

Model selection for spectral parameterization

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Abstract: Neurophysiological brain activity comprises rhythmic (periodic) and arrhythmic (aperiodic) signal elements, which are increasingly studied in relation to behavioral traits and clinical symptoms. Current methods for spectral parameterization of neural recordings rely on user-dependent parameter selection, which challenges the replicability and robustness of findings. Here, we introduce a principled approach to model selection, relying on Bayesian information criterion, for static and time-resolved spectral parameterization of neurophysiological data. We present extensive tests of the approach with ground-truth and empirical magnetoencephalography recordings. Data-driven model selection enhances both the specificity and sensitivity of spectral and spectrogram decompositions, even in non-stationary contexts. Overall, the proposed spectral decomposition with data-driven model selection minimizes the reliance on user expertise and subjective choices, enabling more robust, reproducible, and interpretable research findings.

Lay summary: Brain activity is composed of rhythmic patterns that repeat over time and arrhythmic elements that are less structured. Recent advances in brain signal analysis have improved our ability to distinguish between these two types of components, enhancing our understanding of brain signals. However, current methods require users to adjust several parameters manually to obtain their results. The outcomes of the analyses therefore depend on each user's decisions and expertise. To improve the replicability of research findings, the authors propose a new, automated method to streamline the analysis of brain signal contents. They developed a new algorithm that defines the parameters of the analytical pipeline informed by the data. The effectiveness of this new method is demonstrated with both synthesized and real-world data. The new approach is made available to all researchers as a free, open-source app, observing best practices for neuroscience research.

Keywords: Neurophysiology, Spectral decomposition, Time-frequency analysis, Magnetoencephalography, Model selection, Rhythmic and arrhythmic brain signals, Parameter optimization, Reproducibility in research.

43 Introduction

44
45 Neural oscillations are rhythmic (periodic) signal components ubiquitously observed in
46 electrophysiology across spatial and temporal scales (Buzsaki & Watson, 2012). In the power
47 spectrum, periodic components can be modelled as Gaussian-shaped peaks emerging from an
48 arrhythmic (aperiodic) background (Wen & Liu, 2016; Donoghue et al., 2020; Wilson et al., 2022).
49 Aperiodic activity is spectrally characterized by a reciprocal distribution of signal power that
50 decays with frequency according to a power law ($1/f^\alpha$). In practice, the scalar exponent parameter
51 α and broadband offset of the aperiodic model are inferred from estimates of the signal's power
52 spectrum density (PSD) of the electrophysiological signal. Computational neuroscience models
53 and growing empirical evidence suggest that α reflects the physiological balance between
54 excitatory (E) and inhibitory (I) neural activity (Brake et al., 2024; Chini et al., 2022; Gao et al.,
55 2017; Wiest et al., 2023), and the offset is related to aggregate neuronal population spiking (Miller
56 et al., 2014; Voytek & Knight, 2015). These model parameters of the aperiodic spectral component
57 decrease with age, accounting for the observation of a *flutter* power spectrum in aging (Cellier et
58 al., 2021; Donoghue et al., 2020; Voytek et al., 2015). They also fluctuate during cognitive tasks
59 (Donoghue et al., 2020; Gyurkovics et al., 2022; Preston et al., 2022; Waschke et al., 2021) and
60 reflect behavioral traits (Ostlund et al., 2021; Wilson et al., 2022).

61
62 Recent algorithms and software such as the *specparam* (Donoghue et al., 2020) and Spectral
63 Parameterization Resolved in Time (*SPRiNT*; Wilson et al., 2022) have streamlined the adoption
64 of spectral parameterization in electrophysiological research. These tools require users to define a
65 number of method parameters (hyperparameters), such as model complexity via the pre-
66 specification of the maximum number of spectral peaks N_G to be adjusted from the empirical PSD
67 (Gerster et al., 2022; Ostlund et al., 2022; Wilson et al., 2022). When hyperparameters are not set
68 appropriately, the *specparam* algorithm either fits spurious, outlier spectral peaks or misses
69 genuine spectral peaks (Donoghue et al., 2020). Similarly, time-resolved spectral parametrization
70 tools rely on hyperparameters to minimize the detection of outlier spectral peaks (Brady &
71 Bardouille, 2022; Cole et al., 2019; Kosciessa et al., 2020; Seymour et al., 2022; Stokes et al.,
72 2023; Whitten et al., 2011; Wilson et al., 2022).

73
74 Setting model hyperparameters is a prevalent challenge across many fields of science and
75 engineering. Good-practice approaches recommend prioritizing parsimonious models with a
76 balance between simplicity (less hyperparameters) and the ability to fit the observed data (more
77 flexibility; Vandekerckhove et al., 2015). Here, we propose such a model selection strategy for the
78 parameterization of both the PSD and spectrogram of neurophysiological time series. The method
79 proceeds with adjusting progressively more complex models to the empirical data spectrum or
80 spectrogram, and determines the parameters of the simplest model that adequately accounts for the
81 data on the basis of the Bayesian information criterion (BIC). This also enables the quantitation of
82 evidence for periodic activity in spectral data via Bayes factor analysis. We demonstrate below the
83 method's performance using extensive ground-truth simulated data and a large set of empirical
84 resting-state magnetoencephalography (MEG) from $N=606$ participants.

85 Methods

86

87 Model Selection using Bayesian Information Criterion.

88 In the context of parsimonious modeling of power spectra and spectrograms, our goal is to optimize
89 the trade-off between model fidelity and complexity. This principle emphasizes deriving the most
90 accurate and representative model directly from empirical data while minimizing the inclusion of
91 unnecessary assumptions or parameters (Myung, 2000). Among the methods for comparing
92 models, Bayes factors are noteworthy as they balance model fit evaluation with the principle of
93 simplicity (Jefferys & Berger, 1992). These factors can be effectively estimated using the Bayesian
94 Information Criterion (BIC), which offers a pragmatic tradeoff between goodness-of-fit and
95 complexity in terms of the number of model parameters (Schwarz, 1978; Vandekerckhove et al.,
96 2015).

97

98 In the *specparam* approach, model fitting involves minimizing the least-squares error between
99 model predictions and the empirical power spectrum. The *ms-specparam* method refines this
100 objective by estimating the negative log-likelihood of a model:

101

$$102 \quad -\ln p(y | x, w, \beta) = \frac{\beta}{2} \sum_{i=1}^N \{f(x_i, w) - y_i\}^2 - \frac{N}{2} \ln(\beta) + \frac{N}{2} \ln(2\pi)$$

103

104 where (x) and (y) are the frequency bins and empirical spectral power values, respectively;
105 $(f(x_i, w))$ is the spectral power predicted by the model at frequency (x_i) ; (y_i) is the empirical
106 spectral power value at frequency (x_i) ; (w) represents the model parameters, (N) the number of
107 frequency bins. (β) is the precision, or inverse variance, of residuals.

