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3 **Multi-level decoding of task sets in neurophysiological data during**
4 **cognitive flexibility**
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34 **Summary**

35 To achieve higher-level goals, cognitive flexibility is essential. Cognitive theories assume that
36 the activation/deactivation of goals and task rules is central to understand cognitive flexibility.
37 However, how this activation/deactivation dynamic is implemented on a neurophysiology level
38 is unclear. Using EEG-based MVPA methods, we show that activation of relevant information
39 occurs parallel in time at multiple levels in the neurophysiological signal containing aspects of
40 stimulus-related processing, response selection and motor response execution, and relates to
41 different brain regions. The intensity with which task sets are activated and processed
42 dynamically decreases and increases. The temporal stability of these activations could,
43 however, hardly explain behavioral performance. Instead, task set deactivation processes
44 associated with left orbitofrontal regions and inferior parietal regions, selectively acting on
45 motor response task sets are relevant. The study shows how propositions from cognitive
46 theories stressing the importance task set activation/deactivation during cognitive flexibility are
47 implemented on a neurophysiological level.

48
49 Keywords: task switching, cognitive flexibility, EEG, multivariate pattern analysis, EEG signal
50 decomposition

51
52

53 **Introduction**

54 To achieve higher-level goals, it is not only essential to keep focus. Instead, cognitive flexibility
55 is another important aspect, which has extensively been investigated in cognitive neuroscience
56 using various experimental approaches. One prominent approach is to use task switching
57 paradigms (Allport and Wylie, 2000; Jersild, 1927; Monsell, 2003). The canonical finding in
58 this task is that whenever a response has to be switched, the response times increase and
59 responses become more error-prone than non-switch responses (Monsell, 2003). There has been
60 an intense debate about the cognitive mechanisms underlying these switch costs (Kiesel et al.,
61 2010). Some studies propose that switch costs reflect additional time needed to reconfigure the
62 current task set; other findings suggest that interference between simultaneously active task sets
63 plays a role (Allport and Wylie, 2000; Allport et al., 1994; Goschke, 2000; Grange and
64 Houghton, 2014, 2014; Meiran, 2000; Wylie and Allport, 2000). Moreover, such interference
65 in task sets can emerge at stimulus processing level as well as response selection and motor
66 levels (Goschke, 2000; Kiesel et al., 2010; Koch and Allport, 2006; Philipp et al., 2007; Rogers
67 and Monsell, 1995; Steinhauser and Hübner, 2009; Vandierendonck et al., 2010). The common
68 theme in all these possible explanations is that the degree of activation of the task set at a
69 particular point in time is central to cognitive flexibility. The rapid activation of a task set during
70 switching may require the inhibition (deactivation) of the no longer relevant task representation
71 (Dajani and Uddin, 2015; Klimesch, 2011; Mayr and Keele, 2000; Wolff et al., 2017a; Zhang
72 et al., 2016a, 2016b). Therefore, it is crucial to understand the temporal activation/deactivation
73 of task sets and how this is implemented on a neurophysiological level.

74 Notably, the question of how the activation/deactivation of task rules is implemented on
75 the neurophysiological level is still mostly elusive and therefore reflects a critical theoretical
76 gap in knowledge. Only using more recent multivariate pattern analysis (MVPA, originally
77 known as multi-voxel pattern analysis when applied to fMRI data, Haxby et al., 2001), the
78 precise representational dynamics (i.e. the activation and deactivation of rules) can be analyzed
79 (Carlson et al., 2019; Fahrenfort et al., 2018; Grootswagers et al., 2016; King and Dehaene,
80 2014). This is because these methods allow time-resolved decoding of mental representations
81 from neural activity, including changes of patterns observed in the EEG (King and Dehaene,
82 2014). Specifically, classifiers can be trained by using the difference of the neurophysiological
83 codes between experimental conditions (Fahrenfort et al., 2018; King and Dehaene, 2014).
84 When decoding performance is represented as a function of time, it allows interpretation about
85 the time scale of the neurophysiological activity related to the encoded information (King and
86 Dehaene, 2014). That is, applying this type of analysis to the time series data of EEG, it is

87 possible to determine when is information represented in the brain and how long is it
88 maintained. Then, the nature of the identified representation can be specified by testing the
89 generalizability of the classifier to other time points. This so-called temporal generalization
90 analysis (Fahrenfort et al., 2018; Grootswagers et al., 2016; King and Dehaene, 2014) seems
91 especially useful to examine the neural dynamics of task set activation/deactivation, because
92 this method provides a metric for the stability of mental representations over time. For instance,
93 gradual changes in the strength of the decoded pattern or recurring representations can be
94 detected (King and Dehaene, 2014). When depicting temporal generalization along the axes of
95 training and testing times, the diagonal represents training and testing on the same time points
96 (Fahrenfort et al., 2018; King and Dehaene, 2014). A diagonal pattern has been considered as
97 representation of a series of processing stages (King and Dehaene, 2014). Moreover, other
98 representational dynamics can be found as decoded patterns of different training and testing
99 time points (hence, off-diagonal decoding). Importantly, significant below-chance decoding
100 can be evident in MVPA results, which has been suggested to reflect a representation's
101 deactivation (Carlson et al., 2011; King and Dehaene, 2014). Therefore, the MVPA decoding
102 pattern will explain how the activation and deactivation are implemented on the
103 neurophysiological level and its temporal dynamics.

104 In the current study, we use EEG-based MVPA to examine the dynamic of task set
105 activation/deactivation on a neurophysiological level and combine this with source localization
106 analyses. Since MVPA requires a comparison of conditions (Fahrenfort et al., 2018), it is
107 essential to maximize the difference in the neuronal dynamics between conditions. One means
108 to do so when interested in the importance of executive control in the activation/deactivation of
109 task sets is to compare switching between trials either requiring 'endogenous' switching or
110 'exogenous' switching (Arrington and Logan, 2004, 2005; Terry and Sliwinski, 2012). During
111 exogenous task selection, participants receive external cues before each trial indicating the rule
112 to be applied or activated (Meiran, 1996). Endogenous task switching is more
113 complicated/effortful since task sets retrieval processes are not supported by external stimuli
114 (i.e., cue information). Instead, one has to used endogenous prompts to retrieve and activated
115 relevant task sets. This procedure requires more active control to perform switching (Arrington
116 and Logan, 2004, 2005; Emerson and Miyake, 2003; Kray, 2006; Mayr and Bell, 2006) and
117 makes task switching difficult and slower (Gajewski et al., 2011; Wolff et al., 2017b).
118 Therefore, decoding switching between exogenous (cue-based) and endogenous (memory-
119 based) trials should be particularly useful to examine the neural dynamics of the
120 activation/deactivation of task sets during task switching.

121 As mentioned, evidence suggests that relevant dynamics in task sets can emerge at the
122 stimulus processing level, or the response selection level, or motor levels (Goschke, 2000;
123 Kiesel et al., 2010; Koch and Allport, 2006; Philipp et al., 2007; Rogers and Monsell, 1995;
124 Steinhauser and Hübner, 2009; Vandierendonck et al., 2010). This theoretical distinction is
125 critical when examining the activation/deactivation dynamics on a neurophysiological level
126 using EEG because EEG-signals reflect a mixture of different activity sources (Huster et al.,
127 2015; Nunez et al., 1997; Stock et al., 2017). Especially in tasks taxing executive control,
128 stimulus processing and response selection and motor processes are intermingled in the EEG
129 signal at virtually the same time and in almost overlapping brain structures (Chmielewski et al.,
130 2018; Folstein and Van Petten, 2008; Mückschel et al., 2017a). To examine the dynamics of
131 the task set activation/deactivation using MVPA we, therefore, do this after decomposing the
132 EEG signal into theoretically relevant fractions of informational content. Residue iteration
133 decomposition (RIDE) (Ouyang and Zhou, 2020; Ouyang et al., 2011, 2015, 2017) can be used
134 to distinguish different aspects of information processes in the neurophysiological signal that is
135 processed simultaneously in overlapping functional neuroanatomical structures in a
136 theoretically meaningful way (Mückschel et al., 2017b, 2017a; Opitz et al., 2020; Takacs et al.,
137 2020a). RIDE decomposes the EEG into three clusters of dissociable significance: an S-cluster
138 reflecting stimulus-related processes, an R-cluster reflecting motor execution processes and a
139 C-cluster reflecting response selection mechanisms (Ouyang et al., 2011, 2015). Combining
140 RIDE-decomposition with MVPA it should be possible to examine the dynamics of the task set
141 activation/deactivation in the neurophysiological signals at theoretically relevant levels relating
142 to the role of stimulus processing, response selection level, or motor responding during task
143 switching.

