Optimisation of brain states and behavioural strategies when learning complex tasks

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Abstract

We designed two self-ordered switching (SOS) fMRI paradigms to investigate how people optimise their behaviour whilst managing competing demands. SOS was performed with feedback and minimal training (study 1) or without feedback but with extensive training (study 2). We hypothesised that behavioural performance would improve with practise and that this would be reflected in an optimisation of the brain states associated with the task events. As expected, response speed was slower in study 1, but increased with practise at a greater rate than in study 2. Furthermore, individuals who established more structured routines benefited from superior task performance. This behavioural optimisation was reflected by an ongoing redeployment of the neural resources supporting routine and task-switching trials. Specifically, as structured behaviour developed, there was increased activation of dorsal frontoparietal regions to switching events but decreased activation for routine trials. Conversely, the default mode network showed increased activation to routine trials with learning. Notably, the optimisation of behavioural performance corresponded with increases in frontoparietal and subcortical connectivity. These results demonstrate that a fundamental property of human behaviour is the establishment of structured task schemas that enable neurocognitive resources to be selectively focused on key executive events.

Keywords: Cognitive control, learning, behavioural structure, task-switching, fMRI.

Task-switching paradigms have been used for over a century to study how humans redeploy their attention between tasks (Culler, 1912; Jersild, 1927). Task-switching results in individuals responding more slowly than they would when performing repeated trials of the same task. This difference in response speed between switch and repeat-trials is the "switch cost". Switch costs are amongst the most replicated findings in cognitive neuroscience (Culler, 1912; Jersild, 1927; Spector and Biederman, 1976; Allport, Styles and Hsieh, 1994; Rubinstein, Meyer and Evans, 1994; Rogers and Monsell, 1995; Meiran, 1996; Dove *et al.*, 2000; Monsell, 2003; Arrington and Logan, 2004; Koch *et al.*, 2018). Despite this, our understanding of how the brain performs task-switching is rudimentary, and the insights gained thus far tend to lack ecological validity (Monsell, 2003; Kiesel *et al.*, 2010; Koch *et al.*, 2018).

A major limitation in our understanding relates to experimental paradigms being typically designed to explicitly control when switching events occur (Kiesel *et al.*, 2010). In contrast, successfully navigating daily life often requires people to structure their behaviour and choose how to switch their attention between competing tasks (Fallon *et al.*, 2013). Furthermore, people naturally behave in ways that seek to optimise the efficiency of their behaviours (Kool *et al.*, 2010; Botvinick and Cohen, 2014). While task-switching studies have attempted to address these issues with voluntary switching paradigms, where individuals randomly choose when to task-switch (Arrington and Logan, 2004, 2005; Mayr and Bell, 2006; Lien and Ruthruff, 2008), these paradigms still fail to capture the natural inclination to structure behaviour.

A further limitation comes from the historical focus of identifying one-to-one mappings between task-switching and the functional activation in specific brain regions. The locus of reported activation varies across functional MRI (fMRI) studies but the anterior prefrontal cortex (aPFC) is a recurring theme (Koechlin *et al.*, 1999; Rushworth, Passingham and Nobre, 2002; Braver, Reynolds and Donaldson, 2003). This mapping is supported by observations from classic neuropsychology (e.g. executive dysfunction following aPFC lesions (Nelson, 1976; Reitan and Wolfson, 1994; Shallice *et al.*, 2007; Roca *et al.*, 2010) and the widely-held perspective that regions within aPFC are arranged along an abstract-concrete anterior-posterior axis (Koechlin and Summerfield, 2007; Badre and D'Esposito, 2009); subsequently, activation in the (most-anterior) frontopolar cortex during task-switching is explainable as switching is considered an exemplar of a high-abstraction process (Koechlin *et al.*, 1999; Dove *et al.*, 2000; Rushworth, Passingham and Nobre, 2002; Braver, Reynolds and Donaldson, 2003).

However, such one-to-one mappings may not capture the dynamic brain mechanisms that support cognition and organise behaviour (Mouraux *et al.*, 2011; Yarkoni *et al.*, 2011; Hampshire and Sharp, 2015; Lorenz, Hampshire and Leech, 2017). In contrast, the contemporary network science view proposes that cognitive control are fundamentally non-localisable because they are supported by dynamic interactions that occur across distributed networks of brain regions (Bassett *et al.*, 2011; Cole *et al.*, 2013; Hellyer *et al.*, 2014; Gu *et al.*, 2015; Parkin *et al.*, 2015; Hampshire *et al.*, 2016; Bassett and Sporns, 2017; Khambhati *et al.*, 2018; Soreq, Leech and Hampshire, 2019).

Indeed, actions that require cognitive control, such as task-switching (Dove *et al.*, 2000; Wager, Jonides and Reading, 2004; Hampshire and Owen, 2006; Cusack, Mitchell and Duncan, 2010; Kim *et al.*, 2012; Crittenden, Mitchell and Duncan, 2015; Kehagia *et al.*, 2017), instruction based learning (IBL) (Hampshire *et al.*, 2016, 2019; Parkin *et al.*, 2020), relational integration (Parkin *et al.*, 2015) and planning (Hampshire, MacDonald and Owen, 2013) are associated with highly distributed neural activation that can include the aPFC.

Moreover, engaging with a task is accompanied by substantial reorganization of the brain's functional connectome (Scott *et al.*, 2015; Khambhati *et al.*, 2018; Braun *et al.*, 2019) as attention is focused toward a specific goal. These changes is the brain's functional state can be characterized by transitions from an initial state of high-activation that attenuates toward low-activation high-connectivity state (Petersen *et al.*, 1998; Erika-Florence, Leech and Hampshire, 2014; Hellyer *et al.*, 2015; Hampshire *et al.*, 2016, 2019; Ruge, T. A. Schäfer, *et al.*, 2019; Soreq, Leech and Hampshire, 2019), and this transition rate may depend on learning. Indeed, we have shown that activation in aPFC decays along an anterior-posterior axis as individuals overcome novelty and automate behaviour (Hampshire *et al.*, 2016, 2019).

Critically, the established task-state expresses a stable (Hellyer *et al.*, 2014, 2015) connectivity pattern that is specific enough to be decoded with machine learning to determine the current task (Soreq *et al.*, no date; Cox and Savoy, 2003; Woolgar *et al.*, 2011; Shirer *et al.*, 2012; Crittenden, Mitchell and Duncan, 2016; Soreq, Leech and Hampshire, 2019), the cognitive load (Soreq, Leech and Hampshire, 2019), task performance (Rosenberg *et al.*, 2016) and clinical abnormalities (Hampshire, MacDonald and Owen, 2013; Rosa *et al.*, 2015; Mason *et al.*, 2018).

Subsequently, we can assume that transitions between different functional brain-states

are costly (Figure 1) but often necessary, for example, when performing complex tasks or juggling multiple demands. These costs are mitigated in healthy adults by establishing routines that optimise the organisation of switching within the broader sequence of task events.

Here, we developed two "self-ordered switching" (SOS) paradigms where competing demands were hierarchically arranged into multiple tasks with multiple sub-rules to be managed. Across two independent fMRI studies, we aimed to address the aforementioned limitations of ecological validity and compare the opposing modular and dynamic-network models of cognitive control. Specifically, we examined the relationships between the ongoing optimisation of brain states, behavioural performance and self-ordered structuring of behaviour as individuals learnt SOS demands with feedback (study 1) or performed SOS after receiving extensive training (study 2).

We first tested the hypothesis that behaviour would optimise as individuals practised SOS and predicted that response speed would increase and switching costs would diminish. We then tested the relationship between individuals' behavioural structures and task efficiency and predicted that individuals who structured their behaviour would score more points.

Next, we directly tested for evidence of a modular hierarchy within aPFC or a dynamic-network process that supports switching behaviours. The former would be supported by evidence of strong switching-activation in anterior PFC (e.g., frontal poles), with this being strongest during task-switching relative to rule-switching. The latter would be supported by evidence of highly distributed activation during switching. Finally, we tested the hypothesis that functional brain states and behaviour concurrently optimise through learning. From a dynamic-network perspective, we predicted that optimising behavioural performance would be associated with greater changes in brain function marked by reductions in activation and increases in functional connectivity.