108

$$109 \quad \beta = 1/\sigma^2 ,$$

110

111 Under the assumption of zero-mean (unbiased) Gaussian noise in the empirical power spectrum,
112 minimizing negative log-likelihood provides an equivalent solution to minimizing squared error
113 (Mitchell, 1997). Finally, we express the *specparam* optimization's output in terms of the
114 Bayesian information criterion (BIC):

115

$$116 \quad \text{BIC} = 2 \cdot \text{NLL} + \log(N) \cdot k,$$

117 where NLL is the negative log-likelihood, (N) is the number of frequency bins, and
118 (k) represents the total number of parameters, which includes the aperiodic parameters (exponent
119 and offset) and three additional parameters for each peak (center frequency, amplitude,
120 bandwidth). Note that $(k = 3P + 2)$, where (P) represents the number of peaks.

121 The *specparam* algorithm iteratively fits models of increasing complexity by adding peaks and
122 minimizing the squared error. It performs a final optimization of both aperiodic and periodic
123 parameters, and then converts the squared error into a negative log-likelihood, which is used to

124 calculate the BIC. The algorithm ultimately provides the parameters of the model with the lowest
125 BIC, thus achieving a balance between fit quality and model simplicity.

126 We developed *ms-specparam* and *ms-SPRiNT* as plug-in libraries that interoperate
127 with *Brainstorm* (Tadel et al., 2011) and are therefore open-source and accessible to everyone.

128 **Algorithm Settings and Hyperparameters.**

129 The spectral parameterization of neural power spectra (synthetic and empirical) was conducted in
130 the frequency range of 1-40 Hz using three distinct approaches, each characterized by different
131 hyperparameter settings:

132 **1. Default Hyperparameters:** This approach adhered to the default settings established by the
133 Python implementation of *specparam* (Donoghue et al., 2020). The hyperparameters included a
134 minimum peak height of 0.1 arbitrary units (a.u.), a maximum of 6 peaks, peak width limits set
135 within the range of [1, 8] Hz, and a proximity threshold of 0.75 a.u.

136 **2. Conservative Hyperparameters:** This setting was driven by the *Brainstorm* implementation
137 of *specparam* (Tadel et al., 2011). It involved more conservative hyperparameters, with a
138 minimum peak height of 0.3 a.u., a reduced maximum number of peaks at 3, peak width limits
139 broadened to [0.5, 12] Hz, and an increased proximity threshold of 2.0 a.u.

140 **3. *ms-specparam*:** This approach used the same hyperparameter settings as *default-specparam*,
141 including a minimum peak height of 0.1 a.u., a maximum of 6 peaks, peak width limits between
142 [1, 8] Hz, and a proximity threshold of 0.75 a.u. The most parsimonious spectral model is selected
143 according to the procedure described in *Model Selection using Bayesian Information Criterion*.

144 These different spectral parameterization strategies were selected to provide a comprehensive
145 comparison across various standard and conservative parameter settings.

146 Dynamic synthetic neural time series were similarly parameterized using *SPRiNT* in the 1-40
147 Hz frequency range, using 5x1 s windows (50% overlap), according to four distinct
148 conditions. While each condition used default hyperparameters for *specparam*, they differed
149 in their methodologies for removing spurious, outlier spectral peaks:

150 **1. SPRiNT:** No procedure for pruning spurious, outlier spectral peaks.

151 **2. SPRiNT with post-processing:** This condition identified putative spurious, outlier spectral
152 peaks as those with fewer than a predetermined number of similar peaks (by center frequency)
153 within neighboring time bins of the spectrogram. The process prunes identified spurious,
154 outlier spectral peaks and re-optimizes spectral models in affected time bins. For more details,
155 see Wilson et al. (2022). The hyperparameters used for post-processing consisted of pruning
156 spectral peaks with fewer than four neighboring peaks within 1.5 Hz and six time bins (3 s).

157 **3. *ms-SPRiNT*:** This condition selected the most parsimonious spectral model in each time
158 bin according to the procedure described in *Model Selection using Bayesian Information*
159 *Criterion*.

160 **4. ms-SPRiNT with post-processing:** This process first selected the most parsimonious
161 spectral model using *ms-SPRiNT* before pruning spurious, outlier spectral peaks through post-
162 processing.

163 **Synthetic Data.**

164 We created 5,000 synthetic neural power spectra using a range of aperiodic parameters: exponents
165 from 0.5 to 2 Hz⁻¹) and offsets from -8.1 to -1.5 arbitrary units (a.u.). Each power spectrum was
166 augmented with zero to four peaks, with 1,000 instances for each peak quantity. The parameters
167 for these peaks fell within specified ranges: center frequencies between 3 and 35 Hz, amplitudes
168 from 0.1 to 1.5 a.u., and bandwidths (2 s.d.) from 2 to 6 Hz. We ensured a minimum separation of
169 one bandwidth between adjacent peak frequencies. The frequency domain for simulation spanned
170 from 0.5 to 100 Hz with increments of 0.5 Hz.

171 To mimic realistic noise conditions, we introduced Gaussian white noise at varying intensities:
172 low (0.05 a.u.), medium (0.10 a.u.), and high (0.15 a.u.). We then applied *default-specparam*
173 (minimum peak height of 0.1 a.u., up to six peaks, peak width range of 1 to 8 Hz, and proximity
174 threshold of 0.75 a.u.) alongside *ms-specparam* with identical parameters.

175 We also used 10,000 synthetic neural-like time series to evaluate the model selection approach in
176 the context of time-resolved spectral parameterization. These simulations, previously generated by
177 Wilson et al. (2022) to evaluate *SPRiNT*'s performance, each consist of 60 seconds of unique,
178 dynamic periodic and aperiodic activity. Aperiodic exponents were initialized between 0.8 and 2.2
179 Hz⁻¹, and aperiodic offsets between -8.1 and -1.5 a.u. Within the 12–36 second segment of the
180 simulation (onset randomized), the aperiodic exponent and offset underwent a linear shift of
181 magnitude in the ranges -0.5–0.5 Hz⁻¹ and -1–1 a.u., respectively (sampled continuously and
182 chosen randomly). The duration of the linear shift was randomly selected for each simulated time
183 series between 6 and 24 seconds. Periodic components (0–4 peaks) were added to each trial with
184 parameters randomly sampled within the ranges: center frequency: 3–35 Hz; amplitude: 0.6–1.6
185 a.u.; SD: 1–2 Hz. Onset (5–40 s) and duration (3–20 s) of periodic components (if any) were
186 randomized across trials, with the constraint that they would not overlap in both time and
187 frequency; they were allowed to overlap in one dimension. If a periodic component overlapped
188 temporally with another, its center frequency was set at least 2.5 peak SDs from the other
189 temporally overlapping periodic component(s). The magnitude of each periodic component was
190 tapered by a Tukey kernel (cosine fraction = 0.4). Spectral noise levels were inherent to the
191 methods for time-frequency decomposition (short-time Fourier transform, 5x1 s windows with
192 50% overlap) and were previously approximated to be high (approximately 0.2 a.u.; Wilson et al.,
193 2022).

194
195 For accuracy assessment, a 'hit' was designated when an identified peak's center frequency was
196 within one bandwidth (2 s.d.) of a true peak. In cases where multiple identified peaks met this
197 criterion, the peak with the highest amplitude was selected as the 'hit.' Peaks detected by the
198 algorithm that did not correspond to a true peak were classified as false positives.