144 Based on the above considerations, we suppose that the task set activation/deactivation
145 dynamics relevant to task switching is evident in all decomposed clusters of activity, but the C-
146 cluster and the R-cluster may reflect most pertinent information. These clusters should
147 particularly reveal temporal stability of activated task sets as indicated by significant off-
148 diagonal activity (King and Dehaene, 2014) and evidence for deactivated task sets as indicated
149 by below-chance decoding performance. Since the task set's inhibition is only critical during
150 switching, such deactivation patterns should only emerge when decoding endogenous
151 (memory-based) vs exogenous (cue-based) switching trials, but not when distinguishing
152 between repetition trial types. For time periods yielding relevant activation/deactivation
153 dynamics, we conduct source localization analyses to examine what functional neuroanatomical
154 structures are likely to be associated with them.

155

156 **Results**

157 We describe behavioral and MVPA results obtained from an experiment that required cognitive
158 flexibility. Participants had to perform a task switching task (Gajewski et al., 2011; Petruo et
159 al., 2018, 2019; Wolff et al., 2016), which consists of two different blocks, a cued and a
160 memory-based block. In both blocks, three task rules must be applied interchangeably. For this
161 purpose, either an informative cue (cued block, indicated with ‘NUM’, ‘PAR’, or ‘FS’
162 depending on the task rule at hand) or a non-informative cue (memory-based block, indicated
163 with a ‘XXX’ dummy cue) was presented (see Figure 1). In each trial, one of 8 numbers between
164 1 and 9 (except 5) were shown, to which a motor response had to be executed according to the
165 corresponding pre-defined rule. The task rule 'numeric' (indicated with a ‘NUM’ cue) required
166 a decision on whether the presented digit is less than or greater than 5. The task rule 'parity'
167 (indicated with a ‘PAR’ cue) required whether the given digit is an even or odd number. The
168 task rule 'font-size' (indicated with a 'FS' cue), required the question of whether the digit is
169 written in small or large font. In the memory-based block, participants were always instructed
170 to follow the same order of task rules of 3 × ‘NUM’, 3 × ‘PAR’, and 3 × ‘FS’, i.e., NUM, NUM,
171 NUM, PAR, PAR, PAR, FS, FS, FS, NUM, NUM, NUM, PAR, etc. Here, the order of the rules
172 must be retrieved independently by the participant. Participants were asked to respond target
173 stimuli within 2500 ms. Responses were followed by a display of a black screen for for 500 ms.
174 Then, a feedback stimulus was displayed for 500 ms: A plus sign indicated a correct response
175 while a minus sign an incorrect response. The cues (and correspondingly, the task rules) were
176 presented in a randomized order. For the detailed information about the task structure, see
177 STAR Methods.

178

179

Insert Figure 1 around here

180

181 *Behavioral results*

182 The behavioral data were analyzed using repeated-measures ANOVAs with trial type (cued vs.
183 memory), rule (repetition vs. switch) and motor response (repetition vs. switch) as within-
184 subject factors. The mean and SEM are given. For the response accuracy data (percent of correct
185 responses), there was a main effect rule repetition vs. switch ($F(1,85) = 21.54; p < .001; \eta_p^2 >$
186 $.202$) showing that there were more correct responses in rule repetition trials ($94.83\% \pm 0.46$)
187 than rule switch trials ($93.62\% \pm 0.54$). The trial type by motor response interaction was
188 significant ($F(1,85) = 4.18, p = .044, \eta_p^2 = .047$). There was also an interaction “rule x motor

189 response” ($F(1,85) = 6.15, p = .015, \eta_p^2 = .068$) where it is shown that accuracy was higher
190 when the response was repeated compared to switched responses when the rule was also
191 switched ($t(85) = 3.06; p = .003$). No such response switch effect was obtained when the rule
192 was repeated ($t(85) = 0.66; p = .507$).

193 For the reaction times (RTs), there was a main effect of trial type ($F(1,85) = 24.70, p < .001,$
194 $\eta_p^2 = .225$). Participants responded faster for cued (720 ms \pm 19) than for memory-based trials
195 (760 ms \pm 18). The main effect rule was also significant ($F(1,85) = 123.60, p < .001, \eta_p^2 =$
196 $.593$), showing that responses were faster for rule repetitions (709 ms \pm 17) than for rule
197 switches (771 ms \pm 19). The main effect motor response ($F(1,85) = 4.54, p = .036, \eta_p^2 = .051$)
198 revealed that RTs were shorter when the motor response was repeated (736 ms \pm 18), compared
199 to when it was switched (744 ms \pm 18). There was an interaction “trial type x rule” ($F(1,85) =$
200 $39.98, p < .001, \eta_p^2 = .320$). We compared switch costs (i.e., the difference between task
201 repetition and task switch) between cued and memory trial types to analyse the interaction
202 effect. Switch cost was larger in memory (87 ms \pm 7) than in cued trials (36 ms \pm 6) ($t(85) =$
203 $6.32, p < .001$). Thus, participants showed behavioral cost of alternating rules. This was larger
204 when they had to remember the task's rules instead of having cues to remind them. The
205 behavioral results pattern replicates finding from multiple previous studies using the same task
206 switching paradigm (Gajewski et al., 2011; Petruo et al., 2018; Wolff et al., 2017b).

207 Again, there was also an interaction “rule x motor response” ($F(1,85) = 11.26, p = .001, \eta_p^2 =$
208 $.117$). It is shown that RTs were shortest when rule and motor response were repeated (698 ms
209 \pm 17). When the rule was repeated but the motor response switched, RTs were significantly
210 longer (719 ms \pm 17) ($t(85) = 3.81; p < .001$). RTs were longest when the rule was switched
211 with no difference depending on whether the motor response was repeated (773 ms \pm 20) or
212 switched (769 ms \pm 19) ($t(85) = 0.81; p = .418$). This is important for the interpretation of the
213 MVPA findings, as outlined in the discussion section. Figure 2 presents RTs as a function of
214 trial type and rule.

215 -----

216 Insert Figure 2 around here

217 -----

218 *Multivariate Pattern Analysis results*

219 We introduce first the decoding accuracy results of the classification performance. Then, we
220 describe the temporal generalization matrices. Classification and temporal generalization
221 analyses were performed consecutively for the task repetition in C-cluster, task repetition in R-
222 cluster, task repetition in S-cluster, task switching in C-cluster, task switching in R-cluster, task

223 switching in S-cluster, respectively. Thus, we provide the results separately for the C-, R-, and
224 S-cluster data for each classification (Cued task repetition vs. Memory-based task repetition
225 and Cued task switching vs. Memory-based task switching). When significant above- or below-
226 chance decoding was detected, the corresponding data has been investigated for localizing the
227 signal. That is, if MVPA indicated an above-chance classification between 100 ms and 200 ms
228 after the target presentation in the S-cluster data of task repetition, the same time window in the
229 averaged S-cluster task repetition was used for sLORETA analysis. Similarly, the time windows
230 indicated by significant decoding at the group level were used to compare decoding accuracy
231 between classifications (task repetition vs. task switching) and to investigate correlations
232 between neurophysiological classification and behavioral results. Specifically, individual AUC
233 values averaged over significantly above-chance time windows have been compared between
234 task repetition and task switching classifications, separately for each RIDE cluster. Finally,
235 correlations between individual AUCs averaged over significantly above-chance or below-
236 chance time windows and behavioral measures of switch cost have been reported.

237 -----

238 Insert Figure 3 around here

239 -----

240 *Task repetition*

241 Figure 3 presents the decoding performance and temporal generalization matrices. In the C-
242 cluster, the classification was significantly above chance from -200 ms before the stimulus
243 presentation to 75 ms after that and anterior cingulate (BA32) and extrastriate visual areas
244 (BA18), were associated with that. Additionally, the classification was significantly above the
245 chance level from 150 ms to 1000 ms with superior parietal cortex (BA7) activity being
246 associated with that. In the R-cluster, the classification was significantly above chance from -
247 200 ms before the stimulus presentation to 75 ms after that, similarly to the initial successful
248 classification time window in the C-cluster. Supplemental motor areas were associated with it
249 (BA6). Moreover, in the R-cluster, a second above chance activity started later, from 250 ms
250 after the stimulus presentation and then it lasted until the end of the trial with the insular cortex
251 being associated with it (BA13). In the S-cluster, decoding above chance level was possible in
252 the time windows of -200 ms to 660 ms relative to stimulus presentation and extrastriate visual
253 areas (BA18) were associated with that. Thus, in all three RIDE-clusters, the MVPA provided
254 successful classifications, suggesting that sustained neural activity can be observed at all three
255 isolated coding levels in the EEG signal.