Methods

Participants. 16 healthy volunteers (mean age 24.75 years, range 19-40, 10 female) were recruited for study 1 and 15 healthy volunteers (mean age 26.47 years, range 19-42, 11 female) for study 2. Volunteers were right-handed and gave written informed consent prior to participating.

Self-ordered switch (SOS) paradigms. We designed two paradigms that required participants to self-organise their time between a matching task (MT) or an odd one out (OOO) task. Each task had two visual discrimination rules, colour and shape, and on each trial, individuals discriminated according to one of these rules (Figure 2a). The discrimination rules were simple enough to be performed at high accuracy with minimal effort. This ensured that individuals focused on dividing their time across the tasks and rules to gain maximum points. In both studies, SOS was continuously performed inside the scanner for 20 minutes (there were no resting periods).

Visual discriminations were made on each trial using left or right button presses. Switches between tasks and rules were made using up or down button presses. During MT trials, a target and two probe objects (each with a shape and colour) was presented and a L/R response indicated which of the two probes matched the target (based on the active shape or colour rule). Similarly, during OOO trials, a 2x2 object grid was presented and a L/R response indicated which side of the display contained the object that differed from the others (given the active rule).

Both studies significantly differed with respect to response feedback and the training individuals received prior to the scanning session. In study 1, SOS was performed in the scanner while being guided by response feedback after receiving minimal training (Figure 2b-d). Response feedback was presented after each trial for 1.5s and consisted of a set of hierarchically organised meters and an overall score. Each task had an overall progress meter and two subordinal meters corresponding to each discrimination rule. To increment the task meters, both rule meters for that task had to progress, which occurred when a correct response was made for a corresponding trial. To score maximum points, both task meters had to progress. Response errors, or making too many responses on a particular rule or task, resulted in penalties that hindered progress.

Overall score was calculated as the sum of differences between the task bars current

and initial value. Filling both task bars resulted in a bonus of +10 points. Switching behaviour was encouraged as the inactive rule or task feedback bar was penalized if it was three or more points behind the active rule or task. Thus, those who learnt the most efficient strategy of responding to trials and switching, via trial and error, should accumulate the most points during the experiment.

In study 2, individuals were extensively trained on the SOS paradigm used in study 1 before their scanning session (Figure 2e). However, the SOS variant used in the scanner had the hierarchical feedback elements removed, except for the overall score (Figure 2f-h). This was done to compare and contrast the learning and implementation of a complex task in the presence and absence of feedback across studies. As a further control, the two tasks were presented individually in the centre of the screen, that is, as opposed to in parallel at the top and the bottom of the screen, to control for spatial switching.

Behavioural analysis: Reaction time. Reaction times (RTs) were defined as the time between the stimuli being presented to the display and the response being made. For each individual, RT's were summarised using the median from trials where correct responses were made and these were estimated separately for repeat-trials and for the 1st trial that followed a rule-switch or task-switch. Response accuracy was summarised for the same conditions within-individuals using the percentage of correct responses. These values were analysed at the group-level using a one-way repeated-measures analysis of variance (rm-anova) for each metric.

A further analysis was conducted on RT to examine how response speed varied over the course of the 20 minute experiment. Median RT's were extracted for repeat and switch trials from each individual using the same procedure, but were summarised here within three adjacent temporal windows (each 6.667 minutes in length).

Behavioural analysis: Algorithmic complexity. The degree to which individuals applied structure to their behaviour was estimated using algorithmic complexity (Zenil *et al.*, 2018). Algorithmic complexity estimates the size of the smallest algorithm that could generate a given sequence and tends to be smaller for sequences with consistent structures vs. random sequences.

Here, we use the framework, outlined by (Zenil *et al.*, 2018), which combines a block decomposition method (BDM) and the coding theorem method (CTM) (Lempel and Ziv,

1976) to provide a reasonable estimate of Kolmorogov-Chaitin complexity (K) (Kolmogorov, 1968; Chaitin, 1969) for large strings in a computationally tractable way. The advantage of BDM is that it provides an estimate of K that not only considers statistical regularities, as is captured by Shannon entropy, but it is also sensitive to segments of an algorithmic nature.

Algorithmic complexity was estimated for each individual from the binary vector that represented the sequence of the four trial conditions that they opted to perform. Sequence length naturally varied across individuals, and to account for this, we normalised an individual's algorithmic complexity by the mean algorithmic complexity calculated from 100 randomly shuffled versions of the individual's data (qualitatively similar results were obtained without normalisation). NB:- As expected, the raw data showed a significantly lower complexity than the shuffled data (paired t-test: **Study 1** - t_{15}=-9.775, p<0.001, *d*=3.54; **Study 2** - t_{14}=-35.329, p<0.001, *d*=14.29).

MRI acquisition. Blood oxygenation level dependent (BOLD) fMRI recordings were acquired using the same Siemens 3T Trim Trio scanner and following parameters in both studies: TR=2s, TE=30ms, FA=78°, 3mm^3 voxels, 3.75mm slice-gap, 32 axial slices. 630 volumes were acquired during the 20-minute SOS task run. A T1-weighted magnetization prepared rapid acquisition gradient echo (MPRAGE) sequence was also acquired for each subject using the following parameters: TR=2250ms, TE=2.99ms, IT=900ms, FA=9°, 1mm^3 voxels, 256 axial slices.

Image data analysis. Image Pre-processing was conducted using standard parameters with the Statistical Parametric Mapping 12 (SPM)[1] toolbox in Matlab 2018b[2]. The first 10 volumes were discarded to account for T1-equilibrium effects. The remaining images were slice-time and motion-corrected, and the mean echo planar image (EPI) co-registered to the tissue segmented T1 image, normalised to 2mm^3 MNI space and spatially smoothed (full half width maximum = 8 mm kernel).

Subject level voxelwise modelling. Individuals voxelwise fMRI data was modelled using General Linear Models (GLM) with the psychological events defined by responses to one of the four trial conditions (MT colour, MT shape, OOO colour, OOO shape) and when one of the two task-switches (MT to OOO, OOO to MT) or four rule-switches (MT colour to MT shape, MT shape to colour, OOO colour to shape, OOO shape to colour)

[1] "SPM12 - Wellcome Trust Centre for Neuroimaging - UCL." Accessed July 30, 2019. https://www.fil.ion.ucl.ac.uk/spm/software/spm12/.

[2] "MATLAB - MathWorks - MATLAB & Simulink." Accessed July 30, 2019. https://www.mathworks.com/products/matlab.html.

occurred. Errors were infrequent, but were captured in an additional predictor. Models in study 1 included an additional set of feedback events for when the rule or task bars de/incremented and when bonus points were awarded. These psychological predictors were convolved with the canonical haemodynamic response function (HRF) with the durations set to 0s.

Head motion and nuisance variables were modelled using the rigid-body realignment parameters (defined by the motion-correction stage), the mean timecourses from the white matter and cerebrospinal fluid tissue segmentations and their 1st order temporal derivatives. This resulted in 16 parameters. Additional spike regressors were included where framewise displacement (Power *et al.*, 2012) exceeded the voxel acquisition size (3mm).

There were no resting periods during the scan as individuals continuously performed the SOS paradigm. Therefore, the 1st-level beta maps were estimated for each psychological predictor reactive to the model intercept. Modelling against this implicit baseline results in significant activation differences being relative to the average activation across time.

Group-level voxelwise modelling. To model the activation changes associated with switching, the beta maps from the two task-switching and the four rule-switching conditions were collated from each individual and modelled at the group-level using a one-way repeated-measures anova (rm-anova). The resulting activation maps were initially thresholded at an uncorrected $p<0.01$, followed by a $p<0.05$ false discovery rate (FDR) cluster correction.

Dice coefficient. Dice similarity coefficients (DSC) were used to estimate the spatial similarity of activation maps between study 1 and study 2. Group level cluster-corrected activation maps were binarised and DSC was calculated between each pair of maps using the following formula:

$$DSC(A,B) = \frac{2(A \cap B)}{(A+B)}$$

Modelling activation learning effects. An additional model was created for each individual to model whether voxelwise activation changed over time. Specifically, the four trial response conditions were collapsed into a single predictor, combined with the switch predictors and separated by the three time-windows used in the behavioural analyses. Switch>trial voxelwise contrasts were extracted from each time-window,

individual and study, and then modelled at the group-level in a rm-anova with time-window as the within-subject factor (three levels) and study as a covariate (two levels).