199
200 We defined peak sensitivity as the ratio of 'hits' to the total number of simulated peaks, and the
201 positive predictive value as the ratio of 'hits' to all detected peaks (including false positives). For

202 peaks identified as 'hits,' we calculated the parameter estimation error as the absolute deviation
203 from the true values.

204

205 **Bayes factor evidence for periodic brain activity.**

206 Bayes factor (BF) provides a statistical measure for comparing two models, offering evidence
207 about the presence of periodic activity within neural power spectra. The computation of the Bayes
208 factor follows the formula proposed by Wagenmakers (2007):

$$209 \quad BF_{01} = e^{(BIC_0 - BIC_1)/2}$$

210 where (BIC_0) is the Bayesian Information Criterion (BIC) value for the aperiodic-only model and
211 (BIC_1) is the BIC value of the lowest-BIC model.

212 In this context, (BIC_0) represents the BIC for the aperiodic-only model, which posits that the data
213 can be explained without invoking rhythmic components. (BIC_1) , on the other hand, corresponds
214 to the model that includes both aperiodic and periodic elements and has the lowest BIC among all
215 models considered.

216 The Bayes factor (BF_{01}) compares these models, translating the difference in their BIC values into
217 the odds ratio against periodic activity. A smaller (BF_{01}) implies stronger evidence against the
218 aperiodic-only model, thereby indicating the presence of significant periodic activity within the
219 brain's neural power spectra. Conversely, larger (BF_{01}) values suggest that the periodic
220 components do not significantly improve the model beyond the aperiodic activity alone.

221 This approach allows for the quantitative assessment of oscillations in neural recordings, providing
222 a more rigorous foundation for claims of rhythmic brain activity observed in electrophysiological
223 data.

224 **Empirical data.**

225 The empirical dataset for our study was obtained from the Cambridge Centre for Aging
226 Neuroscience repository (Cam-CAN; Shafto et al., 2014; Taylor et al., 2017). This comprehensive
227 dataset includes 606 healthy individuals aged 18 to 90 years (mean age = 54.69; SD = 18.28), with
228 a balanced gender representation (299 females). Each participant underwent a thorough
229 assessment, beginning with a detailed home interview followed by a resting-state
230 magnetoencephalography (MEG) session. The MEG recordings, lasting approximately 8 minutes
231 each, were conducted using a 306-channel VectorView MEG system (MEGIN). These recordings
232 were complemented with structural T1-weighted magnetic resonance imaging (MRI) to provide
233 anatomical context for MEG source mapping. All data collection occurred at a single, consistent
234 location to maintain uniformity in data acquisition.

235 This rich dataset forms the basis for our analyses, allowing for a comprehensive investigation into
236 the spectral properties of neural signals across a wide age spectrum.

237 **MEG Preprocessing and Source Mapping.**

238 We preprocessed magnetoencephalography (MEG) data with Brainstorm (Tadel et al., 2011;
239 March 2021 distribution), integrated with MATLAB (2020b; Natick, MA), adhering to established
240 best-practice guidelines (Gross et al., 2015). The preprocessing methodology followed protocols
241 detailed previously (da Silva Castanheira et al., 2021).

242 Line noise artifacts at 50 Hz and its first 10 harmonics were filtered using a notch filter bank.
243 Additionally, an 88-Hz artifact present in the Cam-CAN dataset (Wiesman et al., 2022) was
244 removed. To address slow-wave and DC-offset artifacts, a high-pass finite impulse response (FIR)
245 filter with a cutoff frequency of 0.3 Hz was applied. Signal-Space Projections (SSPs) were
246 implemented to attenuate cardiac artifacts and mitigate low-frequency (1–7 Hz) and high-
247 frequency (40–400 Hz) noise components, typically originating from saccades and muscle
248 activities.

249 Brain source models were anchored to the individual T1-weighted MRI data of each participant.
250 Automatic segmentation and labeling of MRI volumes were achieved using FreeSurfer (Fischl,
251 2012). Co-registration with MEG data was facilitated using approximately 100 head points
252 digitized for each participant. MEG biophysical head models were computed using *Brainstorm*'s
253 overlapping-spheres model (default parameters).

254 Cortical source models were estimated using linearly constrained minimum-variance (LCMV)
255 beamforming, following *Brainstorm*'s default parameters (2018 version for source estimation
256 processes). MEG source orientations were constrained normal to the cortical surface, distributed
257 across 15,000 locations. Neural power spectra were then calculated for each of the 148 cortical
258 regions defined by the Destrieux atlas (Destrieux, 2010). These calculations were based on the
259 first principal component of all signals within each region of interest (ROI). Neural spectral power
260 was estimated using Welch's method, utilizing 2-second windows with a 50% overlap.

261 **Statistical Analyses.**

262 To evaluate the accuracy of spectral parameters generated by *ms-specparam*, we employed two-
263 sample non-parametric permutation t-tests from the *RVAideMemoire* package in R. This statistical
264 approach allowed us to test differences in spectral parameter estimates, specifically focusing on
265 five key variables: aperiodic exponent, aperiodic offset, peak center-frequency, peak amplitude,
266 and peak bandwidth.

267 To capture differences in residual variance and the number of peaks fitted between algorithms in
268 our empirical data, we similarly relied on paired non-parametric permutation t-tests.

269 We implemented hierarchical linear regression models using the *lmer* function in R to test how
270 algorithm choice impacts age's effect on both aperiodic exponent and offset. The models were
271 formulated as:

$$272 \quad y \sim \text{intercept} + (\text{Participant intercept}) + \beta_1 \times \text{chronological age} + \beta_2 \times \text{algorithm} \\ 273 \quad \quad \quad + \beta_3 \times \text{chronological age} \times \text{algorithm}$$

274 where (y) represents the dependent variables, including the aperiodic exponent and offset.

275 Separate linear regression analyses were conducted to compare *ms-specparam* against both
276 *default-specparam* and *conservative-specparam*. Chronological age and the chosen algorithm
277 (e.g., *ms-specparam* vs. *default-specparam*) were introduced as fixed predictors, and individual
278 participants were treated as a random factor to account for inter-individual variability.