256 Considering the temporal generalization matrix, the C-cluster showed that above-chance
257 decoding performance ranging from -200 to 75 ms had squared shape with the diagonal axis in
258 its center, and this decoding accuracy has faded after the stimulus's presentation, as indicated
259 by the jittered edges. At the same time, this activation did not include the diagonal axis itself
260 (i.e., when training and testing on the same time points). It was followed by another above-
261 chance decoding starting from 150 ms after the stimulus presentation. This chain-like pattern
262 along the diagonal was extended with jittered edges and showed the most considerable activity
263 between 200 and 600 ms before it continued declining towards the trial's end. Similarly, the R-
264 cluster's first above-chance decoding was characterized by a diagonally centered shape that's
265 decoding performance attenuated after the stimulus was presented. Also, this pattern did not
266 include the area right above the diagonal axis. Then, a chain-like above-chance decoding was
267 observed after 250 ms on the diagonal axis. This activation was extended further from the axis
268 with a gradually changing generalizability. In the S-cluster, above-chance decoding of a single
269 time window was characterized by a combination of three identified patterns: a chain-like
270 decoding between -200 ms and 660 ms along the diagonal axis, and two extended generalization
271 patterns: from -200 ms to 75 ms and from 200 ms to 600 ms.

272 The first of these diagonal clusters showed the same fading after the stimulus presentation as it
273 was already observed in the C-cluster and R-cluster data. The second diagonal pattern showed
274 the most extensive activation in the same window as in the C-cluster data. Thus, the C-, R-, and
275 S-cluster data showed complementary but distinctive activity patterns.

276 -----

277 Insert Figure 4 around here

278 -----

279 *Task switching*

280 Figure 4 presents the decoding performance and temporal generalization matrices. In the C-
281 cluster, the classification was significantly above chance in the 200 ms interval before the
282 stimulus presentation and parietal regions (BA7), as well as inferior parietal areas (BA40), were
283 associated with this activity. Additionally, the classification was significantly above the chance
284 level from 190 ms until the end of the trial and inferior parietal regions (BA40), and medial
285 frontal areas (BA10) revealed activity. In the R-cluster, the classification was significantly
286 above the chance level from -200 ms to 25 ms associated with the supplementary motor area
287 (SMA, BA4), and from 300 ms to the end of the trial, which was again associated with activity
288 SMA activity (BA6). Interestingly, there was a significantly below chance (negative) activation
289 between 75 ms and 190 ms after the stimulus presentation that was associated with activity in

290 the inferior parietal cortex (BA40), left orbitofrontal activity (BA11) and right temporo-
291 occipital activity (BA21). In the S-cluster, the activity was above chance level in the time
292 window of -200 ms to 575 ms relative to stimulus presentation, associated with superior parietal
293 cortex (BA7) activity. Together, the MVPA showed successful classifications for the RIDE
294 clusters, indicating that task sets used during task switching can be decoded at multiple levels
295 in the neurophysiological signal.

296 Following the decoding accuracy results, the C-cluster temporal generalization matrix showed
297 that the in the first time window of decoding (-200 to 0 ms) developed around but not included
298 the diagonal axis. While fading of decoded information was visible in the matrix, this was
299 already outside of the successfully decoded interval. The C-cluster's temporal generalization
300 pattern in the second above-chance decoding followed a chain-like pattern from 190 ms after
301 stimulus presentation with an extended diagonal shape. This extended activation was the largest
302 between 300 ms and 500 ms; then it declined towards the trial's end. The Task switching R-
303 cluster's temporal generalization showed a diagonal pattern from -200 ms prior stimulus
304 presentation to 25 ms after that. This above-chance decoding did not include the diagonal axis
305 and started fading after the stimulus was presented. Additionally, a second above-chance
306 decoding was detected from 300 ms to 1000 ms. A consistent chain-like pattern over the
307 diagonal axis was extended in a ramping fashion. Notably, between the two above-chance
308 decoding of the Task switching R-cluster, activation time window (75 ms to 190 ms after the
309 stimulus presentation) with below-chance decoding was also detected with a chain-like pattern
310 over the axis. The single time window of above-chance decoding in the S-cluster can be
311 described as a combination of three patterns: a chain-like decoding between -200 ms and 575
312 ms, with two jittered extensions: from -200 ms to 0 ms and from 300 ms to 600 ms.

313

314 *Comparison between Task repetition and Task switching*

315 The time windows identified above were selected for each participant and for each
316 classification. Then, within these intervals, the individual AUC values were averaged to
317 facilitate comparisons between different MVPA results. The rule (Task repetition vs. Task
318 switching) by time window (1st vs. 2nd) ANOVA on the individual AUCs of the C-cluster data
319 showed that the main effect of rule was significant ($F(1,85) = 84.79, p < .001, \eta_p^2 = .499$).
320 Decoding performance was higher in task repetition (.84 ± .01) than in task switching (.70 ±
321 .02). Similarly, the main effect of time window was significant ($F(1,85) = 54.89, p < .001, \eta_p^2$
322 = .392). Decoding performance was higher in the second time window (.80 ± .01) than in the
323 first one (.74 ± .02). Finally, the rule by time window interaction was also significant ($F(1,85)$

324 = 6.89, $p = .010$, $\eta_p^2 = .075$). Decoding accuracy was higher for task repetition than for task
325 switching both in the first time window ($.80 \pm .02$ vs $.68 \pm .02$, $p < .001$) and in the second one
326 ($.87 \pm .01$ vs $.72 \pm .02$, $p < .001$). Additionally, for both rules, the second time window yielded
327 higher accuracy than the first one ($ps < .001$). The rule (Task repetition vs. Task switching) by
328 time window (1st vs. 2nd) ANOVA on the individual AUCs of the R-cluster data showed that the
329 main effect of rule was significant ($F(1,85) = 70.79$, $p < .001$, $\eta_p^2 = .454$). Decoding
330 performance was higher in task repetition ($.80 \pm .02$) than in task switching ($.68 \pm .02$).
331 Similarly, the main effect of time window was significant ($F(1,85) = 78.73$, $p < .001$, $\eta_p^2 =$
332 $.481$). Decoding performance was higher in the first time window ($.77 \pm .02$) than in the second
333 one ($.71 \pm .02$). However, the rule by time window interaction was not significant ($F(1,85) =$
334 1.93 , $p = .169$, $\eta_p^2 = .022$). In the S-cluster, AUCs were higher for task repetition ($.73 \pm .01$)
335 than for task switching ($.65 \pm .01$) ($t(85) = 3.81$; $p < .001$, $d = CI [.073; .107]$). Thus, the C-, R-
336 , and S-cluster data could be distinguished from each other based on their decoding performance
337 (and temporal generalization matrices, see Figure 3 and 4), indicating that the temporally
338 decomposed clusters are sensitive to different aspects of the task set dynamics. To analyze the
339 exact relationship between task dynamics and MVPA results, correlations were run between
340 AUC values and behavioral switch cost measures. Importantly, switch cost in the cued block
341 correlated negatively with decoding performance in the first ($r = -.274$, $p = .011$, $CI [-.462; -$
342 $.062]$) and second ($r = -.287$, $p = .007$, $CI [-.474; -.069]$) above-chance decoding of task
343 switching rule in the R-cluster. Additionally, switch cost in the memory block correlated
344 negatively with decoding performance in the first ($r = -.340$, $p < .001$, $CI [-.527; -.131]$) and
345 second ($r = -.379$, $p < .001$, $CI [-.549; -.193]$) above-chance decoding of task switching rule in
346 the R-cluster. Thus, higher above-chance decoding accuracy of task switching in the R-cluster
347 was related to smaller switch cost both in the cued and memory blocks. None of the other pairs
348 showed significant correlations between individual AUCs and switch cost measures ($p > .105$),
349 for detailed results, see Supplemental Information).

350

351 **Discussion**

352 The current study's goal was to investigate the task set activation/deactivation dynamics during
353 cognitive flexibility. The study was motivated by considerations that the content of task sets
354 and the deactivation of no longer relevant content, is a central element in theoretical accounts
355 on task switching and cognitive flexibility, but has nevertheless not directly been examined in
356 neurophysiological (EEG) data thus far. To close this theoretically significant knowledge gap,
357 the study combined temporal EEG signal decomposition (RIDE) with multivariate pattern

358 analysis (MVPA), here, also focusing on temporal generalization analysis (King and Dehaene,
359 2014). Signal decomposition was used because theoretical considerations suggest that task sets'
360 relevant activation/deactivation dynamics can occur at the stimulus processing level, the
361 response selection and motor levels (Goschke, 2000; Kiesel et al., 2010; Koch and Allport,
362 2006; Philipp et al., 2007; Rogers and Monsell, 1995; Steinhauser and Hübner, 2009;
363 Vandierendonck et al., 2010). Using RIDE, it is possible to distinguish such coding levels in
364 neurophysiological data in a theoretically meaningful way (Mückschel et al., 2017b, 2017a;
365 Opitz et al., 2020; Takacs et al., 2020a; Wolff et al., 2017b).

