rate of the multi-demand brain state (e.g. SH<sub>AxCPT</sub>) and cognitive control index in all the DMCC tasks, including (e) AxCPT, (f) CuedTS, (g) Sternberg task, and (h) Stroop. SH<sub>AxCPT</sub>, SH<sub>CuedTS</sub>, SH<sub>Stern</sub> and SH<sub>Stroop</sub> refers to the dynamic brain state that matches to SH<sub>WM</sub> in the AxCPT, CuedTS, Sternberg and Stroop tasks, respectively. AxCPT = Ax Continuous performance task; CuedTS = Cued task switching task; ACC = Accuracy; RT = Reaction time; LL = Low load; HL = High load; Con = Congruent; Incon = Incongruent; OR = Occupancy rate. The regression estimate is presented with 95% confidence interval (shaded area). P values were not adjusted for multiple comparisons. Source data are provided as a Source data file.

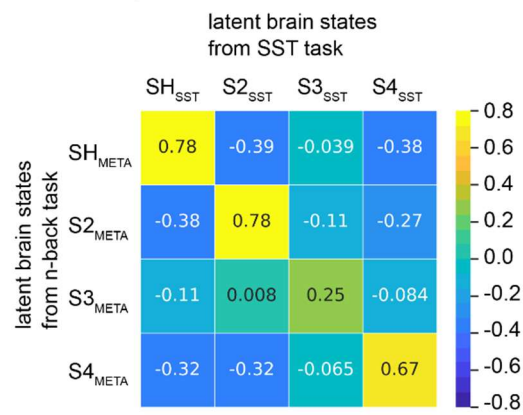


**Supplementary Figure S21. Shared latent brain state in the SST (reference is  $SH_{META}$ ) with ROIs derived from an independent meta-analysis.** BSDS uncovered 4 dynamic brain states in the SST (N=45).  $SH_{SST}$  showed **(a)** the highest state space closeness ( $c=1.2$ ) and **(b)** highest state temporal closeness ( $r=0.78$ ) with  $SH_{META}$ .  $SH_{META}$  refers to the high-load dynamic brain state in the n-back working memory task with ROIs derived from an independent meta-analysis. Color bars are the scales for state space closeness and state temporal closeness.