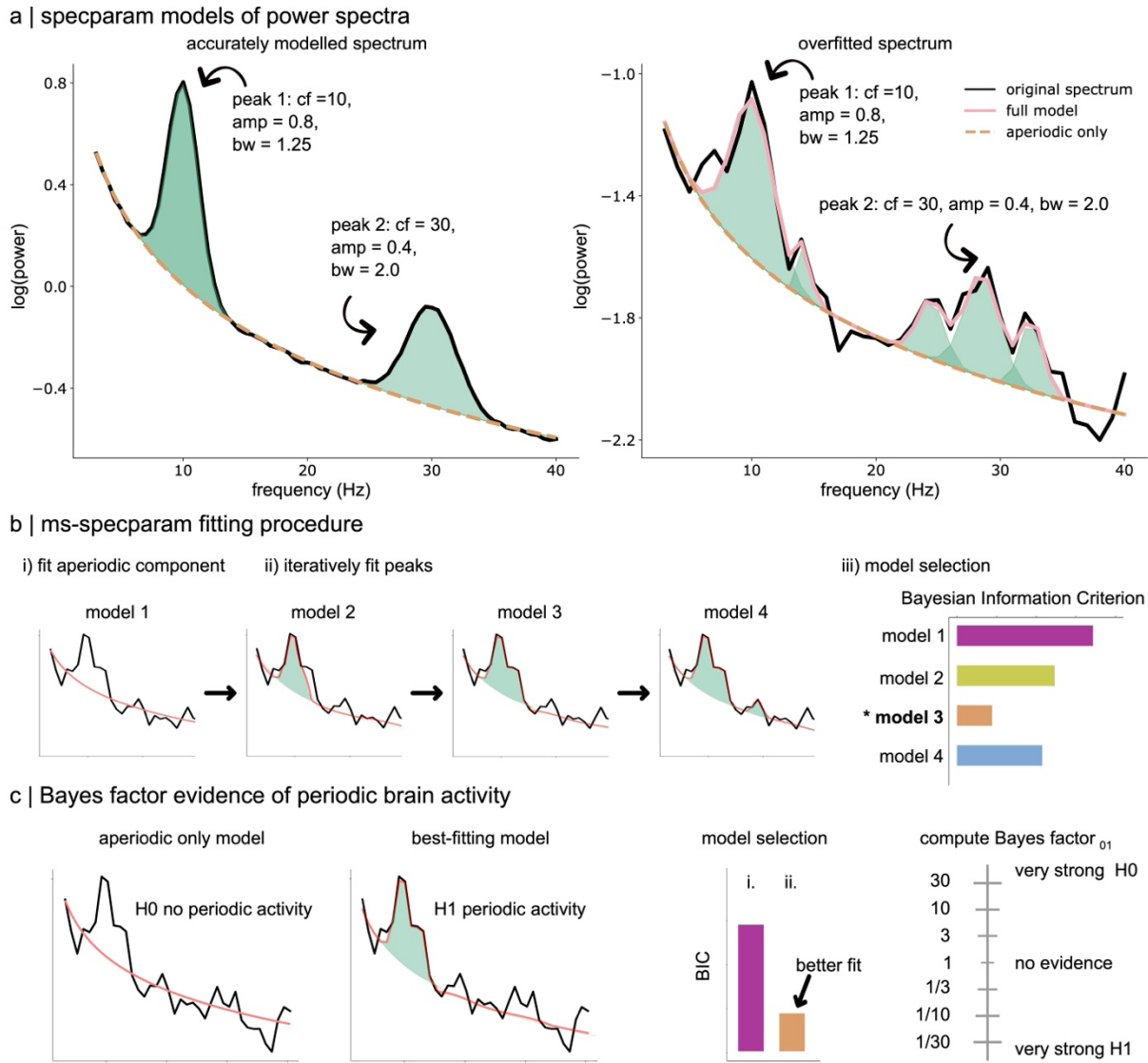
279 To quantify the Bayesian evidence for each predictor in our regression models, we employed
280 Bayes factor analysis with the Wagenmakers approximation (Wagenmakers, 2007). This provided
281 a nuanced understanding of the statistical significance and strength of the effects of age and
282 algorithm on spectral parameterization outcomes.

283 Results

284
285 Figure 1a highlights how user-dependent hyperparameters affect the outcome of spectral
286 parameterization. In the example shown, the hyperparameter specifying the maximum number of
287 peaks expected from spectral parameterization was set manually to a value of 6. However, the
288 spectrum of the present empirical data contains only two peaks (left panel; Figure 1a). Under high
289 signal-to-noise conditions, spectral parameterization may yield only two peaks as expected.
290 However, when data is realistically noisy, the spectral parameterization algorithm may
291 overestimate the number of peaks in the spectrum to account for noise-related fluctuations (right
292 panel; Figure 1a). Ideally, spectral and spectrogram parameterization should automatically and
293 adaptively adjust model hyperparameters to account for the noise level in the data.

294
295 To address these issues, we propose an approach that proceeds iteratively with the
296 parameterization of empirical power spectra and spectrograms with increasing model complexity
297 (i.e., the maximum number of spectral peaks). We derive the Bayesian Information Criterion (BIC)
298 for each hyperparameter setting. The most parsimonious hyperparameter setting to model the
299 empirical power spectrum or spectrogram is the one corresponding to the lowest BIC value (Figure
300 1b). If the most parsimonious model contains spectral peaks, we can further quantify the evidence
301 for periodic activity using the Bayes factor relative to the aperiodic-only model (Figure 1c). Our
302 approach applies to both spectral and spectrogram parameterization, as demonstrated herein with
303 *specparam* (Donoghue et al., 2020) for spectral analysis and *SPRiNT* (Wilson et al., 2022) for
304 spectrograms. The model-selection versions of these methods, coined *ms-specparam* and *ms-*
305 *SPRiNT*, are freely available through *Brainstorm* (Tadel et al., 2011) and on GitHub
306 (github.com/lucwilson/model_selection).

307
308 We tested and validated *ms-specparam* using 5,000 ground-truth, synthetic but
309 neurophysiologically plausible power spectra. We compared its performance against the original
310 *specparam* algorithm, configured to its default hyperparameters (referred to as *default-specparam*;
311 see Methods). Additionally, we validated *ms-SPRiNT* against the original *SPRiNT* algorithm using
312 spectrograms from 10,000 synthetic, neurophysiologically plausible time-series. We also applied
313 *ms-specparam* to task-free MEG recordings from 606 participants to replicate, with less
314 dependence on user-selected hyperparameters, the previously reported findings of an age-related
315 decline in the aperiodic exponent of the neurophysiological power spectrum (Voytek et al., 2015).



316

317

Figure 1: Spectral Parameterization with Model Selection

318 (a) Illustration of a spectral parameterization of a simulated power spectral density

319 estimate (black line) obtained with *specparam* in the context of lower (left panel) and

320 higher (right panel) noise levels. Both spectra are generated using the same spectral

321 parameters (i.e., two spectral peaks). In more noisy conditions, *specparam* (pink line) fits

322 a greater number of spectral peaks (green shaded areas) than what is present (simulated)

323 in the data, resulting in overfitting (right panel). Key: 'cf' refers to a peak's center

324 frequency, 'amp' refers to a peak's amplitude, and 'bw' refers to a peak's bandwidth.

325 (b) *ms-specparam* is a method for spectral parameterization combined with a model

326 selection procedure. It first adjusts a model for the aperiodic component of the spectrum

327 (subpanel i) before adding spectral peaks (green shaded areas) in an iterative fashion

328 (subpanel ii). These successive models are then assessed via the Bayesian Information

329 Criterion (BIC; subpanel iii).

330 (c) The resulting BIC model is then subjected to Bayes factor inference against the

331 aperiodic spectral model (panel i) to adjudicate whether spectral peaks are likely to be

332 present in the data power spectrum. A Bayes factor greater than 1 is evidence in favour
333 of periodic brain activity over the null hypothesis of no periodic activity (panel iv).