366

367 *'Quasi-parallel' activation of task sets at different neurophysiological levels*

368 Participants either had to memorize a simple sequence of task rules or recall the relevant
369 rule based on a cue information. The first one corresponds to endogenous task switching in
370 which flexibility of response selection is supported by existing knowledge. The second one can
371 be described as exogenous task switching which requires a more dynamic, trial-by-trial
372 adaptation. We have used these two types of conditions for classification, separately for task
373 repetition and task switching, and for each temporally decomposed clusters, respectively. Thus,
374 decoding results should depict the difference in exogenous and endogenous task representations
375 when mental set had to be maintained (repetition) or altered (switching). Significant MVPA
376 decoding was evident in all isolated RIDE-clusters of neuronal activity during repetition and
377 switch trials; i.e., in the S-cluster, the C-cluster and the R-cluster. According to Ouyang et al.
378 (2011, 2015), the S-cluster reflects stimulus-related processes; the R-cluster reflects motor
379 execution processes, and the C-cluster reflects response selection mechanisms. Thus, the
380 MVPA data show that relevant task sets can be decoded at multiple coding levels in the
381 neurophysiological signal; i.e., during stimulus-related processing, response selection and
382 motor response execution. This is of particular theoretical importance since it has been
383 suggested that interferences between task sets can emerge at the stimulus processing level, or
384 the response selection and motor levels (Goschke, 2000; Kiesel et al., 2010; Koch and Allport,
385 2006; Philipp et al., 2007; Rogers and Monsell, 1995; Steinhauser and Hübner, 2009;
386 Vandierendonck et al., 2010). The current data suggest that task sets dynamics at all of these
387 levels are relevant to task switching. As shown in Figure 3 and 4 (cf. AUC plots), the C-cluster
388 and the R-cluster show highly similar time courses of significantly decoded activity (cf. AUC
389 plots). Both, the C-cluster and the R-cluster reveal task set activations before stimulus
390 presentation and 200 ms after stimulus presentation until the end of the trial. This can be
391 interpreted that the task set is not only evident at different levels of information coded in

392 neurophysiological activity, but that activated task sets at these different neurophysiological
393 coding levels are evident at least partly in parallel in time. However, the temporal generalization
394 results provide further information about this dynamic. This data revealed a combined diagonal
395 and the off-diagonal activity pattern. The C-cluster showed the largest activity between 200 and
396 600 ms in repetition and switching trials and revealed a jittered diagonal and off-diagonal shape
397 fading ~400 ms after stimulus presentation. Opposed to this, the R-cluster showed a more
398 ramping diagonal and off-diagonal shape activity pattern from ~400 ms onwards in repetition
399 and switch trials. Several lines of evidence suggest that the C-cluster reflects stimulus-response
400 translation or response selection processes in the neurophysiological signal (Ouyang et al.,
401 2015, 2017; Takacs et al., 2020a; Verleger et al., 2014; Wolff et al., 2017b). The R-cluster has
402 been conceptualized to reflect processes associated with the motor execution (Ouyang et al.,
403 2015). Therefore, it is reasonable that the temporal generalization results show a pattern in
404 which the task rule on the stimulus-response mapping is activated before the task set detailing
405 the motor execution process and that the motor execution task set activation starts ramping in
406 when the activity of the task set detailing stimulus-response mapping fades out. Hence, the
407 content of task sets at different neurophysiological coding levels is activated partly in parallel
408 in time, but the intensity with which these various aspects of task sets are activated dynamically
409 fades in and out. Thereby ‘quasi-parallel’ activations of response selection and motor execution
410 task sets emerge at the neurophysiological level. An off-diagonal activity pattern in the R-
411 cluster and the C-cluster was evident for about 300-400 ms in repetition and switch trials and
412 suggested that the activation is relatively stable. Opposed to this, in the S-cluster off-diagonal
413 activity was much less pronounced suggesting visual stimulus task set activations are not held
414 online to the same extend as it is the case for stimulus-response relations or motor execution
415 plans. This may be interpreted that stimulus information is only relevant to trigger processes
416 reflected in the C-cluster and R-cluster activity pattern. Corroborating this interpretation,
417 diagonal activity suggesting for a chain-like processing of information (King and Dehaene,
418 2014) was only evident for about 300 ms (between ~200 and 500 ms). Diagonal activity in the
419 C-cluster and the R-cluster was evident much longer showing this activated content is processed
420 for longer time periods. Notably, the S-cluster main activity pattern was observed in a time
421 period where also the C-cluster activation was strongest (i.e., between ~200 and 500 ms). As
422 mentioned, processes in the C-cluster have been suggested to reflect stimulus-response
423 translation or selection processes (Ouyang et al., 2015, 2017; Takacs et al., 2020a; Verleger et
424 al., 2014; Wolff et al., 2017b). This, however, necessitates that stimulus information is
425 available, which is clearly evidenced by the activity pattern observed in the S-cluster.

426 The dynamics of quasi-parallel activations of the C-cluster and the R-cluster task sets discussed
427 above different brain structures are essential. For the C-cluster, mostly superior and inferior
428 parietal regions (BA7, BA40) and medial frontal regions (BA10, BA32) were activated in
429 repetition and switch trials during the pre-stimulus time window and the time window from
430 ~200 ms onwards. These source location results seem reasonable considering R-cluster and C-
431 cluster activity's functional relevance and fit with the broader literature on task switching. The
432 C-cluster has previously been shown to be associated with task switching effects in the very
433 same paradigm (Wolff et al., 2017b), which is corroborated by the current study's findings.
434 Since the C-cluster likely reflects stimulus-response translation (response selection) processes
435 (Ouyang et al., 2015, 2017; Verleger et al., 2014) the source localization findings are also in
436 line with a theoretical proposition derived from imaging data that (inferior) parietal regions are
437 central for mechanisms updating internal task sets during response selection (Geng and Vossel,
438 2013). Moreover, other evidence shows that inferior and posterior parietal cortical regions are
439 involved in task switching (Armbruster et al., 2012; Cooper et al., 2016; Kubanek and Snyder,
440 2015; Liu et al., 2015; Petruo et al., 2019; Philipp et al., 2013; Vallesi et al., 2015; Yin et al.,
441 2015; Zhang et al., 2016a, 2016b). Since response selection processes are a relevant function
442 of medial frontal areas (Ridderinkhof et al., 2004; Rushworth et al., 2004, 2005; Shenhav et al.,
443 2013), that finding is reasonable. In the R-cluster, particularly superior frontal pre-
444 motor/supplementary motor areas (BA4, BA6) were activated in repetition and switch trials
445 during the pre-stimulus time window and the time window from ~200 ms onwards. This is well
446 in line with the R-cluster's conceptualisation to reflect execution processes of motor programs
447 (Ouyang et al., 2015) and with studies reporting involvement of these regions during task
448 switching and cognitive flexibility (Cutini et al., 2008).

449 Besides the activations of task-related representations after the target stimulus has been
450 presented, all three clusters showed significant decoding that started before the trial. In case of
451 the S-cluster, pre- and post-stimulus activities could not be separated from each other. However,
452 in the C-cluster and R-cluster data, the representations from the pre-stimulus time window were
453 not sustained after the start of the trial, as evidenced by the steep drop in decoding accuracy. It
454 is conceivable, that information decoded in the inter-trial time windows represent rather general
455 differences between cued and memory-based task switching, such as additional cognitive
456 processes in one condition. For instance, the difference between maintaining the sequence of
457 task rules (in memory block) and monitoring the cue for selecting the appropriate mental set (in
458 cued block) might be reflected by the pre-stimulus decoding. However, any interpretation of
459 the pre-stimulus decoding remains tentative at this point, especially considering the fact, that a

460 pre-stimulus time-window might be sensitive to filtering criteria (van Driel et al., 2021). The
461 fact that this general activity was separable from post-stimulus decoding in the C-cluster and
462 R-cluster data lends support to interpret the post-stimulus representations in these two clusters
463 as the activation of task set.

464 Finally, the MVPA results of the undecomposed EEG data (see Supplemental Information)
465 showed both similarities and dissimilarities with the RIDE-clusters' classification. Specifically,
466 while pre-stimulus decoding was not identified, broad above-chance decoding in the post-
467 stimulus period suggested stable task-related representations both in task repetition and
468 switching conditions. Interestingly, the temporal generalization matrices resembled features of
469 all the three RIDE-clusters albeit with less specificity. Moreover, given the lower decoding
470 accuracy for undecomposed than for temporally decomposed data, the decomposed MVPA
471 results can provide a more precise picture of the dynamics of task representation during
472 cognitive flexibility.