Activation clusters derived from the F-contrast testing for the main effect of time-window were used to extract mean beta weights from each individual. The direction of the effect for each cluster was then assessed using one-sample t-tests on the difference between activation in the 1st and last time-window.

Modelling functional connectivity learning effects. Generalised psychophysiological interaction (gPPI) models (Friston *et al.*, 1997; McLaren *et al.*, 2012) were fitted pairwise to the mean timecourses from 274 ROIs defined by external atlases that parcelated the cortex, subcortex and cerebellum (Buckner *et al.*, 2011; Fan *et al.*, 2016; Schaefer *et al.*, 2018). gPPI's were simultaneously estimated for the events of interest in each time-window for each pair of ROIs using the following:

$$Y^T = \beta_0 + [Y^S * H(X)]\beta_G + [Y^S, H(X), E]\beta + e,$$

where, X, is the matrix of psychological timecourses and, $H(X)$, its HRF convolution. Y^T is the target ROI timecourse and, Y^S, the seed ROI timecourse. E is the matrix of motion & tissue signal timecourses. β_G are the gPPI betas weights, β, the beta weights of no-interest, β_0, is the model intercept and, e, the residual. The resulting betas from each pair of ROIs were averaged ([model A->B + model B->A] / 2) and z-scored across time-window. Subsequently, each dFC estimate represented the *change* in FC relative to that connection's baseline FC.

To estimate how dFC associated with trial responses changes over time-window, generalised linear mixed effect (glme) models were fitted to each connection. This mass-univariate approach modelled the three time-windows as a fixed effect and individuals as a random effect. The resulting model set was corrected for multiple-comparisons at a $p<0.05$ FDR threshold. The F-values were visualised with red (increase) or blue (decrease) colours to indicate the direction of the effect as determined by the models accompanying *t*-statistic.

A further analysis was conducted on those connections that demonstrated a significant difference in magnitude over time-windows. For each connection, the change in dFC magnitude was partially correlated with the change in trial RT while factoring out the

total number of trials performed by each individual. The resulting set of r-values were corrected for multiple comparisons using a $p<0.05$ FDR threshold.

Effect size calculations. *Partial eta squared* was used to calculate the proportion of variance explained for the main and interaction effects tested with anova models using the F-statistic and degrees of freedom by the following:

$$\eta_p^2 = \frac{(F * DF1)}{(F * DF1) + DF2}$$

Cohen's d was used to calculate the standard effect size of statistical comparisons by dividing the difference between two means by the pooled standard deviation, in the 2-sample case, or dividing the mean by the standard deviation in the 1-sample case, e.g:

$$d = \frac{\overline{X}1 - \overline{X}2}{\sqrt{(SD_1^2 + SD_2^2) / 2}}$$

Results

SOS is costly to response speed. As expected, reaction times (RT) varied across repeat-trials and rule-switch or task-switch trials (one-way repeated-measures analysis of variance: **Study 1** - $F_{2,30}$=48.588, p<0.001, η_p^2=0.76; **Study 2** - $F_{2,28}$=52.886, p<0.001, η_p^2=0.79). In contrast, response accuracy did not vary across repeat or switch trials (one-way rm-anova: **Study 1** - $F_{2,30}$=1.218, p=0.310, η_p^2=0.08; **Study 2** - $F_{2,28}$=1.867, p=0.173, η_p^2=0.12) and was high across individuals (**Study 1** - mean=94.87%, SD=4.18; **Study 2** - mean=94.69%, SD=4.04).

In study 1, task-switching slowed response speed on average by 883ms (SD=538) (paired t-test: t_{15}=6.573, p<0.001, confidence interval 95% (CI)=0.54 to 1.17, Cohen's *d*=1.64), and rule-switches were 179ms (SD=273) faster (t_{15}=-2.630, p=0.019, CI=0.03 to 0.33, *d*=0.66), relative to repeat-trials (FDR corrected). In study 2, response speed slowed by 267ms (SD=143) after rule-switching (paired t-test: t_{14}=7.214, p<0.001, CI=0.19 to 0.35, *d*=1.86), and by a further 362ms (SD=268) after task-switching (t_{14}=5.227, p<0.001, CI=0.21 to 0.51, *d*=1.35) (FDR corrected).

Response time decreases with learning. We then examined how response speed varied as individuals practised SOS. Across studies, repeat-trial RT was slower in study 1 (Figure 3a) compared to study 2 (Figure 3f), where individuals received extensive training (two-sample t-test: t_{29}=4.119, CI = 0.29 to 0.85, p<0.001, *d*=1.20). Moreover, individuals who performed more trials tended to have faster median repeat-trial RT's (pearson: **Study 1** - r_{15}=-0.890, p<0.001, CI=-0.96 to -0.71; **Study 2** - r_{14}=-0.934, p<0.001, CI=-0.98 to -0.81).

This relationship between learning and performance was then confirmed within-subjects by summarising the repeat-trial RTs with three time-windows (each ~7 minutes). Repeat-trial RT varied across time-window (one-way rm-anova: **Study 1** - $F_{2,30}$=19.595, p<0.001, η_p^2=0.57; **Study 2** - $F_{2,28}$=12.253, p<0.001, η_p^2=0.47) and reduced with practise in both studies between the 1st and 2nd time-windows (paired t-test: **Study 1** - t_{15}=-6.770, p<0.001, CI=-0.33 to -0.17, *d*=0.49; **Study 2** - t_{14}=-5.276, p<0.001, CI=-0.20 to -0.08, *d*=0.79). Repeat-trial RT continued to reduce between the 2nd and 3rd time-windows in study 1 (t_{15}=2.173, p=0.046, CI=-0.222 to -0.002, *d*=0.15), but not in study 2 (t_{14}=0.887, p=0.390, CI = -0.09 to 0.04, *d*=0.16) (FDR corrected, within study).

Despite individuals in study 1 responding more slowly overall to repeat-trials, their rate

of RT reduction across the time-windows was greater than in study 2 (two-sample t-test: t_{29}=2.878, p=0.007, CI=0.06 to 0.37, *d*=0.93). Thus, repeat-trial RT is slower without training (study 1) but decreases at a greater rate with practise, and this may be due to trained individuals performing at a level that is closer-to-ceiling (study 2).

Switching costs decrease with learning. Costs to switching between tasks or rules also varied with practise (relative to each time-windows repeat-trial RT). Specifically, task-switching costs varied over time-window (one-way rm-anova: **Study 1 -** $F_{2,30}$=3.579, p=0.040, η_p^2=0.19; **Study 2 -** $F_{2,28}$=5.413, p=0.010, η_p^2=0.28) and reduced between the 1st and last window by ~370ms (SD=607) in study 1 (paired t-test: t_{15}=-2.433, p=0.028, CI=0.04 to 0.69, *d*=0.52), and by ~280ms (SD=418) in study 2 (t_{14}=-2.570, p=0.022, CI=-0.51 to -0.05, *d*=0.81) (FDR corrected, within study). Rule-switching costs did not vary across time-window in study 1 ($F_{2,30}$=0.128, p=0.881, η_p^2=0.01), but did in study 2 ($F_{2,28}$=5.543, p=0.009, η_p^2=0.28) and reduced by ~220ms (SD=286) between the 1st and last time-window (t_{14}=-2.945, p=0.021, CI=-0.38 to -0.06, *d*=0.88) (FDR corrected).

Moreover, individuals mean rule-switch and task-switch cost negatively correlated with the total number of switches they made (pearson: **Study 1** - r_{15}=-0.557, p=0.025, CI=-0.83 to -0.09, Figure 3b; **Study 2** - r_{14}=-0.658, p=0.008, CI=-0.88 to -0.22, Figure 3g). Together, this indicates that switching costs diminish as individuals learn through practise.

Efficient performers structure their behaviour. Turning to behavioural strategies, we used algorithmic complexity (Zenil *et al.*, 2018) to estimate the structure in each sequence of trials completed as individuals managed their time between the tasks and rules. Across studies, normalised algorithmic complexity (see methods) was significantly greater in study 1 compared to study 2 (two-sample t-test: t_{29}=4.500, p<0.001, CI=0.14 to 0.36, *d*=1.26). This indicates that individuals who did not receive training and were receiving ongoing feedback performed more diverse SOS behavioural routines (study 1).