334

335 **Synthetic, Ground-Truth Data.**

336

337 Each of the 5,000 synthetic power spectra comprised an aperiodic component, with offset values
338 ranging from -8.1 to -1.5 arbitrary units (a.u.) and exponents set between 0.5 and 2 Hz⁻¹. We
339 randomly added between 0 and 4 spectral peaks to the aperiodic background of each power
340 spectrum (1,000 simulated spectra for each number of peaks; see Methods). Zero-mean Gaussian
341 noise was added to the resulting power spectra with varying standard deviation values (s.d.).

342

343 In moderate noise conditions (s.d. = 0.10), *ms-specparam* demonstrated a slightly lower sensitivity
344 (89%) in detecting spectral peaks compared to *default-specparam* (91%). However, it had a
345 substantially higher positive predictive value for peak detection (*ms-specparam*: 96%; *default-*
346 *specparam*: 63%). On average, *default-specparam* overestimated the number of peaks in the
347 spectrum by 59%, whereas *ms-specparam* underestimated the number of peaks by 13% (Figure
348 2a). We observed similar results for sensitivity and PPV in both algorithms at lower and higher
349 noise levels (Supplemental Materials).

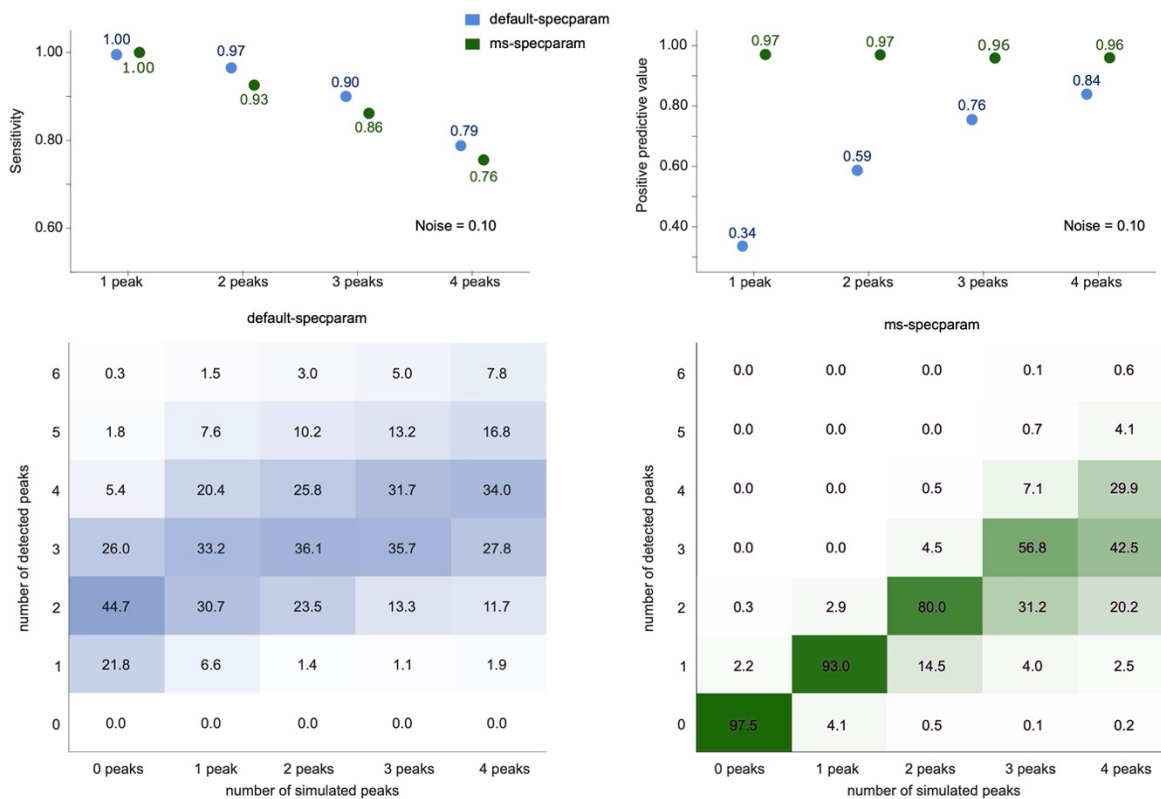
350

351 We found that, on average, parameter estimates derived from *ms-specparam* are more accurate
352 than those derived from *default-specparam*: aperiodic exponent ($t = 8.62$, $p = 0.0019$; aperiodic
353 offset $t = 8.38$, $p = 0.0019$; peak center frequency $t = 15.33$, $p = 0.0019$; peak amplitude $t =$
354 10.33 , $p = 0.0019$; peak bandwidth $t = 14.50$, $p = 0.0019$; one-tailed permutation t-tests; Figure
355 2b).

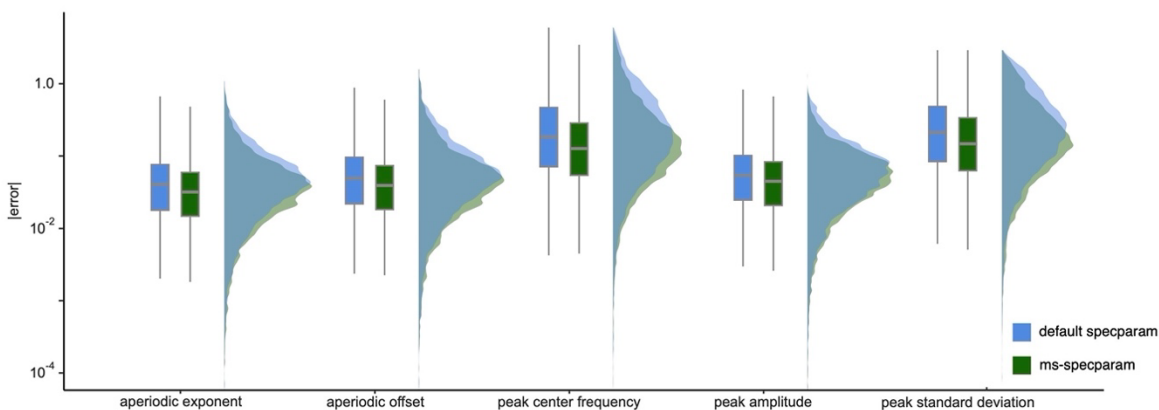
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357

a | *ms-specparam* fits fewer spurious peaks



b | *ms-specparam* fits spectral parameters better



358

359

Figure 2: Performances on Synthetic Stationary Data

360 (a) Sensitivity and positive predictive value (PPV) for detection of spectral peaks (top

361 peak). *ms-specparam* (green) has similar sensitivity (89%) than *default-specparam* (blue;

362 91%), but superior PPV (96% vs. 63%). The heat maps below report the ground-truth vs.

363 estimated number of spectral peaks (with percent incidence listed in each element) and

364 highlight *ms-specparam*'s improved peak detection accuracy.