473

474 *Decoding of motor task sets: the role of inhibition and response strategies*

475 A critical aspect reflected by the temporal generalization matrices is that the off-
476 diagonal activity pattern in the time period from 200 ms after stimulus presentation onwards
477 was highly comparable for switch and repetition trials. That is, maintaining an already active
478 task set (in repetition trials) and recalling an alternative task set (in switch trials) show many
479 similarities in terms of when and for how long a mental task representation is available. At the
480 same time, repetition trials were decoded more accurately than switching trials. Please note,
481 that this difference could be influenced by the trial numbers entered into the MVPA (see STAR
482 Methods). Interestingly, switch cost at the behavioral level correlated negatively with both pre-
483 and post-stimulus above-chance decoding performance in task switching of the R-cluster but
484 not with decoding in task repetition. Thus, at least in motor execution, the decoded
485 neurophysiological activity in task switching was associated with inter-individual differences
486 in cognitive flexibility. Moreover, in this regard, the time period between ~75 ms after stimulus
487 presentation and ~200 ms after stimulus presentation might be of particular relevance. In this
488 time period, the MVPA was only able to decode significant R-cluster processes in switch trials
489 (cf. Figure 4). Importantly, and unlike all other time periods in all RIDE-clusters, below-chance
490 activity was decoded. The source localization suggests that regions in the left orbitofrontal areas
491 (BA11) and left and right inferior parietal regions (BA40) partly extending to superior temporal
492 areas were active. Until now, the meaning of such below-chance decoding patterns have been
493 a bit contentious (Carlson et al., 2011; King and Dehaene, 2014). On a descriptive level, a stable

494 below-chance decoding indicates a reversal of the decoded neurophysiological pattern, that is,
495 difference between the classes is the opposite of the ones behind the above-chance decoding
496 patterns. Here we offer two tentative explanations of how below-chance decoding in the R-
497 cluster is related to the neurophysiological dynamics of task-switching.

498 It has been argued that a below-chance decoding may reflect the deactivation of a
499 representation (Carlson et al., 2011; King and Dehaene, 2014). That is, when a no longer
500 relevant content needs to be suppressed, a reversal is expected between the initial emergence of
501 that representation (above-chance decoding) and the inhibitory phase (below-chance decoding).
502 This interpretation makes sense considering cognitive theoretical propositions on processes
503 occurring during switching, which may contribute to a behavioral difference in switching
504 between the decoded cue-based and memory-based switching trials. Some conceptual
505 approaches state that the activation of a new task set necessitates the inhibition of the no longer
506 relevant task set (Dajani and Uddin, 2015; Kiesel et al., 2010; Klimesch, 2011; Mayr and Keele,
507 2000). Such inhibition is not required during repetition trials since the response rule from the
508 n-1 trial is still valid. This scenario predicts that possible benefits of repeating stimulus,
509 response, or both should be restricted to task repetitions. Note that our behavioral findings are
510 consistent with this prediction. We obtained an interaction between rule repetition/switching
511 and motor response repetition/switching, indicating that significant response repetition benefits
512 were obtained if the rule/response was repeated, but all of these benefits were eliminated when
513 a switch was included. This observation is consistent with findings from Rogers and Monsell
514 (1995) and others. They suggest that codes of just-performed responses might still be activated
515 in the next trial to some degree if the task repeats, but are inhibited by the process of switching
516 to another task. The obtained MVPA data pattern lends support to this idea because significantly
517 below-chance decoding was only evident in the switch trial decoding. This interpretation does
518 not contradict accounts according to which the control of inference between task sets is
519 important during switching (Kiesel et al., 2010; Vandierendonck et al., 2010) since inhibition
520 is one means to control interference effects (Cisek and Kalaska, 2005; Friedman and Miyake,
521 2004; Klein et al., 2014; Ocklenburg et al., 2011; Stürmer et al., 2000; Tandonnet et al., 2011;
522 Taylor et al., 2007). Therefore, the obtained data suggest that inhibitory control of task sets is
523 accomplished in the period between ~75 and ~200 ms after stimulus presentation during
524 switching. Intriguingly, however, this inhibition of task set was specific for the R-cluster and
525 hence a fraction of the neurophysiological signal carrying motor-response related information.
526 Therefore, the data might suggest that the no longer valid motor response task set is inhibited
527 during switching.

528 Importantly, however, the current below-chance decoding occurred in a diagonal
529 analysis (i.e., training and testing on the same time points (Fahrenfort et al., 2018). In this
530 training-testing scheme, all trials were divided into equal sized folds; into five parts in the
531 current study. Then, one fold was used for training and the remaining four folds were used for
532 testing to ensure that training and testing sets are independent from each other (Fahrenfort et
533 al., 2018). This procedure was iterated five times to cover the entire dataset for training. Thus,
534 the identified below-chance decoding is not necessarily the reversal of the two above-chance
535 decoding patterns that were identified in task switching in the R-cluster. However, it is possible
536 that the decoded difference between cued and memory-based switching was reversed as the
537 task progressed. This is in line with the observation that task-switching behavior is
538 characterized by large intra-individual variability that is even more pronounced in memory-
539 based than in cued task-switching (Petruo et al., 2018; Wolff et al., 2017c). Moreover, in a
540 previous study that investigated prolonged testing, the variability difference grew further
541 between the two types of task-switching (Petruo et al., 2018), suggesting that internal switching
542 is more sensitive to time-on-task effects, such as fatigue, than external switching. On a related
543 note, phasic modulatory effects of the norepinephrine system was shown in memory-based but
544 not in cued task-switching (Wolff et al., 2018a), that might contribute to the large variability in
545 internal switching. Thus, variability effects in previous studies (Petruo et al., 2018; Wolff et al.,
546 2017c, 2018a) point to the direction that participants' behaviour was more diverse in the
547 memory blocks than in the cued blocks, and this variability involves time-on-task effects, as
548 well (Petruo et al., 2018). How could variability differences between classes lead to below-
549 chance decoding? During the task, it is likely, that participants maintained the order of task
550 rules by repeating them internally (Petruo et al., 2018, 2019). However, with more practice, the
551 active maintenance of the order is not necessary anymore, and more automatized processes
552 might guide the response preparation. Thus, early and late trials in the memory blocks might
553 differ from each other in terms of what type of memory processes (i.e., intentional vs.
554 automatic) they involve. Consequently, the difference between internal and external switching
555 might also differ across consecutive folds, which then contributes to a pattern reversal (below-
556 chance decoding). Nonetheless, any change in response strategy during the task could be more
557 reliably detected in longer testing times and with a mixed presentation of memory-based and
558 cued trials (Petruo et al., 2018) instead of the current block-wise design. At this stage, below-
559 chance decoding as a signal of task-set inhibition seems theoretically feasible, however, it does
560 not completely explain the mechanisms of the pattern reversal. On the other hand, time-on-task
561 effects, such as changes of response strategy provide a potential explanation of a reversed

562 difference between classes, however, the proposed connection to behavioural markers remains
563 elusive. Nevertheless, the two interpretations (task set deactivation vs changes of response
564 strategies) are not necessarily independent from each other. Namely, if memory processes
565 involved in task switching become more automatic, it can result in a more effortless task-
566 switching, and therefore, it can make the deactivation of previous task sets easier.

567 Of note, decoding performance in the below-chance time window did not show
568 correlation with the behavioral measures of task switching. Thus, this inhibitory activity alone
569 cannot explain the effect of task switching on response times. In contrast, the above-chance
570 decoded representation that directly follows it, has a significant and linear relationship with the
571 executed response. As such, the RIDE-decomposed neurophysiological data provide clear-cut
572 evidence for theoretical propositions according to which processes in the cascade of motor
573 response preparation and execution, detached from cognitive response selection mechanisms,
574 affect switching (Koch and Philipp, 2005; Philipp et al., 2007; Schuch and Koch, 2003;
575 Steinhauser and Hübner, 2006, 2008; Verbruggen et al., 2005). These insights would not have
576 been possible with prior EEG signal decomposition. The R-cluster dynamics seem to relate to
577 orbitofrontal regions (BA11) and left and right inferior parietal regions (BA40) as suggested by
578 the source localization results. Interestingly, parietal contributions to motor processes have been
579 suggested to be inhibitory (Bernier et al., 2012; Beste et al., 2009; Cisek and Kalaska, 2002; De
580 Jong et al., 2001; Desmurget et al., 2018; Jaffard et al., 2008; Sulpizio et al., 2017), which nicely
581 fits the above line of arguments. In a similar vein, also orbitofrontal regions have been
582 associated with (motor) inhibitory control processes (Casey et al., 1997; Chikazoe et al., 2009;
583 Majid et al., 2013; Rubia et al., 2005), even though strong evidence also suggest for a role of
584 right inferior frontal regions (Aron et al., 2004) (but see: (Hampshire et al., 2010)).