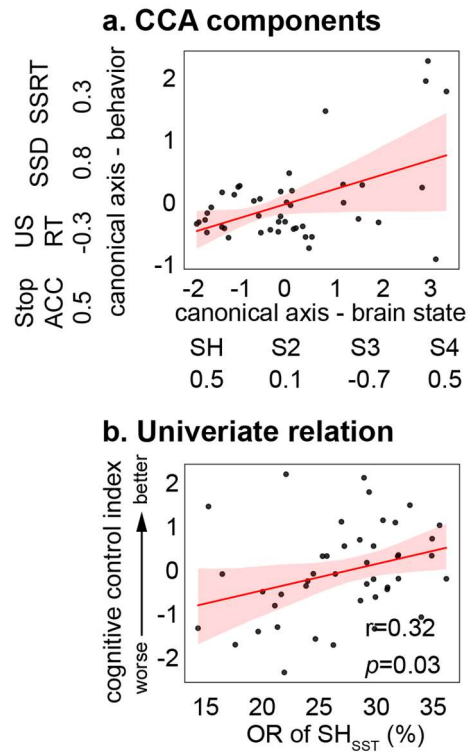
**a. State space closeness**



**b. State temporal closeness**

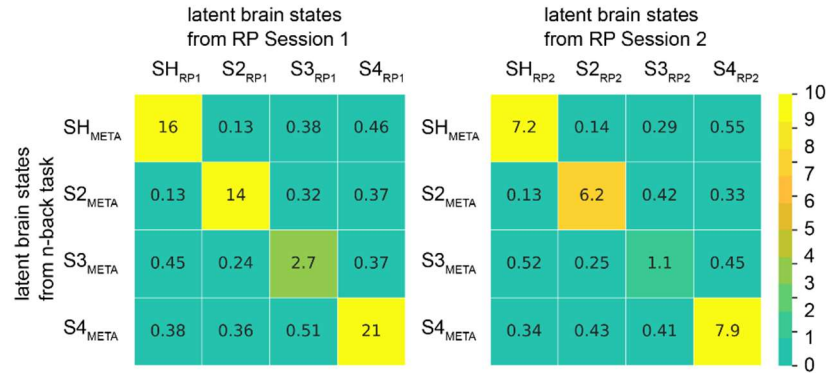


**Supplementary Figure S22. Latent brain states are associated with task performance in the SST with ROIs derived from an independent meta-analysis.** (a) Multivariate CCA revealed significant canonical correlations between occupancy rates of latent brain states and behavioral variables in SST (N=45). (b) Univariate *Pearson's* correlation analysis revealed that OR of SH<sub>SST</sub> is significantly correlated with cognitive control index in the SST. SH<sub>SST</sub> refers to the dynamic brain state that matches to SH<sub>META</sub> in the SST. ACC = Accuracy; RT = Reaction Time; US = Unsuccessful Stopping; SSD = Stop Signal Delay; SSRT = Stop Signal Reaction Time; OR = Occupancy rate. The regression estimate is presented with 95% confidence interval (shaded area). Source data are provided as a Source data file.

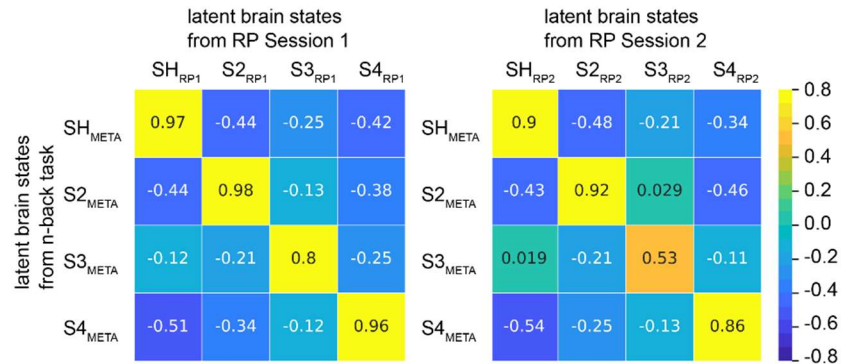


**Supplementary Figure S23. Shared latent brain state across two sessions of the RP task (reference is  $SH_{META}$ ) with ROIs derived from an independent meta-analysis. (a, b) BSDS uncovered 4 dynamic brain states in both Sessions 1 and 2 (N=90).  $SH_{RP1}$  has the highest state space closeness ( $c=16$ ) and high state temporal closeness ( $r=0.97$ ) with  $SH_{META}$  in Session 1.  $SH_{RP2}$  has the highest state space closeness ( $c=7.2$ ) and high state temporal closeness ( $r=0.9$ ) with  $SH_{META}$  in Session 2.  $SH_{META}$  refers to the high-load dynamic brain state in the n-back working memory task with ROIs derived from an independent meta-analysis.  $SH_{RP1}$  and  $SH_{RP2}$  refers to the dynamic brain states that matches to  $SH_{META}$  in the Relational task session 1 and 2, respectively. Color bars are the scales for state space closeness and state temporal closeness.**