365 (b) Boxplots and empirical density distributions reporting the errors on the estimates of

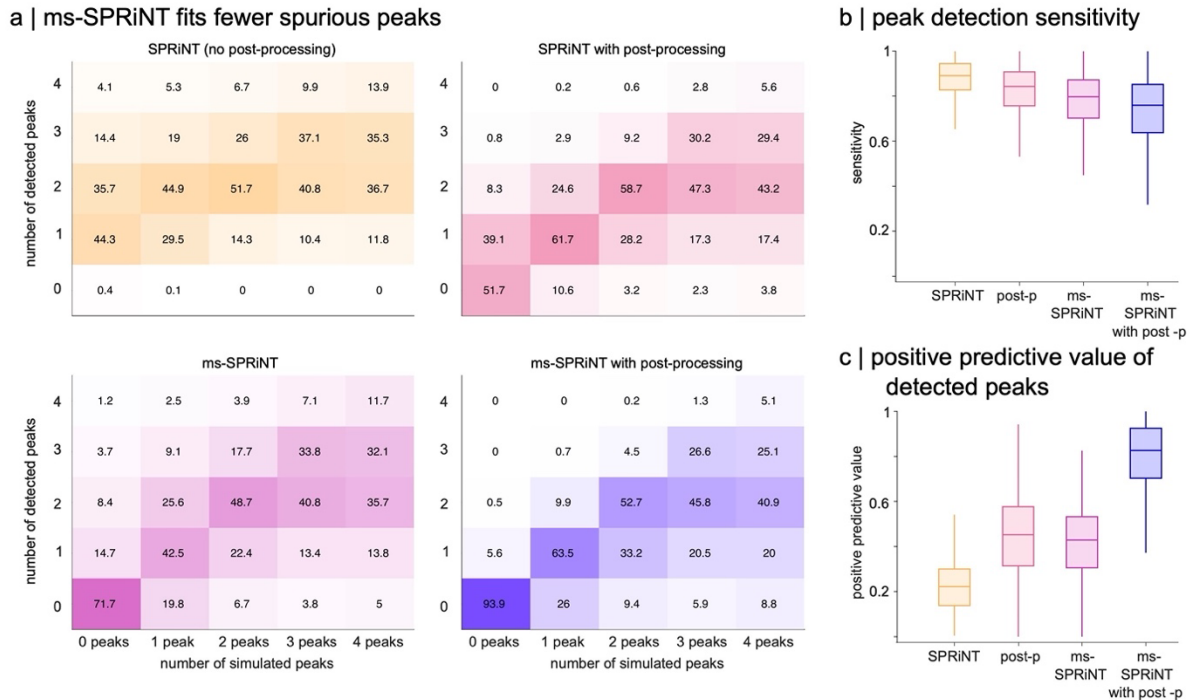
366 the spectral parameters derived using *ms-specparam* and *default-specparam*. For every

367 spectral parameter, *ms-specparam* estimated values with significantly lower mean
368 absolute error (one-tailed permutation t-test, all $p < 0.05$).

369
370 We subsequently evaluated the performance of *ms-SPRiNT* using 10,000 time series simulated
371 from realistic ranges of spectral parameters. We replicated the simulation procedure of Wilson et
372 al. (2022): in short, we synthesized neurophysiologically plausible time series (60-s duration)
373 composed of time-varying periodic and aperiodic components (see Methods).

374
375 We evaluated the respective performances of *SPRiNT*, *SPRiNT* with post-processing (i.e.,
376 removing spurious outlier spectral peaks, following Wilson et al., 2022), *ms-SPRiNT*, and *ms-*
377 *SPRiNT* with post-processing (Table S1). On average, *SPRiNT* with post-processing best estimated
378 the number of spectral peaks (4% more than expected), than *ms-SPRiNT* (15% more than expected)
379 and *ms-SPRiNT* with post-processing (20% fewer than expected). Similar to *specparam*, *SPRiNT*
380 tended to overestimate the number of spectral peaks (60% more than expected; Figure 3a).
381 *SPRiNT*'s peak detection had the highest sensitivity (89%) of all contexts (post-processing: 84%;
382 *ms-SPRiNT*: 80%; *ms-SPRiNT* with post-processing: 76%; Figure 3b) but also the lowest positive
383 predictive value (22%). Notably, peaks detected using *ms-SPRiNT* with post-processing had a
384 much higher positive predictive value (83%) than all other contexts (post-processing: 45%; *ms-*
385 *SPRiNT*: 43%; Figure 3d).

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Figure 3: Performances on Synthetic Data with Time-Varying Spectral Contents

396 (a) Heat maps reporting the number of spectral peaks detected vs. ground-truth. *ms-*

397 *SPRiNT* with post-processing (purple; bottom right) best recovers the true number of

398 spectral peaks. Numbers of datasets synthesized with 0 spectral peaks = 798,753, 1

399 peak = 256,599, 2 peaks = 78,698, 3 peaks = 14,790, and 4 peaks = 1160.

400 (b) Sensitivity of spectral peak detection (N = 10,000 simulated time series). *ms-SPRiNT*

401 with (purple) and without post-processing (fuchsia) exhibit marginally lower sensitivity

402 than the default *SPRiNT* algorithm (orange).

403 (c) Positive predictive value (PPV) of spectral peak detection. *ms-SPRiNT* with post-

404 processing (purple) exhibits a higher positive predictive value than all other algorithms.

405

Empirical MEG Data.

406

407

408 We applied *ms-specparam* to resting-state MEG data from the Cam-CAN repository (N=606;

409 Shafto et al., 2014; Taylor et al., 2017). We first preprocessed and source-mapped the MEG time

410 series using *Brainstorm* (Tadel et al., 2011) following good-practice guidelines (Gross et al.,

411 2013). We then derived the PSDs of each cortical parcel of the Destrieux atlas (Destrieux, 2010;

412 see Methods). We then compared models generated with *ms-specparam* to those from *specparam*,

413 using two hyperparameter settings: *default-specparam* (minimum peak height: 0.1 a.u.; maximum

414 number of peaks: 6; peak width limits: [1 8]; proximity threshold: 0.75 s.d.) and a more

415 conservative configuration (*conservative-specparam*; minimum peak height: 0.3 a.u.; maximum

416 number of peaks: 3; peak width limits: [0.5 12]; proximity threshold: 2).