585

586 *Conclusions*

587 In summary, we show that the relevant activation of task sets occurs parallel in time at
588 multiple levels in the neurophysiological signal containing aspects of stimulus-related
589 processing, response selection and motor response execution, and different brain regions. The
590 intensity with which these task sets are activated decreases and increases dynamically. The
591 temporal stability of these activations could, however, only explain behavioral performance on
592 a limited scale. Instead, inhibitory control processes associated with left orbitofrontal regions
593 and inferior parietal regions, selectively acting on invalid motor task sets are relevant. The study
594 shows how propositions from cognitive theories stressing the importance of the

595 activation/deactivation of task sets during cognitive flexibility are implemented on a
596 neurophysiological level.

597

598 **Limitations of the study**

599 The study shows how task sets activation and deactivation is implemented on a
600 neurophysiological level and how these processes unfold in time on distinct neurophysiological
601 levels coding for different information relevant to cognitive flexibility. The applied EEG
602 methods provide high temporal resolution and thus detailed insights into the temporal aspects
603 of activated and deactivated task set representations. However, when comparing the obtained
604 results of task repetition and task switching, the difference between trial numbers used in the
605 separate analyses have to be taken into account. Similarly, decoding accuracy might not reflect
606 the different task rules with the same weight across the analyses, since the number of trials has
607 been balanced between memory and cue conditions but not between the different rules or
608 stimulus types. Furthermore, using EEG, the study is limited regarding the information on the
609 functional neuroanatomical structures likely playing a role. Although the presented study also
610 presents data using EEG source localization methods, the question which functional
611 neuroanatomical structures are implied in the identified dynamics requires further verification
612 using fMRI methods.

613

614 **Resource Availability**

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622

623 *Materials Availability*

624 Not applicable

625

626 *Data and Code Availability*

627 The datasets generated during and/or analysed for the current study are available at the Open
628 Science Framework https://osf.io/xuqah/?view_only=9600a8257e9440f2b9c99a8903a17c24.

629 We used standard software packages as described in the methods section. Non-standard Matlab
630 scripts can be retrieved from the Open Science Framework
631 https://osf.io/xuqah/?view_only=9600a8257e9440f2b9c99a8903a17c24

632

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636

637 **Author contributions**

638 VP, AT, MM, CB designed the study and wrote the protocol. Author VP, collected the data,
639 Author VP, AT undertook the data analysis, BH, CB contributed data analysis methods, VP,
640 AT, BH and CB and wrote the first draft of the manuscript. All authors contributed to and have
641 approved the final manuscript.

642

643 **Declarations of interest**

644 There is no financial and non-financial competing interest.

645

646 **Figure Legends**

647 **Figure 1. Schematic illustration of the trials in the cue-based and the memory-based**
648 **conditions.**

649

650 **Figure 2. Individual and group reaction times as a function of trial type (cue vs memory)**
651 **and rule (task repetition vs task switching).** Group level RTs are presented as box plots,
652 where the central vertical bar denotes the median and the black cross the mean. The bottom and
653 top edge denote the 25th and 75th percentile, the whiskers depict 1 times the interquartile range,
654 and values outside of this range are marked by a red plus. Individual RTs are presented as
655 scatterplots. Individual data points are organized according to the four subsamples (marked as
656 red, blue, green, and purple dots, for details, see Participants section).

657

658 **Figure 3. MVPA results for repetition condition. RIDE decomposed C-, R-, and S-cluster**
659 **EEG data for the classification of cue versus memory block.** Left: Temporal generalization
660 plot. The plots show the degree to which the classifier when trained on a given time point (y-
661 axis) generalizes to time points in the trial (x-axis). The colors indicate the classifier
662 performance. The diagonal (bottom left to top right) shows classification performance when the
663 classifier is trained and tested simultaneously—middle: Area under the curve (AUC) decoding
664 accuracy across time. Time zero denotes the presentation of the target stimulus. Thicker lines
665 indicate significant time windows ($p < 0.05$; two-sided cluster-based permutation). Right:
666 results of sLORETA source localization for significant time windows as indicated by roman
667 numbers in AUC plots. For the C-cluster, activity differences (against zero) were found in BA18
668 and BA32 for the time window I and BA7 for time window II. For the R-cluster, sources in
669 BA6 for time window I and BA13 for time window II were found. For the S-cluster, the
670 sLORETA revealed sources in BA18 and BA19.

671

672 **Figure 4. MVPA results for switching condition. RIDE decomposed C-, R-, and S-cluster**
673 **EEG data for the classification of cue versus memory block.** Left: Temporal generalization
674 plot. The plots show the degree to which the classifier when trained on a given time point (y-
675 axis) generalizes to time points in the trial (x-axis). The colors indicate the classifier
676 performance. The diagonal (bottom left to top right) shows classification performance when the
677 classifier is trained and tested simultaneously—middle: Area under the curve (AUC) decoding
678 accuracy across time. Time zero denotes the presentation of the target stimulus. Thicker lines
679 indicate significant time windows ($p < 0.05$; two-sided cluster-based permutation). Right:
680 results of sLORETA source localization for significant time windows as indicated by roman
681 numbers in AUC plots. For the C-cluster, activity differences (against zero) were found in BA7
682 and BA40 for the time window I and BA10 and BA40 for time window II. For the R-cluster,
683 sLORETA revealed sources in BA4 for time window I, in BA11, BA21, BA40 for time window
684 II and BA6 for time window III. For the S-cluster, activity differences were found in BA7.

685

686 **STAR METHODS**

687 **RESOURCE AVAILABILITY**

688 *Key Resources Table*

REAGENT or RESOURCE	SOURCE	IDENTIFIER
Software		
Matlab 2019a	https://de.mathworks.com/products/matlab.html	RRID:SCR_001622
BrainVision Recorder	https://www.brainproducts.com/productdetails.php?id=21	RRID:SCR_016331
BrainVision Analyzer	http://brainproducts.com/productdetails.php?id=17	RRID:SCR_002356

689 *Lead contact*

690 Further information and request for resources should be directed and will be fulfilled by the
 691 lead contact, Christian Beste (Christian.Beste@uniklinikum-dresden.de).

692 *Materials availability*

693 There are no newly generated materials.

694 *Data and code availability*

695 De-identified human behavioral data and neurophysiological datasets for classification have
 696 been deposited at Open Science Forum: <https://osf.io/xuqah/>. Neurophysiological datasets in
 697 different stages of processing (e.g., raw, pre-processed, undecomposed, temporally
 698 decomposed) are available after specification of requested format upon reasonable request by
 699 the lead contact.

700 The original code for MVPA has been deposited at Open Science Forum: <https://osf.io/xuqah/>.

701 Please, note, that the code requires Matlab and ADAM: <https://github.com/fahrenfort/ADAM>.

702

703 **EXPERIMENTAL MODEL AND SUBJECT DETAILS**

704 *Participants*

705 Datasets from $N=86$ healthy young adults (42 males, 44 females, $M_{age} = 24.6$ years $SD_{age} = 2.8$)
 706 were used. Part of the data was re-used from previous studies using the same experimental task

707 (Petruo et al., 2017; Wolff et al., 2017b, 2018b) ($N = 11$, $N = 24$, $N = 17$), and other data were
708 collected newly ($N = 34$), to increase the sample size and to obtain reliable results for the MVPA
709 analysis representing a data-driven method. All studies used an identical version of the
710 paradigm, including stimuli, timing, conditions, and trial numbers. For a general overview of
711 comparability across the four subsamples, see Figure 2. The previous studies did not use any
712 form of MVPA decoding and data-driven methods, but were designed to test more specific
713 hypotheses referring to event-related potentials (ERPs). The inclusion criteria for the current
714 study were normal or corrected-to-normal vision, no psychiatric or neurological disorders, and
715 no usage of centrally acting medication. All participants provided written informed consent
716 before they participated in the studies. The participants were treated in accordance with the
717 declaration of Helsinki and the study was approved by the ethics committee of the TU Dresden.

718

719 *Task*

720 We applied a well-studied switching task (Gajewski et al., 2011; Petruo et al., 2018, 2019;
721 Wolff et al., 2016) for assessing cognitive flexibility. It consisted of two different blocks, a cued
722 and a memory-based one, each with 198 trials. In both blocks, participants were instructed to
723 follow three task rules interchangeably. First, either an informative cue (cued block) or a non-
724 informative cue (memory-based block) was presented. The task cue was presented in white
725 letters 3 mm below the fixation cross.