Normalised algorithmic complexity showed a strong relationship with individuals' SOS efficiency, that is, total points scored (partial correlation, factoring N-trials: **Study 1** - r_{15}=-0.646, p=0.017, CI=-0.87 to -0.22, Figure 3c; **Study 2** - partial: r_{14}=-0.805, p=0.002, CI=-0.93 to -0.50, Figure 3h), indicating that those who had more structured behaviour also were more efficient at scoring points. For clarity, behavioural timecourses from

exemplar low-, medium- and high-performers in both studies are displayed in (Figure 3d/i).

As a further control, individuals' scores did not relate in a trivial manner to the number of switches in either study (pearson: **Study 1 - rule-switch** r_{15}=0.473, p=0.065, CI=-0.03 to 0.79; **Study 1 - task-switch** r_{15}=0.213, p=0.428, CI=-0.32 to 0.64; **Study 2 - rule-switch** r_{14}=0.160, p=0.569, CI=-0.38 to 0.62; **Study 2 - task-switch** r_{14}=0.034, p=0.905, CI=-0.49 to 0.54) (uncorrected, Figure 3e/j). This demonstrates that applying a sequential structure helps people to efficiently organise their behaviour during complex tasks.

We expected that those who began practising SOS with a less-structured behavioural routine to show larger decreases in complexity over time, as they refined their routines with practise. Confirming this, algorithmic complexity in the 1st time-window negatively correlated with the change in complexity across all time-windows (pearson, one-tailed: **Study 1** - r_{15}=-0.450, p=0.040, lower bound=-0.811 **Study 2** r_{14}=-0.857, p<0.001, lower bound=-0.951)

SOS activates lateral frontoparietal cortex and deactivates the default mode network.
To identify brain regions where activation changed during SOS, preprocessed fMRI data were used to generate voxelwise task-switching and rule-switching event contrasts that were modelled at the group-level with a one-way rm-anova in each study (six levels: two task-switch, four rule-switch). Collapsing across switch type with a *t*-contrast, switching was associated with widespread activation in lateral frontoparietal and cerebellar cortices, and also in the insula, putamen, and thalamus (Figure 4a/d). This pattern shared high spatial similarity across studies (DSC=0.580). Switching was also associated with reduced activation in dorsomedial frontoparietal and temporal cortices (Figure 4b/e), according closely with, the default mode network (DMN), in a consistent pattern across studies (DSC=0.562).

Next, we directly tested a prominent hypothesis that regions within the lateral frontal cortex are arranged along an anterior-posterior axis, with the most anterior selectively activating for tasks with high abstraction demand (Koechlin, Ody and Kouneiher, 2003; Badre and D'Esposito, 2007). In accordance with this, we should expect greater activation in the lateral frontal cortex for task-switches compared to rule-switches. However, the t-contrast testing this prediction showed no significant differences in

frontal lobe activation, in either study. Increased activation for task-switching vs rule-switching was observed in the dorsal visual streams in study 1 (Figure 4c). However, the same contrast in study 2 showed focal increases in the dorsal motor cortex (Figure 4f), with modest spatial similarity to study 1 (DSC=0.210). The inverse contrast testing for increased activation for rule-switches vs task-switches showed no differences that survived correction in either study.

Greater activation changes with learning when behaviour is structured. Previous studies have reported decreased frontoparietal activation when simple tasks are established through practice (Petersen *et al.*, 1998; Hampshire *et al.*, 2016, 2019). To determine whether the same was evident for complex tasks, we extracted switching activation (switch>trial) contrasts from each time-window and individual. These contrasts were then combined across studies in a 3 * 2 rm-anova with time-window as a within-subject factor and study as a covariate.

The main effect of time-window *F*-contrast rendered bilateral clusters where switching-activation significantly varied over time-window (Figure 5a). Contrary to past studies (Hampshire *et al.*, 2016, 2019), comparing the 1st and last time-windows, switching-activation *increased* in dorsolateral parietal cortex (paired t-test: DLPC - t_{30}=4.657, p<0.001, CI=1.65 to 0.64, *d*=1.56), anterior cingulate cortex (ACC - t_{30}=5.267, p<0.001, CI=1.37 to 0.61, *d*=1.59) and in occipital cortex (Occ. - t_{30}=4.707, p<0.001, CI=1.42 to 0.56, *d*=1.57). We combined these three ROIs into a "multiple-demand" composite and extracted the mean switching activation from each time-window and then summed the differences across time-windows. Individuals' changes in multiple-demand activation negatively correlated with their behavioural structure (pearson: r_{30}=-0.523, p=0.003, CI=-0.74 to -0.21, Figure 5b). This indicates that applying structure to SOS behaviour is associated with greater increases in multiple-demand switching activation as SOS is practised.

Repeating this procedure, but focusing on regions where switching activation (switch>trial) *decreased* over the time-windows (Figure 5d), three bilateral ROIs showed significantly reduced activation in the last window, compared to the first: The posterior cingulate cortex (PCC - t_{30}=-4.097, p<0.001, CI=-0.93 to -0.31, *d*=1.34), putamen (Put. - t_{30}=-3.412, p=0.002, CI=-0.91 to 0.23, *d*=1.14) and temporal cortex (Tem. - t_{30}=-5.401, p<0.001, CI=-1.12 -0.51, *d*=1.77). This pattern is also contrary to results reported when

simpler tasks are being learnt (Hampshire *et al.*, 2016, 2019). The sum of mean activation change across time-window, within this composite "DMN" ROI, positively correlated with individuals' algorithmic complexity (pearson: r_{30}=0.379, p=0.036, CI=0.03 to 0.65, Figure 5e). NB:- All comparisons of the increasing and decreasing ROIs survive bonferroni correction, n=6, alpha=0.05/n=0.008.

To help understand why the practise effect was inverted relative to previous studies, we independently examined trial response activation, as these events are more comparable to simple learning curve paradigms (Petersen *et al.*, 1998; Hampshire *et al.*, 2016, 2019; Ruge, T. A. Schäfer, *et al.*, 2019). Directly replicating these studies, activation in the multiple-demand ROI varied with learning (one-way anova: $F_{2,58}$=15.553, p<0.001, η_p^2 =0.35) and was significantly decreased in the last window, compared to the first (paired t-test: t_{30}=-4.573, p=0.001, CI=-0.99 to -0.38, *d*=0.77, Figure 5c). Similarly, activation within the DMN ROI varied with learning (one-way anova: $F_{2,58}$=9.790, p<0.001, η_p^2 =0.25) and was significantly increased in the last window, compared to the first (paired t-test: t_{30}=3.595, p=0.001, CI=-0.40 to -0.11, *d*=0.56, Figure 5f). Thus, activation decreases for simple trial response demands in multiple-demand cortex and increases in the DMN, as previously demonstrated. However, the opposite pattern occurs for the more-executive switching events when individuals are self-ordering their behaviour (Figure 5).

Functional connectivity between frontoparietal and subcortical networks increase with learning. Turning to dynamic functional connectivity (dFC), we sought to complement the learning associated changes in brain activation with changes in the brain's network coherence as individuals progressively optimised their behavioural performance. Taking a mass univariate approach, glme models were fitted to the trial response dFC weights from each connection with time-window as a fixed effect and individuals as a random effect. To aid interpretation, the connections that survived FDR correction at p<0.05 were grouped into nine networks, including seven cortical (Yeo *et al.*, 2011; Schaefer *et al.*, 2018) and the subcortical and cerebellar ROIs being grouped into additional networks (Figure 6a).

In study 1, a dense set of connections showed dFC changes for trial responses across time-widows. This predominantly involved increases between multiple frontoparietal networks, including the DMN, dorsal and ventral attention networks and between the dorsal attention, frontoparietal and subcortical networks (Figure 6b). In contrast, a

sparse set of connections showed changes in dFC over time in study 2 (Figure 6d). This indicates that the functional brain states associated with trial responses were subject to a greater degree of change in study 1, where individuals received minimal training and performed SOS with ongoing feedback. Whereas those who received extensive training and performed SOS without feedback where performing the task with accompanying brain states that were relatively fixed over time.