**a. State space closeness**

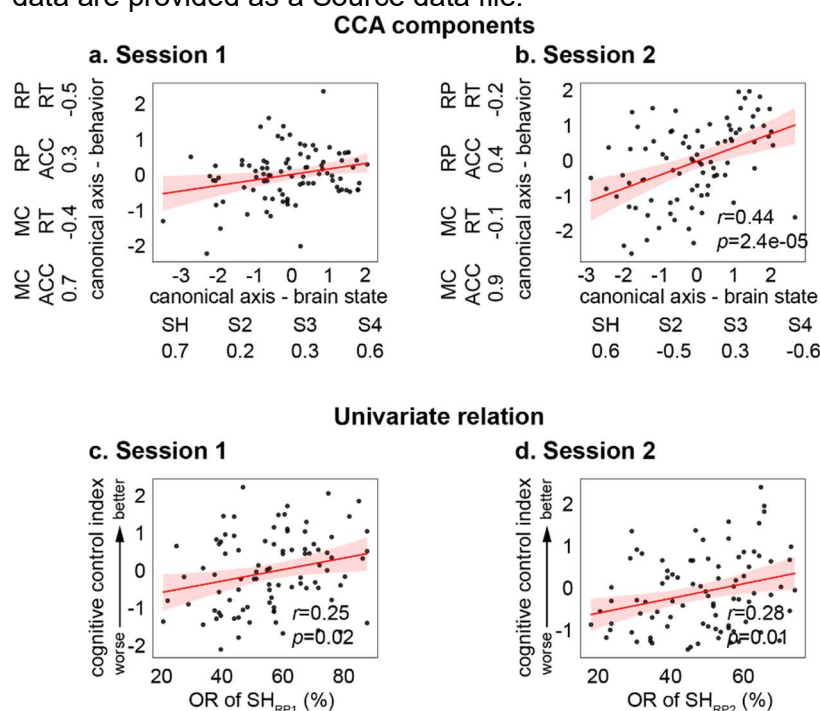


**b. State temporal closeness**



# Supplementary Figure S24. Latent brain states are associated with task performance in each session of the RP task with ROIs derived from an independent meta-analysis.

Multivariate CCA revealed significant correlations between occupancy rates of latent brain states and behavioral variables in the HCP RP task session 1 (a) and 2 (b) (N=90). Univariate *Pearson's* correlation analysis revealed that OR of SH<sub>SST</sub> is significantly correlated with cognitive control index in the HCP RP session 1 (c) and 2 (d). SH<sub>RP1</sub> and SH<sub>RP2</sub> refers to the dynamic brain states that matches to SH<sub>WM</sub> in the Relational task session 1 and 2, respectively. HCP = Human Connectome Project; RP = Relational Processing; MC = Matching Control; ACC = Accuracy; RT = Reaction Time; OR = Occupancy rate. The regression estimate is presented with 95% confidence interval (shaded area). Color bars are the scales for state space closeness and state temporal closeness. P values were not adjusted for multiple comparisons. Source data are provided as a Source data file.



#### IV. Supplementary Tables

**Table S1. Seven cognitive tasks across four datasets used in the present study.** Tasks are listed in the order analyzed. HCP = Human Connectome Project; DMCC = Dual Mechanisms of Cognitive Control; N-back = n-back working memory task; AxCPT = Ax continuous performance task; CuedTS = Cued task switching task; Sternberg = Sternberg working memory task; Stroop = Stroop interference task; SST = Stop signal task; RP = Relational processing; TR = Time Repetition.

| <b>Dataset</b>  | <b>Cognitive Tasks</b>                 | <b>Sample Size</b> | <b>Age</b> | <b>Gender (F/M)</b> | <b>TR (ms)</b> |
|-----------------|----------------------------------------|--------------------|------------|---------------------|----------------|
| <b>HCP</b>      | N-back                                 | 90                 | 22-36      | 53/37               | 720            |
| <b>DMCC</b>     | AxCPT<br>CuedTS<br>Sternberg<br>Stroop | 50                 | 19-42      | 31/19               | 1200           |
|                 |                                        |                    |            |                     |                |
| <b>Stanford</b> | SST                                    | 45                 | 9-12       | 22/23               | 490            |
|                 |                                        |                    |            |                     |                |
| <b>HCP</b>      | RP                                     | 90                 | 22-36      | 53/37               | 720            |

**Supplementary Table S2.** Behavioral results for AxCPT, CuedTS, Sternberg and Stroop tasks in the DMCC study. Con: congruent; Incon = Incongruent. P values were not adjusted for multiple comparisons. Source data are provided as a Source data file.

| <i>Task/Condition</i> | <i>Accuracy (%)</i> | <i>RT (ms)</i> | <i>Task Comparisons</i> | <i>t-value</i> | <i>Cohen's d</i> | <i>p-value</i> |
|-----------------------|---------------------|----------------|-------------------------|----------------|------------------|----------------|
| <b>AxCPT</b>          |                     |                |                         |                |                  |                |
| AX                    | 95±7                | 437±100        | AY - AX Acc             | 0.04           | 0.011            | 0.097          |
| AY                    | 95±8                | 583±93         | AY - AX RT              | 17.44          | 4.933            | <0.001         |
| BX                    | 86±13               | 614±170        | BX - BY Acc             | 4.61           | 1.303            | <0.001         |
| BY                    | 85±8                | 480±106        | BX - BY RT              | 8.02           | 2.268            | <0.001         |
|                       |                     |                |                         |                |                  |                |
| <b>CuedTS</b>         |                     |                |                         |                |                  |                |
| Con                   | 96±6                | 1113±224       | Incon - Con Acc         | 4.7            | 1.517            | <0.001         |
| Incon                 | 93±7                | 1150±216       | Incon - Con RT          | 3.2            | 0.533            | 0.002          |
|                       |                     |                |                         |                |                  |                |
| <b>Stern</b>          |                     |                |                         |                |                  |                |
| LL                    | 88±10               | 989±153        | HL -LL Acc              | 4.02           | 1.138            | 0.0002         |
| HL                    | 84±10               | 1014±169       | HL - LL RT              | 2.69           | 0.761            | 0.01           |
|                       |                     |                |                         |                |                  |                |
| <b>Stroop</b>         |                     |                |                         |                |                  |                |
| Con                   | 99±1                | 862±121        | Incon - Con Acc         | 4.45           | 1.259            | <0.001         |
| Incon                 | 97±5                | 987±123        | Incon - Con RT          | 13.76          | 3.892            | <0.001         |