726 In each trial, one of 8 numbers between 1 and 9 (except 5) were shown, to which a motor
727 response had to be executed according to the corresponding pre-defined rule. The task rule
728 'numeric' required a decision on whether the presented digit is less than or greater than 5. The
729 task rule 'parity' required a decision whether the given digit is an even or odd number. The task
730 rule 'font-size', required the question of whether the digit is written in small or large font. Both
731 the left and right control key (Ctrl keys on a stand QWERTZ-keyboard) had to be used for the
732 responses. Responses indicating 'smaller than 5', 'odd number' or 'small font-size' had to be
733 given by pressing the left Ctrl key. For the respective other options, i.e., 'greater than 5', 'even
734 number' or 'large font size' the response had to be given by pressing the right Ctrl key. Switches
735 or repetitions of the 'rule' were therefore varied orthogonal to switches or repetition of the
736 motor response. In the current study, we used a within-subject design with the factors of trial
737 type (memory vs. cued) and rule (repetition vs switch) for the main analyses (see sections
738 *Multivariate Pattern Analysis* and *Statistics*). Thus, the three types of task rules were not
739 decoded from each other. This was necessary to increase the number of features (i.e., trials)
740 when applying MVPA (see sections *Multivariate Pattern Analysis*).

741 The experiment began with the cued block. Each trial started by presenting a fixation cross,
742 which was followed by one of three randomly presented cues; they are ‘NUM’ (abbreviation
743 for ‘numeric’), ‘PAR’ (abbreviation for ‘parity’), and ‘FS’ (abbreviation for ‘font-size’)ⁱⁱ
744 presented 1300ms before the target stimulus. In each trial, the cue remained visible during the
745 following presentation of one of the eight digits. Participants were asked to respond within a
746 period of 2500 ms. Once the response was executed, the screen turned black for 500 ms. Then,
747 a feedback stimulus was displayed for 500 ms: A plus sign indicated a correct response while
748 a minus sign an incorrect response. The cues (and correspondingly, the task rules) were
749 presented in a randomized order.

750 In the memory-based block, the cue was replaced by a non-informative dummy cue ‘XXX’.
751 This was necessary to keep the experiment's visual structure and timing comparable between
752 the cue-block and the memory-block. Participants were always instructed to follow the same
753 order of task rules of $3 \times$ ‘NUM’, $3 \times$ ‘PAR’, and $3 \times$ ‘FS’, i.e., NUM, NUM, NUM, PAR,
754 PAR, PAR, FS, FS, FS, NUM, NUM, NUM, PAR, etc. Here, the order of the rules must be
755 retrieved independently by the participant. As soon as the participant produced three
756 consecutive errors, the task was paused, and the order of the rules was presented to them again.
757 The corresponding informative cue (‘Num’, ‘Par’, or ‘FS’) was displayed over the next three
758 trials to help get back into the task. After these three trials, the dummy cue was shown for each
759 trial, and the participant continued to work independently on the task. In the memory-based
760 block, the participants thus had to rely on working memory information and they also had to
761 use internal prompts such as inner speech to retrieve the currently relevant task set (Emerson
762 and Miyake, 2003; Kray, 2006). As with the cue-based block, there was a balanced proportion
763 of each rule (33.33%), yet the frequency of switching was reduced to 33.3% of all trials due to
764 the fixed order of task rules in the memory block.

765 While a fixed order of rules was necessary in the memory-based block to rely on working
766 memory, we deliberately did not use a fixed order in the cue-based block for the following
767 reasons: Within-subject manipulation, such as the introduction of memory and cued blocks, is
768 subject to ‘carry-over effects’ (Petruo et al., 2018). For instance, participants could apply their
769 strategy from the memory block to the cued block without the need to process the cue
770 information. Furthermore, a fixed trial order in the cued block could cause a mixture of
771 memory-and cue-based strategies, and consequently, inflate the inter-individual variations.

ⁱⁱ Please note that the rules were translated from german. German participants saw the abbreviations ‘Num’, ‘Ger’, and ‘SG’. ‘Num’ indicated ‘numerisch’ (engl. ‘numeric’), ‘Ger’ indicated ‘Geradzahligkeit’ (engl. ‘parity’), and ‘SG’ indicated ‘Schriftgröße’ (engl. ‘font size’).

772 Thus, to rule out potential carry-over effect, trials of the cued block did not follow a
773 predetermined order. This ensured that participants had to process the cue information, and
774 update their behavior flexibly on a trial-by-trial basis. In sum, successful task switching had to
775 be carried out either with an anticipated order of task rules (memory block) or in a dynamically
776 changing environment (cued block). Since the difference between blocks should have
777 influenced of how participants recalled ('activated') or switched between ('suppressed') task
778 rule representations, memory and cued block trials were used for subsequent classification (see
779 *Multivariate Pattern Analysis*).

780

781 *EEG recording and analysis*

782 EEG activity was recorded at 500 Hz sampling rate from 60 Ag/AgCl electrodes and with using
783 the BrainVision Recorder and a QuickAmp amplifier (BrainProducts, Germany). Electrodes
784 were mounted on elastic caps (EasyCap, Germany) in equidistant positions. During EEG
785 recordings, electrode impedances were kept below 5 k Ω . The ground and reference electrodes
786 were placed at the coordinates of $\theta = 58$, $\phi = 78$ and $\theta = 90$, $\phi = 90$. Offline EEG analyses,
787 including filtering, ICA-decomposition for ocular and cardiovascular artifact correction,
788 segmenting, and residual artifact rejection, were conducted in BrainVision Analyzer 2 software
789 package (Brain Products, Germany). The steps and parameters of EEG pre-processing followed
790 the pipeline of previous studies that used the same task (Petruo et al., 2018, 2019; Wolff et al.,
791 2016). Comparable data processing across studies can facilitate more direct comparisons
792 between studies and between different EEG analyses. The offline data pre-processing began
793 with down-sampling the EEG recordings to 256 Hz. The data was filtered using a band-pass
794 filter of 0.5-20 Hz and a notch filter at 50 Hz—both, with a slope of 48 dB/oct. After a manual
795 raw data inspection, ICA decomposition (infomax algorithm) was applied to remove blinks,
796 horizontal/vertical eye movements and cardiac artifacts. These artifacts were identified by
797 visual inspection of the components and the ones showing these artifacts were discarded before
798 back-projecting the data to the EEG sensor space. Next, segments were formed using all
799 channels for corresponding conditions. Segments were stimulus-locked, separating switch from
800 repetition trials, and only included trials with correct responses. This was performed for the
801 cue-based and the memory-based blocks separately. The segments' length added up to 1200 ms,
802 starting at -200 ms before the locking point and ending 1000 ms after the stimulus presentation.
803 Subsequently, an automated artifact rejection was run, that discarded all segments with signal
804 amplitudes higher or lower than $\pm 200 \mu\text{V}$. Segments were also discarded if an activity smaller
805 than $0.5 \mu\text{V}$ was registered for at least 200 ms. Additionally, if amplitude differences between

806 two consecutive peaks in a time frame of 200 ms were higher than 200 μ V, the segment was
807 removed. To discard the reference potential from the data, current source density (CSD)
808 transformation was carried out using the spherical Laplace operator (parameters for this
809 procedure were $n = 4$ splines and $m = 10$ Legendre polynomials; $\Lambda = 1 \times 10^{-5}$). Lastly,
810 the baseline was corrected by calculating new locking points using the period between -200 ms
811 and the locking point for each segment. This baseline-corrected EEG data of all 60 channels
812 have been exported from Brain Vision Analyzer as single trial, single-subject time-locked data.
813

814 **QUANTIFICATION AND STATISTICAL ANALYSIS**

815 *Residue iteration decomposition (RIDE)*

816 Residue Iteration Decomposition (RIDE) was applied to the single-trial level, single-subject
817 data. RIDE decomposition was performed following a previous study that used the same
818 experimental paradigm (Wolff et al., 2017b). Although RIDE was initially developed to control
819 and correct intra-individual variability in the data, it is also used to distinguish intermingled
820 coding levels in neurophysiological data (Mückschel et al., 2017b, 2017a; Opitz et al., 2020;
821 Takacs et al., 2020a). This is the primary reason why we applied RIDE (the toolbox and manual
822 of RIDE available on <http://cns.hkbu.edu.hk/RIDE.htm>). Comprehensive mathematical details
823 on the RIDE method can be found in Ouyang et al. (Ouyang et al., 2011, 2015). Briefly, RIDE
824 uses a self-optimizing iteration scheme, which decomposes single-trial ERPs into static latency
825 and variable-latency components at each electrode separately. These components are thought
826 to reflect different and partly overlapping stages of cognitive processing. The separation of
827 these stages in the EEG signal leads to three RIDE-components (clusters of components) with
828 similar time-locking properties (Ouyang et al., 2011, 2015): the S-cluster refers to processes
829 related to the stimulus (such as perception and attention processes), the R-cluster relates to the
830 processes associated to the response (such as motor preparation and execution processes), and
831 the C-cluster refers to intermediate processes between S and R (such as stimulus evaluation and
832 response selection processes) (Ouyang et al., 2011, 2015; Verleger et al., 2014). The different
833 components within a RIDE cluster correspond to standard ERP components with different
834 peaks, topographies, and functional significance (Ouyang et al., 2011, 2015). For the
835 decomposition, the RIDE algorithm employs a time window function to obtain each RIDE
836 component's waveform. It is assumed that the time frames include each component's occurrence
837 (Ouyang et al., 2011, 2015). Therefore, the search windows' parameters must be adjusted to fit
838 the experimental task's data. In the present case, the following time windows were defined: 0
839 to 600 ms (including the target stimulus) for the S-cluster, 200 to 900 ms for the C-cluster, and