To confirm this we sought to relate to dFC changes in those connections that showed a significant effect over time-window to changes in individuals' behavioural performance. Specifically, the change in trial response speed between the 1st and last time-window was partially correlated with the connection's dFC change, while controlling for the total number of trials completed. The correlations were then FDR-corrected at $p<0.05$. In study 1, the majority of correlations were positive increases in response speed relating to dFC increases between the dorsal attention and subcortical networks and between the DMN, dorsal attention and frontoparietal networks (Figure 6c). In contrast, study 2 exhibited a very sparse number of connections which related to changes in trial response speed (Figure 6e).

Discussion

The results demonstrate a fundamental property of concurrent optimisation in the brain where external behaviours are structured to minimise the demands on the internal neural resources. Moreover, the results accord well with dynamic-network perspectives on the brain's functional organisation, but are hard to reconcile with predictions from classic modular perspectives.

By allowing individuals to self-order their behaviour, we observed a process by which the complexity of SOS paradigms was overcome by individuals developing efficient behavioural routines that became more structured over time. Concurrently, this behavioural optimisation was reflected by an ongoing redeployment of the brain's neural resources. Indeed, the tendency to generate structured behaviour, and to further refine it, naturally varied across individuals. Those who generated structured routines were most efficient at managing the competing demands. Structured behaviour was accompanied by a greater tuning of dorsal frontoparietal activation as SOS was practised, with activation relatively reducing for simple trial responses and increasing for the executive switch events.

Learning to automate the processing of individual trials has important implications for the overall efficiency when performing complex tasks. Rapidly 'mastering' the simple components of a more complex routine, frees up cognitive control resources for the more executive switching events that are crucial for navigating between the competing demands. Subsequently, the earlier that an individual can achieve this during the experiment, the more efficient their behaviour will be, overall.

We have previously demonstrated that the implementation of novel simple behavioural routines is accompanied by a transition in the brain from an initial state of heightened multiple-demand activation that attenuates, particularly in aPFC, as individuals become familiar with the routine (Petersen *et al.*, 1998; Hampshire *et al.*, 2016, 2019; Ruge, T. A. J. Schäfer, *et al.*, 2019; Parkin *et al.*, 2020). Here, we were able to go further by demonstrating that implementing an efficient *sequence* of behaviours accelerates this optimization of neural resources.

Given the natural variation in the behavioural efficiency of healthy adults, there are a number of clear predictions that follow which would pertain to neuropsychiatric patient

populations that exhibit cognitive inflexibility (impaired cognitive control). During similar self-ordered contexts, we should expect to see patients taking longer to generate efficient behavioural routines (1). If a routine is established then we would expect it to be more complex and inefficient (2) and be refined at a slower rate (3), if subject to any refinement, compared to healthy controls.

Consider anxiety (Kashdan and Rottenberg, 2010), depression (Fossati, Ergis and Allilaire, 2002), obsessive compulsive disorder (Chamberlain *et al.*, 2008) and autism spectrum disorders (Geurts, Corbett and Solomon, 2009; Watanabe and Rees, 2017; Watanabe *et al.*, 2019) where repetitive behaviours and rigid thought patterns are typical, or attention deficit hyperactivity disorder (ADHD) (Nigg and Casey, 2005), neurodegeneration (Kehagia, Barker and Robbins, 2014) and brain injury (Hellyer *et al.*, 2015) where distractibility and goal-set maintenance is problematic. In fact, our group has previously reported that the tendency to self-structure switching behaviour during a dimensional switching paradigm is reduced in some people with Parkinson's disease, and that this impoverished structure is associated with reduced dorsolateral prefrontal cortex activation during search behaviour (Fallon *et al.*, 2013).

These symptoms may result from the suboptimal cognitive control involved with creating, maintaining, updating or switching between behavioural routines. Future research could benefit from incorporating self-ordered elements to studies of cognitive control in these clinical populations. Tapping the ability to efficiently organise behaviour may provide a clinical marker with high ecological validity.

Beyond behavioural structure, learning was reflected by increases in response speed that differed across studies. In study 1, we scanned individuals as they learnt SOS with feedback. This promoted an ongoing update to behavioural routines. Whereas, in study 2, we scanned individuals performing SOS without feedback and after they had been trained. This promoted a stable context of behavioural implementation. Subsequently, while study 1 exhibited slower repeat-trial response times, the rate of response speed increase was greater than in study 2. Despite this, repeat-trial response speed increased and switching-costs diminished in both studies. Moreover, those who responded to more trials or performed more switches were generally faster.

Remarkably, within-task learning is not a typical feature of task-switching studies. An average switch-cost is normally calculated from all trials in an experiment and compared across conditions of interest (Kiesel *et al.*, 2010). However, we can draw from

tangential evidence from studies that manipulate the frequency, and therefore predictability, of task-switches being presented that report switching-costs reducing as a function of predictability (Mayr, 2006; Monsell and Mizon, 2006; Bonnin, Gaonac'h and Bouquet, 2011; Duthoo *et al.*, 2012). Relatedly, the present reduction of switching-costs were accompanied by individuals behaving with increasing structure; in other words, their self-ordered behavioural structures were increasingly refined and became more predictable allowing switches to be anticipated more effectively. This further emphasises the importance of structuring behaviour to maximise efficiency.

This behavioural optimisation may reflect a natural tendency towards efficiency (Botvinick and Cohen, 2014) as individuals were not explicitly instructed to speed up, to respond as quickly as possible, or to even generate optimal behavioural routines, but instead were instructed to gain as many points as possible. These learning dynamics have broader implications for understanding switch costs; they may indicate that switch costs index different mixes of top-down cognitive control (Meiran, 1996) and bottom-up interference (Allport, Styles and Hsieh, 1994) depending on where an individual is on the learning curve. The cognitive control mechanisms that support switching may optimise with practise and this may serve to reduce top-down delays and also minimise potential interference between competing task programs. Further research is required to determine how these components of the switch-cost vary with learning.

Building on this optimisation of behavioural performance, a clear distinction emerged between studies when examining the changes in functional connectivity associated with trial responses. In study 1, dFC increased between several frontoparietal and subcortical systems as individuals practised SOS. Furthermore, this increase in network coherence strongly correlated with the increases in repeat-trial response speed. In study 2, connectivity patterns were more stable over time and they shared a minimal correspondence with behavioural performance increases. This between-studies contrast provides a clear dissociation between ongoing learning and implementation of existing routines.

More broadly, switching was costly to response speed and was associated with widespread activations that were not specific to aPFC, as has been previously claimed (Koechlin *et al.*, 1999; Dove *et al.*, 2000; Rushworth, Passingham and Nobre, 2002; Braver, Reynolds and Donaldson, 2003; Charron and Koechlin, 2010). Strikingly, we found no evidence in support of predictions that logically follow from related abstraction hierarchy models of the frontal lobes (Koechlin and Summerfield, 2007;

Badre and D'Esposito, 2009); namely, that activation in aPFC should be greater during task-switching vs. rule switching, or task-switching should activate regions that are more anterior within aPFC. Instead, we saw no aPFC differences, despite SOS evoking substantial costs to response speed and greater task-switching activation in posterior regions including the motor cortices and dorsal visual streams.

The modular perspective on cognition and brain functioning counters a wealth of evidence indicative of highly distributed functional changes during various kinds of attentional-switching, such as set-shifting (Hampshire and Owen, 2006), rule learning (Hampshire *et al.*, 2019), relational integration (Parkin *et al.*, 2015) working memory updating (Soreq, Leech and Hampshire, 2019) and even task-switching (Cusack, Mitchell and Duncan, 2010). aPFC activation has even been reported during simple tasks that lack abstraction (Crittenden and Duncan, 2014). Moreover, we have recently found broad swathes of PFC activating, but not fractionating, for switches that vary in abstraction demands, suggesting a lack of a functional hierarchy (Daws *et al.*, no date).

Together, these findings accord with the hypothesis that cognitive control processes are emergent properties of dynamic network states that are modulated by learning (Cocchi *et al.*, 2013; Hampshire and Sharp, 2015; Lynn and Bassett, 2019) . More generally, the present study highlights the value of cognitive paradigms that allow individuals sufficient latitude to structure their own behaviour. Moving forward, we should consider the in-task learning that may occur during all studies of cognitive control. We consider learning to be an inevitable feature of cognition that will manifest even during simple procedures. Developing fMRI variants of paradigms that allow deeper hierarchical behavioural structures to be learnt and activation associated with the component processes of learning within the hierarchy differentiated should also be considered.