**Supplementary Table S3. Canonical correlation analysis of brain-behavior relations in the four dual model of cognitive control (DMCC) tasks.** Canonical correlation weights for brain state and behavioral performance measures are shown. OR = Occupancy Rate; Con: congruent; Incon = Incongruent.

| <b>AxCPT</b>          |       | <b>CuedTS</b>         |       | <b>Stern</b>          |       | <b>Stroop</b>         |       |
|-----------------------|-------|-----------------------|-------|-----------------------|-------|-----------------------|-------|
| <i>Brain State OR</i> |       | <i>Brain State OR</i> |       | <i>Brain State OR</i> |       | <i>Brain State OR</i> |       |
| SH <sub>AxCPT</sub>   | 0.52  | SH <sub>CuedTS</sub>  | 0.78  | SH <sub>Stern</sub>   | 0.5   | SH <sub>Stroop</sub>  | 0.13  |
| S2 <sub>AxCPT</sub>   | 0.48  | S2 <sub>CuedTS</sub>  | -0.13 | S2 <sub>Stern</sub>   | 0.19  | S2 <sub>Stroop</sub>  | -0.37 |
| S3 <sub>AxCPT</sub>   | 0.3   | S3 <sub>CuedTS</sub>  | 0.43  | S3 <sub>Stern</sub>   | -0.77 | S3 <sub>Stroop</sub>  | -0.84 |
| S4 <sub>AxCPT</sub>   | -0.63 | S4 <sub>CuedTS</sub>  | 0.43  | S4 <sub>Stern</sub>   | -0.33 | S4 <sub>Stroop</sub>  | -0.37 |
|                       |       |                       |       |                       |       |                       |       |
| <i>Behavior</i>       |       | <i>Behavior</i>       |       | <i>Behavior</i>       |       | <i>Behavior</i>       |       |
| AX RT                 | 0.21  | Con ACC               | -0.44 | LL ACC                | 0.65  | Con ACC               | -0.63 |
| AY RT                 | 0.59  | Con RT                | 0.85  | LL RT                 | -0.36 | Con RT                | 0.63  |
| BX RT                 | -0.35 | Incon ACC             | 0.31  | HL ACC                | 0.24  | Incon ACC             | -0.33 |
| BY RT                 | -0.7  | Incon RT              | -0.03 | HL RT                 | 0.62  | Incon RT              | -0.3  |

**Supplementary Table S4. Behavioral results for the SST task.** ACC = Accuracy; RT = Reaction Time; US = Unsuccessful Stopping. Source data are provided as a Source data file.

|              | Mean $\pm$ Std |
|--------------|----------------|
| Go ACC (%)   | 94 $\pm$ 5     |
| Go RT (ms)   | 521 $\pm$ 86   |
| Stop ACC (%) | 51 $\pm$ 6     |
| US RT (ms)   | 464 $\pm$ 72   |
| SSRT (ms)    | 292 $\pm$ 59   |

**Supplementary Table S5. Canonical correlation analysis of brain-behavior relations in the SST.** Canonical correlation weights for brain states and behavioral performance measures are shown. OR = Occupancy Rate.

| <b>SST</b>            |       |
|-----------------------|-------|
| <i>Brain State OR</i> |       |
| SH <sub>SST</sub>     | 0.62  |
| S2 <sub>SST</sub>     | 0.34  |
| S3 <sub>SST</sub>     | -0.62 |
| S4 <sub>SST</sub>     | -0.33 |
|                       |       |
| <i>Behavior</i>       |       |
| Stop ACC              | 0.45  |
| US RT                 | -0.51 |
| SSD                   | 0.71  |
| SSRT                  | 0.18  |