417

418 We found that *ms-specparam* generated models with less residual variance (i.e., mean squared

419 error, MSE; average MSE = 2.08×10^{-3} , SD = 7.68×10^{-4}) than both *specparam* settings (default:

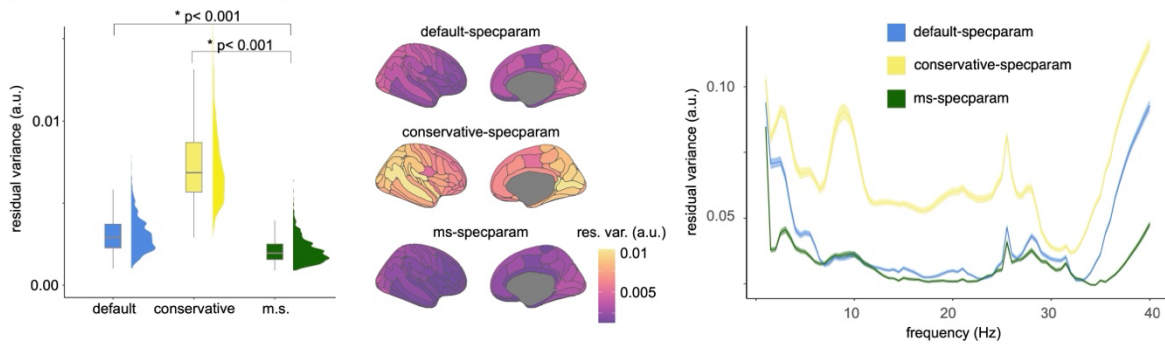
420 average MSE = 3.06×10^{-3} , SD = 1.07×10^{-3} ; $t = -48.82$, $p < 0.001$; conservative average MSE =
421 7.63×10^{-3} , SD = 3.08×10^{-3} ; $t = -51.17$, $p < 0.001$; Figure 4a). This observation was consistent across
422 all cortical parcels, with posterior parietal areas showing the greatest enhancements in model
423 goodness-of-fit (Figure 4a). Reduced residual variance was consistent over the entire frequency
424 range (1–40 Hz), with marked improvements with respect to both *specparam* settings over the
425 edges of the spectrum (<5 Hz and >35 Hz; Figure 4a). We also observed that *ms-specparam*
426 detected fewer spectral peaks than *default-specparam*, and therefore, as expected, provided more
427 parsimonious spectral parameterizations ($t = -58.26$, $p < 0.001$; Figure 4b).

428
429 With *ms-specparam*, we performed Bayes factor analyses (Vandekerckhove et al., 2015) as an
430 objective measure of evidence for the presence of rhythmic activity in the neurophysiological
431 power spectrum. We found that the bilateral cuneus exhibited the highest Bayesian evidence for
432 rhythmic activity in the resting-state, while we found the lowest evidence of rhythmic activity in
433 the orbitofrontal and medial frontal cortices (Figure 4c).

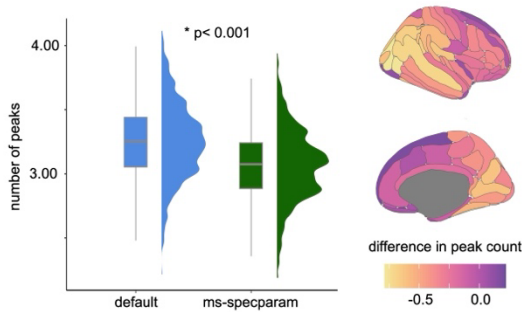
434
435 For illustration purposes, Figure 4d shows representative spectral parameterizations obtained from
436 neurophysiological time series recorded the right post-central gyrus. In this instance, *ms-*
437 *specparam* identified two spectral peaks while *default-specparam* adjusted five spectral peaks
438 (*default-specparam* MSE: 1.76×10^{-3} ; *ms-specparam*: 1.17×10^{-3}).

439

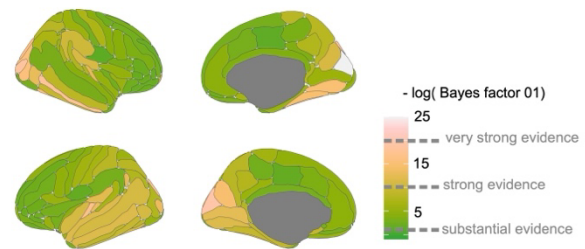
a | empirical data: ms-specparam vs specparam model error



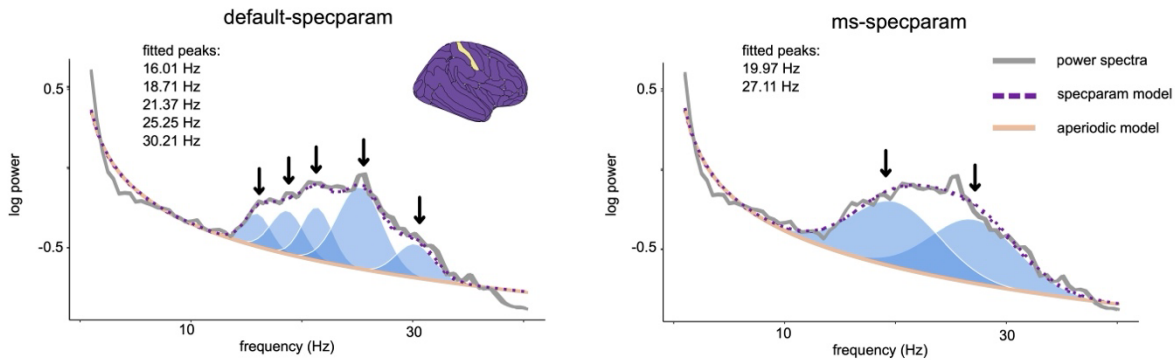
b | ms-specparam is more parsimonious



c | Bayesian evidence of periodic brain activity



d | example parameterized spectra



440

441

Figure 4: Performances on Empirical MEG Data.

442 (a) Residual variance analysis across the 606 participants and all brain regions shows

443 *ms-specparam* (green) with consistently lower residual variance, indicating a superior fit

444 relative to the other spectral parameterization methods (blue and yellow; left panel). The

445 brain maps display residual variance values for each cortical parcel. A frequency

446 breakdown (right panel) reveals *ms-specparam* outperforms the other two tested

447 *specparam* variations across the spectrum, particularly at the edges of the frequency

448 spectrum.

449 (b) *ms-specparam* estimates less spectral peaks than *default-specparam*, demonstrating

450 more parsimonious modeling, as reported in the box/density plots (left panel). The brain

451 maps indicate that less spectral peaks were detected in posterior cortical parcels with *ms-*

452 *specparam* (right panel).

453 (c) Bayesian evidence for periodic, rhythmic brain activity mapped across the cortical

454 surface emphasizes occipital and left temporal regions.

455 (d) Parameterized spectra from the right post-central gyrus of a sample subject highlight
456 the differences between algorithms: *ms-specparam* fits two peaks (right panel), reflecting
457 the dominant oscillations, whereas *default-specparam* fits five (left panel), some of which
458 may be redundant or overfitted, as seen in the overlaid spectral models.

459

460 **Age-Related Flattening of the Aperiodic Spectrum Depends on Hyperparameter Choice.**

461

462 We aimed to replicate with *ms-specparam* previous observations using *specparam* of age-related
463 decreases in aperiodic exponent (Donoghue et al., 2020; Voytek et al., 2015). We examined the
464 degree to which the methods' hyperparameters influenced the detection of these aging effects. To
465 do this, we fitted hierarchical linear regression models where age, the choice of spectral
466 parameterization algorithm, and their interaction were included as predictors of both aperiodic
467 exponent and aperiodic offset, respectively. A significant interaction would suggest that age-
468 related changes in the spectral aperiodic exponent, for example, are contingent upon the method's
469 hyperparameters, rather than reflecting actual neurophysiological effects.