Finally, to build upon the generalisability of the present study, it will be important for future studies to probe switches between tasks that tap different aspects of intelligence (Daws and Hampshire, 2017) and which systematically vary in similarity, as indexed by psychometric distance. There is some behavioural evidence that switch costs increase with the magnitude of the switch (Arrington, Altmann and Carr, 2003); however, the neural mechanisms supporting switches of varying distance are yet to be characterised.

In summary, we developed SOS paradigms to examine how behaviour and brain states optimise to maximise efficiency. Behavioural performance and routines were sensitive

to learning and as individuals learnt to manage SOS demands and this was reflected by an ongoing optimisation of the brain's functional organisation. These findings characterise a fundamental property of human neurocognitive systems as the ongoing and concurrent self-optimisation of behavioural structure and network dynamics in order to maximise performance outcomes and minimise the use of neural resources.

Funding. This work was supported by funding to R.E.D. from the Engineering and Physical Sciences Research Council (EPSRC) via the centre for doctoral training (CDT) Neurotechnology programme at Imperial College London (grant number EP/L016737/1).

Author contributions. AH conceived and designed the self-ordered switching (SOS) paradigms and acquired the study data. RED analysed the data, created the figures and drafted the manuscript. GS and ES contributed analytical and visualisation tools. ES verified the data visualisation. AH, RL and PH verified analytical approaches. All authors provided interpretations of the findings and co-wrote the paper.

Competing interests. The authors declare no competing interests.

Code availability. Visual basic code used for the presentation of the SOS paradigms and Matlab code for conducting the data analyses are available upon request from the corresponding author.

Data availability. Behavioural and pre-processed imaging data will be made available in an online repository upon acceptance for publication.

Figure captions

Figure 1. **Schematic of hypothesised task-switching reconfiguration in the brain.** Distinct tasks can recruit similar brain regions, but distinct patterns of activation and hierarchical connectivities. a) In this hypothetical example, "TASK A" is supported by a pattern where the green region drives the activities of the red region which drives the blue region, in turn. This stable state is represented as a stack, below. b) During a task-switch from TASK A to TASK B, activation increases as the outgoing connectivity state is destabilized and reconfigured (c) to support the incoming TASK B demands. d) This process resolves with TASK B being supported by a connectivity state where the blue region drives the activities of both green & red regions equally.

Figure 2. **Self-ordered switching (SOS) paradigms.** a) Schematic of the two tasks (MT - Matching task, OOO - Odd one out) and the two rules (colour, shape) in each row and column, respectively. Arrows represent possible sequences of trials and switches that could be performed by an individual: Repeat-trials (grey) and switches between rules (orange) or tasks (blue). b) Study 1 involved a 20 minute fMRI session where subjects performed SOS that was guided by hierarchical response feedback (c). d) An example of a MT -> OOO task-switch following feedback. Each task was displayed simultaneously with the active task being denoted

by a red border. Feedback was hierarchical with correct responses accumulating progress on one the blue bars, where each bar represented one of a task's sub-rules. By balancing time on both sub-rules from a given task progress the green bar for that task and balancing time on both tasks lead to an increase in the overall score. e) Study 2 involved a training session prior to scanning (f) where SOS was performed in the absence of response feedback. h) This SOS paradigm also differed in that tasks were shown individually.

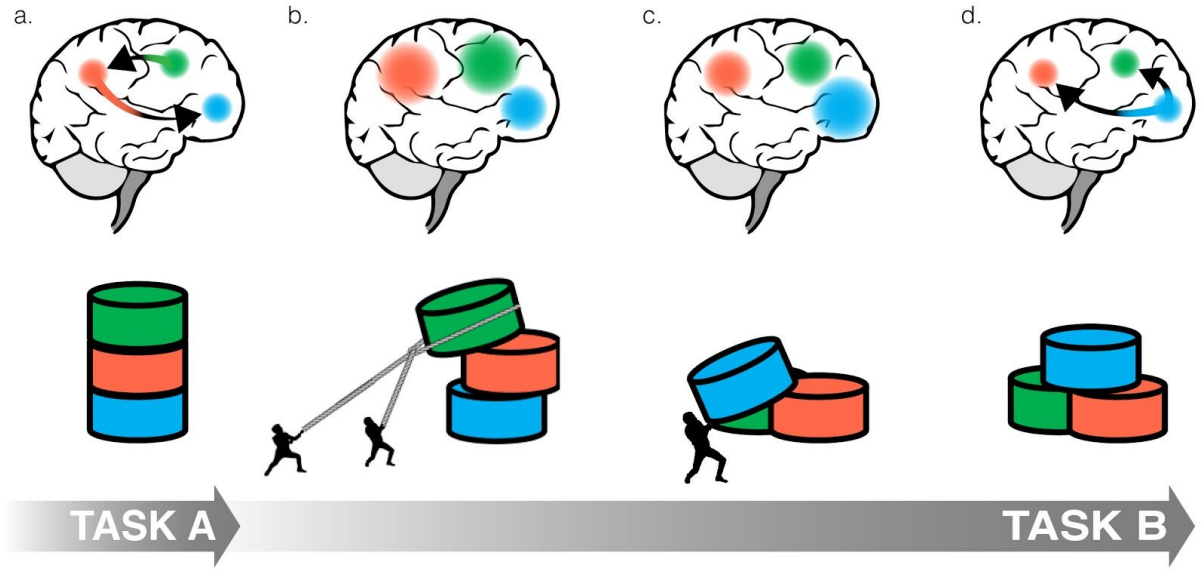
Figure 3. **Switching costs reduce with practise and structuring behaviour increases efficiency.** Study 1 - a) Individuals median reaction time (RT) in seconds (s) broken down by 3 ~7-minute windows for repeat-trials (TR - grey) and the trials following a rule-switch (RS - orange) or task-switch (TS - blue). b) The mean task-switch and rule-switch cost negatively correlates with the total number of switches made. c) negative correlation between individuals normalised algorithmic complexity & task scores. e) The sequence of trials performed by three individuals with high, average and low algorithmic complexity. f-j) Data analysis and visualisation procedure repeated for study 2.

Figure 4. **Lateral frontoparietal activation and default mode deactivation during self-ordered switching.** Study 1 - a) Group-level t-contrast maps depicting activation increases associated with SOS (collapsed across rule-switches & task-switches). b) The inverse contrast to (b) showing activation decreases accompanying SOS. c) T-contrast testing for increased activation during task-switching compared to rule-switching (the inverse contrast showed no significant differences in either study). d-f) Data analysis and visualisation procedure repeated for study 2. All maps are thresholded at an uncorrected $p<0.01$, followed by a $p<0.05$ FDR cluster correction.

Figure 5. **Switching activation magnitude varies as individuals practise SOS, with larger changes associated with greater structure being applied to behaviour.** Data from both studies were combined to test for a main effect of time-window on switching activation. a) F-contrast map showing regions where switching activation increased over time. b) The sum of activation change across time-windows for these "multiple-demand" regions correlates with individuals' normalised algorithmic complexity. Indicating greater increases in switching activation over time relating to behaviours that were more structured. c) Over time-window (W), multiple-demand activation increased for executive switching events but decreased for routine trial responses. d) Regions where switching activation decreased identified by the main effect of time-window F-contrast. e) The sum of activation change across time-windows for these "DMN" regions correlates with individuals' normalised algorithmic complexity. c) Over time-window, DMN activation decreased for executive switching events but increased for routine trial responses.

Figure 6. **Substantial increases in dynamic connectivity when learning a novel task.** a) Connectivity weights were arranged by the seven cortical networks defined by Yeo et al. with the addition of cerebellum and subcortical ROIs as additional networks (CB=Cerebellum, DM=Default Mode, DA=Dorsal Attention, FP=Frontoparietal, LI=Limbic, SM=Somatomotor, SC=subcortical, VA=Ventral Attention, VS=Visual). b) In study 1, dFC accompanying trial responses increased over time as a novel task was learnt. Increases were predominantly between networks located on frontoparietal cortices (DMN, dorsal attention, frontoparietal) and the visual network and subcortical regions. FDR-corrected $p<0.05$ F-values were estimated using generalised linear mixed effect (glme) models for each connection testing for connectivity differences across three time-windows (the accompanying glme t-statistic was used to colour the effect direction. Red=increase, blue=decrease). The distribution of F-values across models are plotted to the right of the schemaball. c) The correlation between changes in connectivity and trial RT between the 1st and last time-windows in the subset of connections identified in (b). Coefficients were controlled for the total number of trials completed by each individual and FDR-corrected at $p<0.05$. d) In contrast to study 1, individuals in study 2 were scanned after extensive training and showed relatively sparse dFC changes over time. e) Correlations between changes in dFC, identified in (d), & trial RT between the 1st and last time-windows.