**Supplementary Table S6. Behavioral results for the RP task.** MC = Matching Control; ACC = Accuracy; RT = Reaction Time. P values were not adjusted for multiple comparisons. Source data are provided as a Source data file.

|                  | <b>ACC (%)</b> | <b>RT (ms)</b> | <b>Contrast</b> | <b><i>t</i>-value</b> | <b>Cohen's <i>d</i></b> | <b><i>p</i>-value</b> |
|------------------|----------------|----------------|-----------------|-----------------------|-------------------------|-----------------------|
| <i>Session 1</i> |                |                |                 |                       |                         |                       |
| RP               | 73±20          | 1938±344       | RP – MC<br>ACC  | 9.19                  | 1.937                   | <0.001                |
| MC               | 93±10          | 1450±209       | RP – MC RT      | 16.71                 | 3.523                   | <0.001                |
|                  |                |                |                 |                       |                         |                       |
| <i>Session 2</i> |                |                |                 |                       |                         |                       |
| RP               | 64±19          | 2001±368       | RP – MC<br>ACC  | 11.7                  | 2.467                   | <0.001                |
| MC               | 88±10          | 1473±212       | RP – MC RT      | 14.8                  | 3.121                   | <0.001                |

**Supplementary Table S7. Canonical correlation analysis of brain-behavior relations in the RP task.** Canonical correlation weights for latent brain state and task performance measures are shown. MC = Matching Control; ACC = Accuracy; RT = Reaction Time.

| RP session 1          |       | RP session 2          |       |
|-----------------------|-------|-----------------------|-------|
| <i>Brain State OR</i> |       | <i>Brain State OR</i> |       |
| SH <sub>RP1</sub>     | 0.2   | SH <sub>RP2</sub>     | 0.61  |
| S2 <sub>RP1</sub>     | 0.16  | S2 <sub>RP2</sub>     | -0.66 |
| S3 <sub>RP1</sub>     | -0.9  | S3 <sub>RP2</sub>     | 0.3   |
| S4 <sub>RP1</sub>     | -0.35 | S4 <sub>RP2</sub>     | -0.31 |
|                       |       |                       |       |
| <i>Behavior</i>       |       | <i>Behavior</i>       |       |
| MC ACC                | -0.16 | MC ACC                | 0.85  |
| MC RT                 | -0.95 | MC RT                 | 0.03  |
| RP ACC                | -0.09 | RP ACC                | 0.44  |
| RP RT                 | 0.23  | RP RT                 | -0.29 |

**Supplementary Table S8. Summary of brain-behavior relations across tasks.** Multivariate relation analysis showed significant canonical correlation between occupancy rates of latent brain states and behavioral performance in each of the seven cognitive control tasks. Univariate relation analysis showed significant *Pearson's* correlation between occupancy rate of the multi-demand latent brain state (e.g. SH<sub>AxCPT</sub>) and cognitive control index in each cognitive control task. AxCPT: A-x continued performance task; SST: Stop-signal task; RP1/2: Relational Processing session 1/2. P values were not adjusted for multiple comparisons.

| Dataset/Task | Canonical Correlation Analysis |         | Univariate Analysis |       |
|--------------|--------------------------------|---------|---------------------|-------|
| DMCC         |                                |         |                     |       |
|              | $r$                            | $p$     | $r$                 | $p$   |
| AxCPT        | 0.51                           | 0.0001  | 0.34                | 0.02  |
| CuedTS       | 0.59                           | 8.3E-06 | 0.28                | 0.05  |
| Sternberg    | 0.65                           | 3.0E-07 | 0.37                | 0.01  |
| Stroop       | 0.59                           | 6.9E-06 | 0.32                | 0.02  |
|              |                                |         |                     |       |
| Stanford     |                                |         |                     |       |
| SST          | 0.61                           | 1.2E-05 | 0.33                | 0.03  |
|              |                                |         |                     |       |
| HCP          |                                |         |                     |       |
| RP1          | 0.35                           | 0.0007  | 0.32                | 0.002 |
| RP2          | 0.44                           | 1.3E-05 | 0.28                | 0.01  |

**Supplementary Table S9. Cognitive control measures used to assess univariate brain-behavior relations in each cognitive task.** AxCPT: A-x continued performance task; SST: Stop-signal task; RP1 and RP2: Relational Processing tasks in sessions 1 and 2; SSRT: Stop-signal reaction time; RT = Reaction Time.