840 300 ms before and after the response for the R-cluster. The RIDE procedure created the
841 following types of separate datasets for each condition and each subject: C-cluster averaged
842 data, C-cluster single-trial data, R-cluster averaged data, R-cluster single-trial data, S-cluster
843 averaged data, S-cluster single-trial data, and averaged latency-corrected data of the
844 undecomposed EEG. The single-trial single subject data were used for subsequent MVPA,
845 while the single subject average data were used for source localization (see *Source localization*
846 *analysis (sLORETA)*). Prior to the MVPA, the single-trial datasets of all task conditions needed
847 to be concatenated for each subject, separately for the C-cluster, R-cluster, and S-cluster data.

848

849 *Multivariate Pattern Analysis*

850 Temporally decomposed, single-trial single-subject datasets were used for MVPA. The MVPA
851 was performed using the ADAM toolbox (version 1.05, Fahrenfort et al., 2018) in Matlab
852 (Mathworks). For a similar approach, see Takacs et al. (Takacs et al., 2020b). First, the EEG
853 data was down-sampled offline to 55 Hz (Fahrenfort et al., 2018). A linear discriminant
854 classifier was trained and tested on each time point. The classifier was trained on 80% of the
855 data, and tested on the remaining 20% of the data, iterating this process until all data points had
856 been tested (5-fold training). The average of the consecutive test folds was used as a final
857 performance index. Classification accuracy was quantified as Area Under the ROC Curve
858 (AUC). Larger AUC indicates better (more accurate) classification performance (Fahrenfort et
859 al., 2018). The classifier was trained on the following categories, separately for the C-cluster,
860 R-cluster and S-cluster data:

861 (1) Task repetition: cue repetition vs memory repetition; (2) Task switching: cue switch vs
862 memory switch. Thus, decoding performance with these categories should reflect the difference
863 between following the task rule after receiving a cue versus remembering that. That is, decoding
864 was expected to reveal the activation/deactivation of the appropriate response under memory
865 load. This allowed us to investigate how neural patterns differ from each other while following
866 the same task rules with external reminders (cue conditions) or relying on internal ones
867 (memory conditions), separately for trials where task switching was either necessary or not.
868 Specifically, decoding categories of Task repetition was expected to reveal the difference
869 between being reminded or recalling the continuously present task set. On the other hand, the
870 decoding results of Task switching categories was expected to show the difference between
871 neural patterns for being reminded or being recalled an alternative (i.e., competitive) task set.
872 Altogether, the potential differences between Task repetition and Task switching MVPA results
873 should be informative on the dynamics of neural implementations during upholding vs

874 switching mental sets of task rules. The decoding of task repetition denotes appropriate response
875 activation in a continuous manner. In contrast, task switching represents response activation
876 when participants had to change their mental set from one rule to another between two
877 consecutive trials. Skewed classification was avoided by balancing the categories with ADAM
878 (Fahrenfort et al., 2018). If trial numbers in the categories were unbalanced, the majority class
879 was down-sampled (that is, between cue repetition and memory repetition, and between cue
880 switch and memory switch, respectively). The following trial numbers entered the analyses for
881 each classification (mean, minimum and maximum given): Task repetition in the C-cluster
882 (121.9; 36; 378), Task switching in the C-cluster (89.2; 30; 234), Task repetition in the R-cluster
883 (151; 36; 378), Task switching in the R-cluster (90.9; 30; 234), Task repetition in the S-cluster
884 (150.2; 36; 378), Task switching in the S-cluster (90.2; 30; 234). Classification features
885 consisted of EEG amplitude data at the sixty single channels in all stimulus classes. A backward
886 decoding model (Fahrenfort et al., 2018) was used for training and testing. After the calculation
887 of the AUCs, temporal generalization matrices were computed based on cross-classification
888 across time. Temporal generalization matrices are commonly used to visualize how accurately
889 classification performance for a given time window generalizes to all other time points of the
890 analysed data (Fahrenfort et al., 2018; King and Dehaene, 2014). Good (i.e., highly accurate)
891 classification performance across samples suggests stability of the identified neural pattern.
892 Higher stability was visualized as either darker colours on a heat map (see Figures 3-4) or as a
893 larger extension of the generalized pattern in comparison to the diagonal angle. The stability of
894 the C-, R-, and S-clusters activity patterns was examined over time by training the model in one
895 time point and testing its discriminatory power in the other time points. Cross-classification
896 was iterated at every time point. In the final AUC, performance significantly above or below
897 chance level indicates sustained neural activity. Statistical analyses for the MVPA, including
898 corrections for multiple comparisons, were performed in ADAM (Fahrenfort et al., 2018). Two-
899 sided t-tests against chance level defined as $AUC = .05$ were performed for each time sample
900 across subjects. Cluster-based permutation was used to correct multiple comparisons as
901 implemented in ADAM (Fahrenfort et al., 2018).

902

903 *Source localization analysis (sLORETA)*

904 Source localization analysis using standardized low resolution brain electromagnetic
905 tomography (sLORETA) (Pascual-Marqui, 2002) was used to examine what functional
906 neuroanatomical structures were associated with MVPA-decoded neuronal activity in time
907 periods showing significantly above/below chance level classification performance.

908 Mathematical details on the sLORETA algorithm can be found elsewhere (Pascual-Marqui,
909 2002) and the validity of this approach has been corroborated by combined fMRI/EEG and
910 TMS/EEG studies (Dippel and Beste, 2015; Sekihara et al., 2005). Briefly, sLORETA uses a
911 three-shell spherical head model (MNI152 template) in which the intra-cerebral volume is
912 partitioned into 6239 voxels using a spatial resolution of 5mm. The standardized current density
913 is calculated for every voxel in this head model. The algorithm provides a single linear solution
914 for the inverse problem without localization bias (Marco-Pallarés et al., 2005; Pascual-Marqui,
915 2002; Sekihara et al., 2005). We used the sLORETA contrast against zero for the statistical
916 analysis, and we performed voxel-wise randomization tests with 2,500 permutations and
917 statistical non-parametric mapping procedures (SnPM) to correct for multiple comparisons.
918 Locations of voxels that were significantly different ($p < .05$) are shown in the MNI-brain
919 www.unizh.ch/keyinst/NewLORETA/sLORETA/sLORETA.htm, with color coding reflecting
920 t-values.

921

922 *Statistics*

923 Statistical analyses of the behavioral data were performed using IBM SPSS Statistics (IBM
924 Corp., Armonk, NY). Mean accuracy (percentage of correct responses) and means of reaction
925 time (RT) data (for correct responses) were calculated for each participant and each condition.
926 To examine task switching effects, accuracy and RT data were analysed repeated measures
927 ANOVAs with trial type (cued vs memory), rule (repetition vs switch) and motor response
928 (repetition vs switch) as within-subject factors. Switch cost was quantified as the difference
929 between task repetition and task switch RT or accuracy, separately for cued and memory
930 conditions. Mean AUC in the time windows of significant above- or below-threshold
931 classifications was calculated for each participant and each condition. To analyse the difference
932 between MVPA decoding results, repeated measures ANOVAs with time window (as indicated
933 by a successful decoding) and rule (repetition vs switch) were conducted separately for the C-
934 and R-cluster data. In the S-cluster, only since a single time window was identified, decoding
935 results between repetition and switch rules were compared with a paired sample *t*-test
936 (bootstrapped: sample size of 5000, confidence interval [CI] level of 95%). Here we report η_p^2
937 effect size for ANOVA main effects and interactions and Cohen's *d* for *t*-tests. All post-hoc
938 tests were Bonferroni-corrected. Finally, to analyse the relationship between behavioral and
939 neurophysiological markers of task switching, bootstrapped (sample size of 5000, confidence
940 interval [CI] level of 95%) Pearson's correlations were ran between the individual AUCs
941 averaged over significant above- or below-threshold classifications and task switching.

942

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