Figures:



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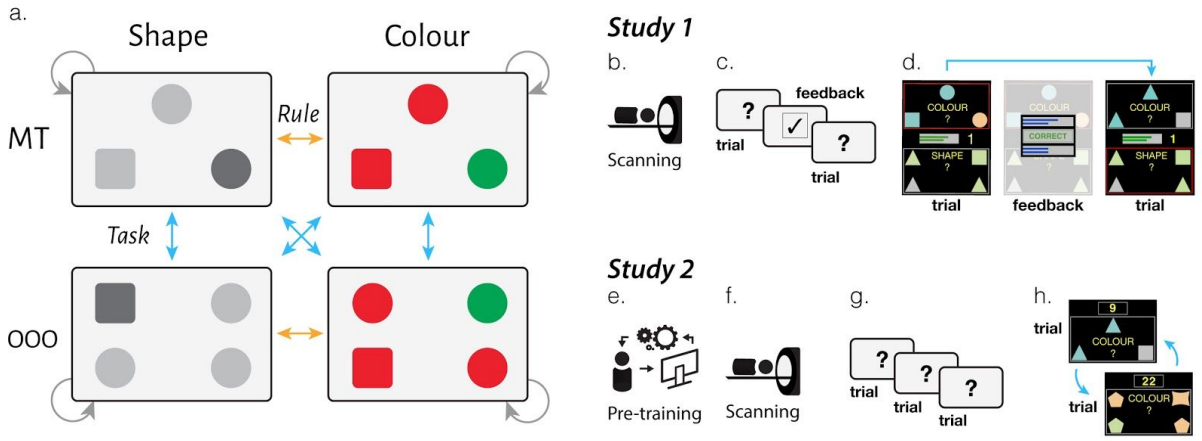

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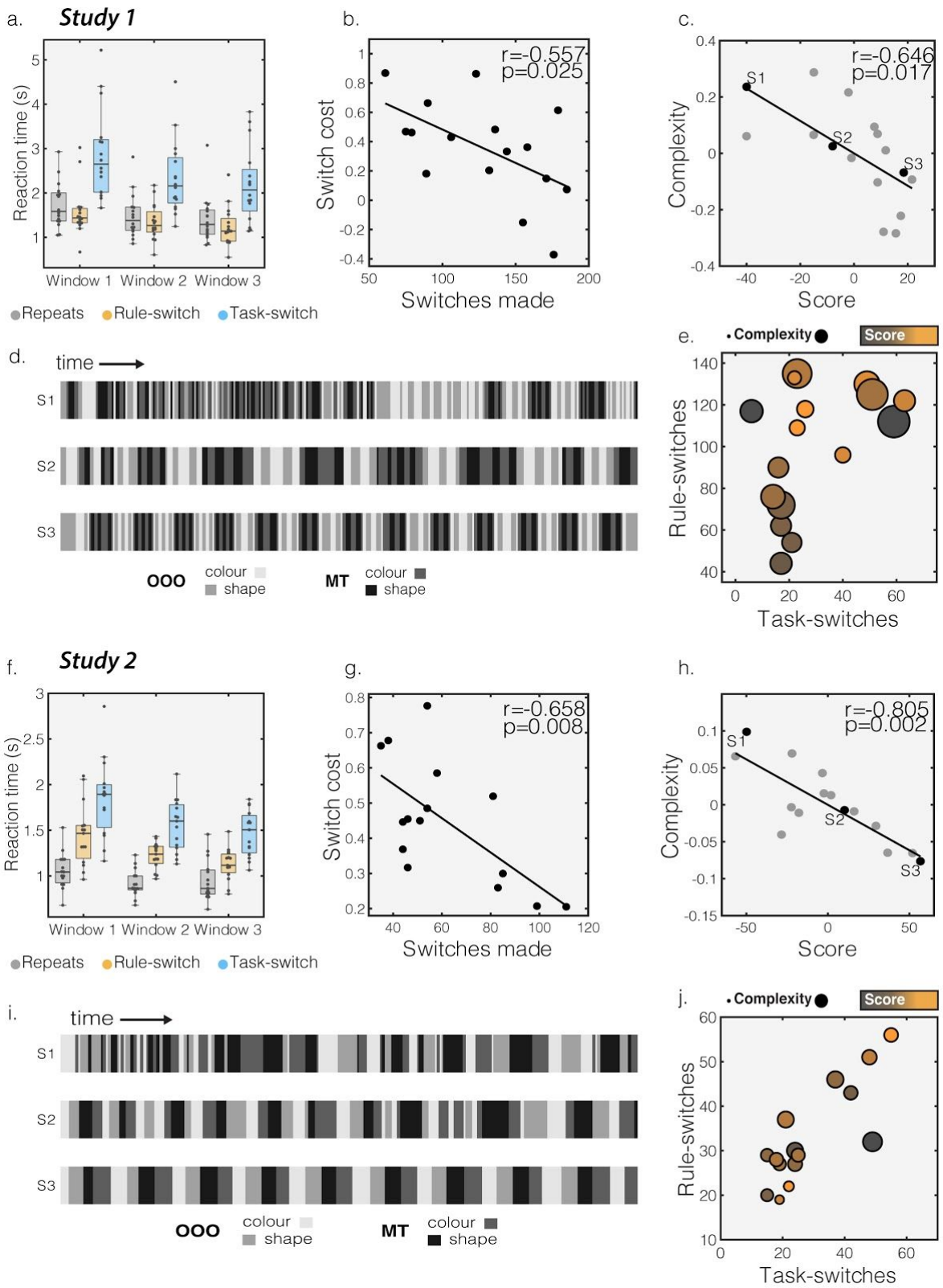

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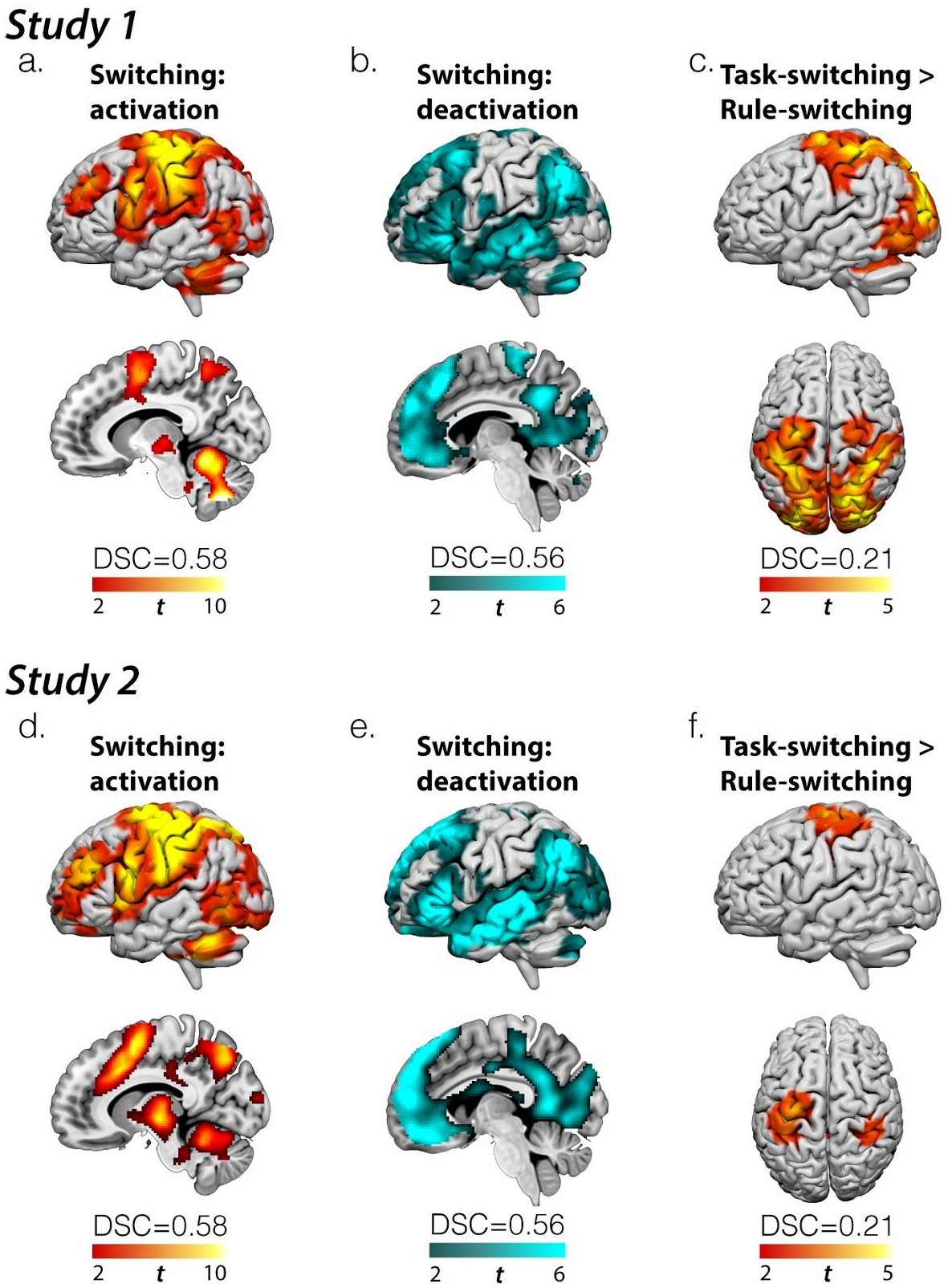