| <b>Task</b> | <b>Cognitive Control Measure</b>      |
|-------------|---------------------------------------|
| AxCPT       | $(AY\ RT - BX\ RT)/(AY\ RT + BX\ RT)$ |
| CuedTS      | Congruent RT - Incongruent RT         |
| Sternberg   | High-load Accuracy/High-load RT       |
| Stroop      | Congruent RT - Incongruent RT         |
| SST         | 1/SSRT                                |
| RP1         | Relational Accuracy/Relational RT     |
| RP2         | Relational Accuracy/Relational RT     |

**Supplementary Table S10. OR of latent brain states in relation to indices of cognitive control in each task.** In each task, the state that matched  $SH_{WM}$  was the only state with significant and positive contribution to the cognitive control index. P values were not adjusted for multiple comparisons.

|               | r     | p     |
|---------------|-------|-------|
| <b>AxCPT</b>  |       |       |
| $SH_{AxCPT}$  | 0.34  | 0.02  |
| $S2_{AxCPT}$  | -0.01 | 0.9   |
| $S3_{AxCPT}$  | 0.1   | 0.5   |
| $S4_{AxCPT}$  | -0.3  | 0.03  |
|               |       |       |
| <b>CuedTS</b> |       |       |
| $SH_{CuedTS}$ | 0.28  | 0.05  |
| $S2_{CuedTS}$ | -0.1  | 0.5   |
| $S3_{CuedTS}$ | -0.03 | 0.8   |
| $S4_{CuedTS}$ | 0.1   | 0.5   |
|               |       |       |
| <b>Stern</b>  |       |       |
| $SH_{Stern}$  | 0.36  | 0.009 |
| $S2_{Stern}$  | 0.07  | 0.6   |
| $S3_{Stern}$  | -0.06 | 0.7   |
| $S4_{Stern}$  | -0.26 | 0.06  |
|               |       |       |
| <b>Stroop</b> |       |       |
| $SH_{Stroop}$ | 0.33  | 0.02  |
| $S2_{Stroop}$ | 0.09  | 0.5   |
| $S3_{Stroop}$ | 0.08  | 0.6   |
| $S4_{Stroop}$ | 0.07  | 0.6   |
|               |       |       |
| <b>SST</b>    |       |       |
| $SH_{SST}$    | 0.33  | 0.03  |
| $S2_{SST}$    | -0.21 | 0.16  |
| $S3_{SST}$    | -0.4  | 0.006 |
| $S4_{SST}$    | 0.13  | 0.4   |
|               |       |       |
| <b>RP1</b>    |       |       |
| $SH_{RP1}$    | 0.28  | 0.009 |
| $S2_{RP1}$    | -0.2  | 0.06  |
| $S3_{RP1}$    | -0.04 | 0.7   |
| $S4_{RP1}$    | -0.33 | 0.002 |
|               |       |       |
| <b>RP2</b>    |       |       |
| $SH_{RP2}$    | 0.32  | 0.002 |
| $S2_{RP2}$    | -0.22 | 0.04  |
| $S3_{RP2}$    | -0.05 | 0.6   |
| $S4_{RP2}$    | -0.21 | 0.05  |

**Supplementary Table S11. OR of latent brain states in SST in relation to the clinical measures of inattention.** The SH<sub>SST</sub> state that matched SH<sub>WM</sub> was the only state with significant and positive contribution to clinical attention scores. P values were not adjusted for multiple comparisons.

|                   | <i>r</i> | <i>p</i> |
|-------------------|----------|----------|
| SH <sub>SST</sub> | 0.39     | 0.008    |
| S2 <sub>SST</sub> | -0.09    | 0.6      |
| S3 <sub>SST</sub> | -0.31    | 0.04     |
| S4 <sub>SST</sub> | 0.14     | 0.4      |

**Supplementary Table S12. MNI coordinates of the brain network nodes.** Nodes were determined based on activation and deactivation peaks in the contrast of 2-back versus 0-back in the HCP n-back working memory task.

| <b>Node</b> | <b>x</b> | <b>y</b> | <b>z</b> |
|-------------|----------|----------|----------|
| IAI         | -32      | 24       | 2        |
| rAI         | 36       | 22       | 0        |
| IMFG        | -42      | 24       | 30       |
| rMFG        | 40       | 36       | 34       |
| IFEF        | -26      | 2        | 58       |
| rFEF        | 30       | 10       | 56       |
| IPL         | -46      | -44      | 44       |
| rIPL        | 52       | -40      | 50       |
| PCC         | -12      | -56      | 16       |
| VMPFC       | -2       | 48       | -8       |
| DMPFC       | 4        | 16       | 50       |