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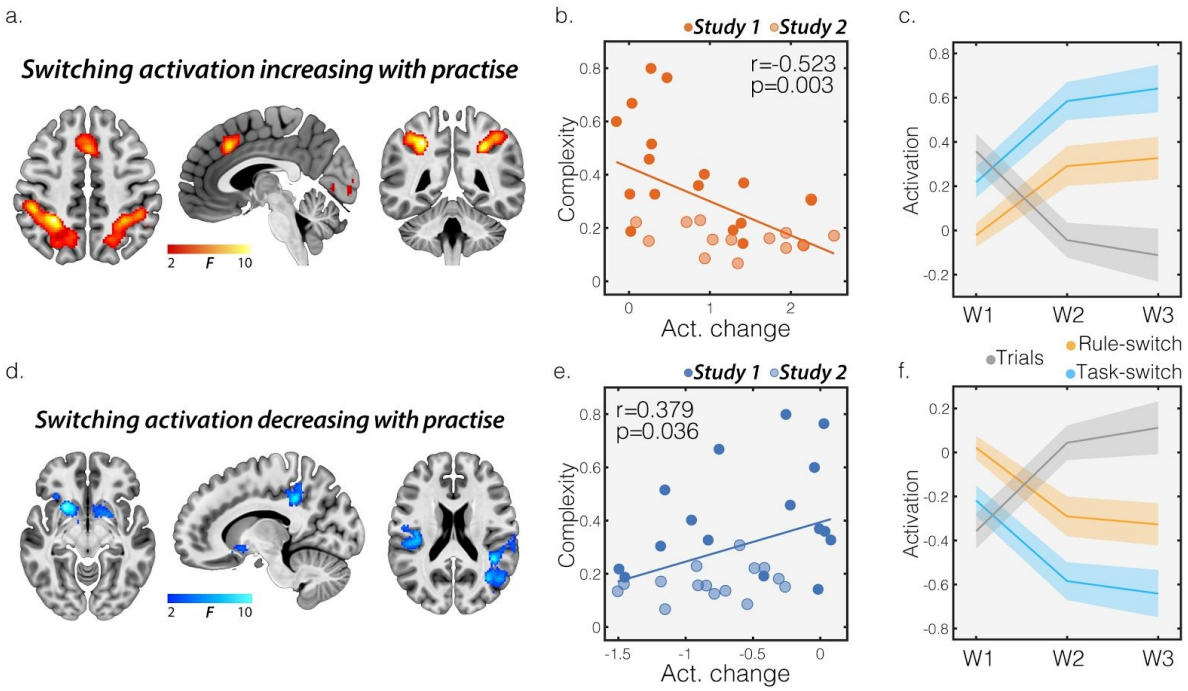

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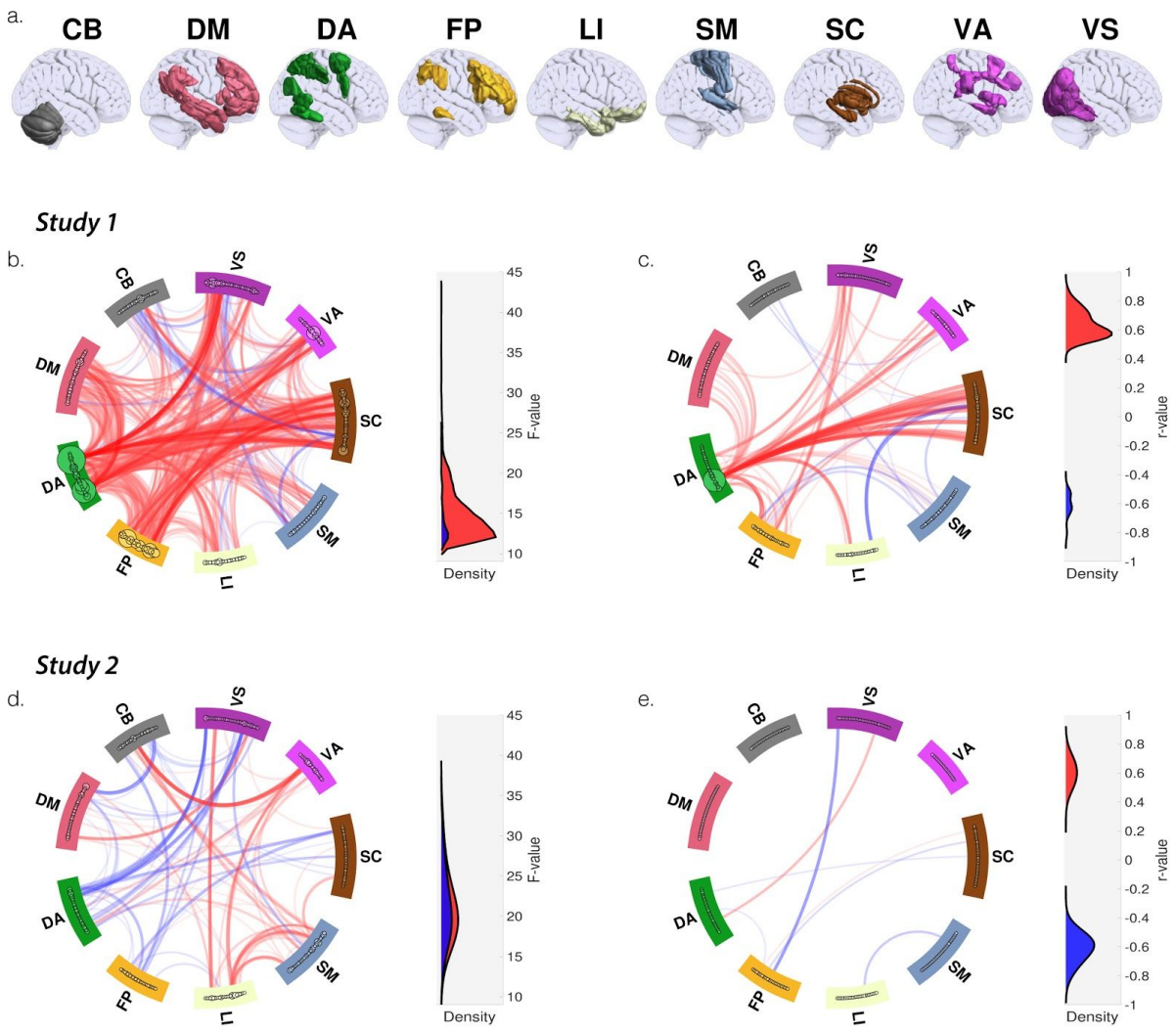

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