**Supplementary Table S13. State matching to SH<sub>WM</sub> in each cognitive task.** Space and temporal closeness of states that matched SH<sub>WM</sub> were statistically significant. P values were not adjusted for multiple comparisons.

| Task                 | space closeness |          | temporal closeness |          |
|----------------------|-----------------|----------|--------------------|----------|
|                      | <i>d</i>        | <i>p</i> | <i>r</i>           | <i>p</i> |
| <b>AxCPT</b>         |                 |          |                    |          |
| SH <sub>AxCPT</sub>  | 1.2             | 0.01     | 0.83               | 0.01     |
| S2 <sub>AxCPT</sub>  | 0.27            | 0.38     | -0.3               | 0.81     |
| S3 <sub>AxCPT</sub>  | 0.19            | 0.6      | -0.3               | 0.81     |
| S4 <sub>AxCPT</sub>  | 0.12            | 0.7      | -0.37              | 0.96     |
|                      |                 |          |                    |          |
| <b>CuedTS</b>        |                 |          |                    |          |
| SH <sub>CuedTS</sub> | 0.88            | 0.01     | 0.72               | 0.01     |
| S2 <sub>CuedTS</sub> | 0.51            | 0.05     | 0.22               | 0.26     |
| S3 <sub>CuedTS</sub> | 0.14            | 0.91     | -0.29              | 0.8      |
| S4 <sub>CuedTS</sub> | 0.18            | 0.71     | -0.37              | 0.9      |
|                      |                 |          |                    |          |
| <b>Stern</b>         |                 |          |                    |          |
| SH <sub>Stern</sub>  | 0.86            | 0.05     | 0.7                | 0.01     |
| S2 <sub>Stern</sub>  | 0.34            | 0.59     | -0.16              | 0.38     |
| S3 <sub>Stern</sub>  | 0.19            | 0.84     | -0.2               | 0.44     |
| S4 <sub>Stern</sub>  | 0.14            | 0.93     | -0.46              | 0.91     |
|                      |                 |          |                    |          |
| <b>Stroop</b>        |                 |          |                    |          |
| SH <sub>Stroop</sub> | 1               | 0.01     | 0.82               | 0.01     |
| S2 <sub>Stroop</sub> | 0.39            | 0.15     | -0.047             | 0.34     |
| S3 <sub>Stroop</sub> | 0.17            | 0.78     | -0.31              | 0.73     |
| S4 <sub>Stroop</sub> | 0.16            | 0.87     | -0.43              | 0.92     |
|                      |                 |          |                    |          |
| <b>SST</b>           |                 |          |                    |          |
| SH <sub>SST</sub>    | 1.4             | 0.01     | 0.77               | 0.05     |
| S2 <sub>SST</sub>    | 0.27            | 0.56     | -0.3               | 0.61     |
| S3 <sub>SST</sub>    | 0.26            | 0.61     | -0.12              | 0.34     |
| S4 <sub>SST</sub>    | 0.17            | 0.83     | -0.38              | 0.79     |
|                      |                 |          |                    |          |
| <b>RP1</b>           |                 |          |                    |          |
| SH <sub>RP1</sub>    | 13              | 0.1      | 0.97               | 0.01     |
| S2 <sub>RP1</sub>    | 0.4             | 0.33     | -0.46              | 0.87     |
| S3 <sub>RP1</sub>    | 0.26            | 0.81     | -0.29              | 0.51     |
| S4 <sub>RP1</sub>    | 0.12            | 0.96     | -0.4               | 0.75     |
|                      |                 |          |                    |          |
| <b>RP2</b>           |                 |          |                    |          |
| SH <sub>RP2</sub>    | 7.7             | 0.04     | 0.95               | 0.01     |
| S2 <sub>RP2</sub>    | 0.42            | 0.2      | -0.47              | 0.96     |
| S3 <sub>RP2</sub>    | 0.27            | 0.75     | -0.19              | 0.43     |
| S4 <sub>RP2</sub>    | 0.13            | 0.98     | -0.44              | 0.77     |

## V. Supplementary references

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