470

471 We found that age-related decreases in aperiodic exponent are modulated by the algorithm used,
472 whether *ms-specparam* or *specparam* with default or conservative hyperparameter settings (i.e., a
473 significant interaction between age and spectral parameterization algorithm). This indicates that
474 the observed age-related changes in aperiodic exponent may be influenced by the choice of
475 parameterization method rather than solely reflecting genuine neurophysiological effects (default
476 hyperparameters: $\beta = 0.04$, SE = 0.01, 0.02, 0.06]; $BF_{01} = 0.12$; conservative hyperparameters: $\beta =$
477 0.12 , SE = 0.01, [0.09, 0.14]; $BF_{01} = 5.91 \times 10^{-12}$; Figure 5a-b and Table S2 & S3).

478

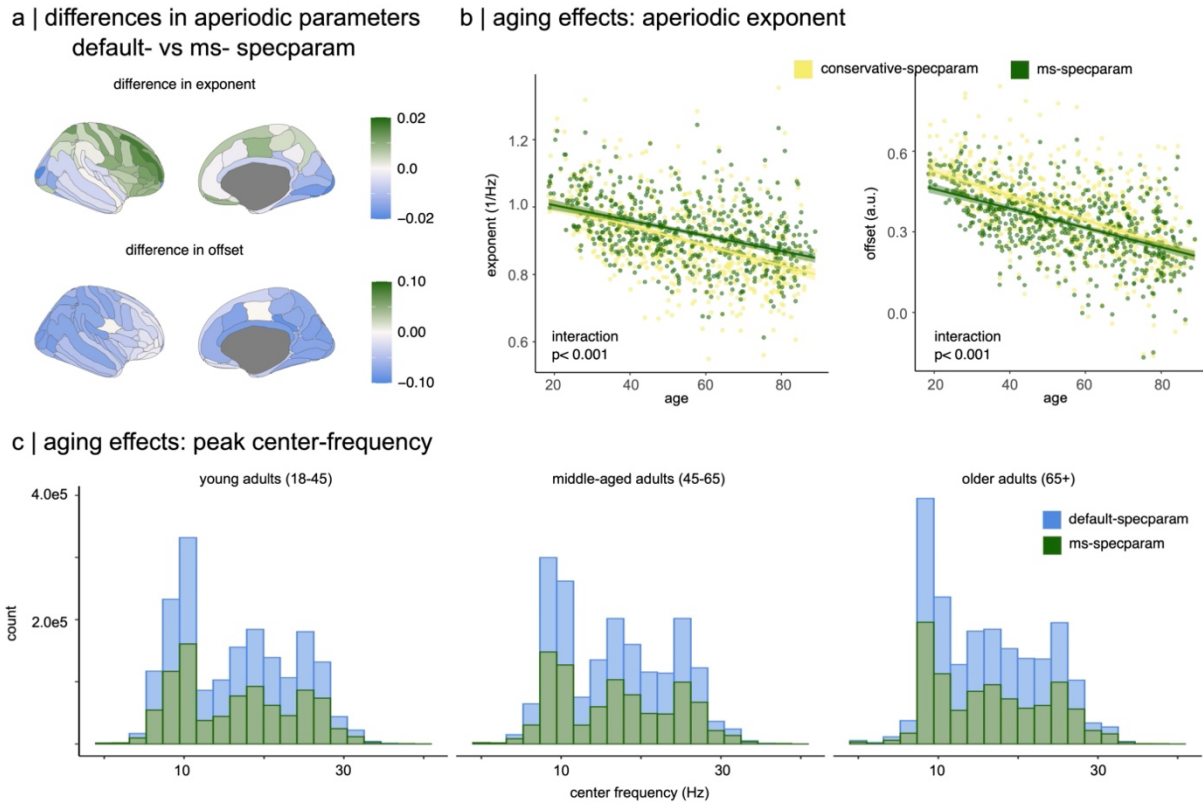
479 We obtained similar results for the age-related decline in aperiodic offset. Our analysis confirmed
480 a significant interaction effect between age and spectral parameterization algorithm, both when
481 comparing *ms-specparam* to *default-specparam* ($\beta = 0.04$, SE = 0.01, CI [0.01, 0.06]; $BF_{01} = 11.91$)
482 and to *conservative-specparam* ($\beta = 0.11$, SE = 0.01, CI [0.09, 0.14]; $BF_{01} = 2.96 \times 10^{-13}$; Figure 5b
483 and Table S4 & S5).

484

485 Taken together, these observations suggest that the magnitude of age-related declines in the
486 aperiodic exponent and offset are influenced by the choice of the hyperparameters in the spectral
487 parametrization method. Note that the effect size of age was the smallest in the spectral models
488 derived from *ms-specparam*.

489

490 As in our simulation results, we also found that *ms-specparam* identified fewer spectral peaks than
491 *default-specparam*, particularly in the 8-30 Hz range, and most pronounced in senior participants
492 (65-89 years old). This reinforces the earlier finding that *ms-specparam* curtails the number of
493 detected peaks and underscores the influence of model selection on the characterization of peak
494 parameters across all age groups (Figure 5c).



495
496

Figure 5: Age-related Neural Spectral Changes and Algorithmic Parsimony

497 (a) Topographical differences in aperiodic neural components, showing the variations in
498 exponent (top) and offset (bottom) estimates when using *ms-specparam* versus *default-*
499 *specparam*. Areas where *ms-specparam* yields higher parameter estimates are
500 highlighted in blue.

501 (b) Moderating effect of spectral parameterization method (*ms-specparam* vs. *Default-*
502 *specparam*) on the relationship between age and aperiodic spectral components. The left
503 graph shows the exponent, and the right graph displays the offset, with statistical
504 interactions highlighted.

505 (c) Frequency-specific empirical distribution of the number of peaks fitted across different
506 age groups. The histograms show that *ms-specparam* (green) generally fits fewer peaks,
507 especially in the mid-frequency range (8-30Hz), illustrating a more parsimonious
508 approach to model fitting and potentially more accurate reflection of age-related spectral
509 changes.

510
511

512 Discussion

513

514 Spectral parameterization enables the spectral decomposition of neurophysiological signals into
515 aperiodic and periodic components. Its adoption has grown rapidly over recent years, thanks to
516 open software tools, with the aim of disambiguating the respective functions of rhythmic
517 oscillatory and arrhythmic background neural activity. However, present tools require the manual
518 adjustment of algorithm parameters (hyperparameters), which hinders the reproducibility,
519 interpretability, and proper fitting of spectral parameterization models to the empirical data. In the
520 present report, we addressed this issue with the addition of a principled model selection strategy
521 to *specparam* (*ms-specparam*) and *SPRiNT* (*ms-SPRiNT*) to set key hyperparameters, including
522 the maximum number of peaks, minimum peak height, and proximity threshold. We validated both
523 new methods with synthetic and empirical data. We show that the resulting spectral
524 parameterizations are more parsimonious and fit better the data, while being considerably less
525 dependent on user decisions and expertise.

526

527 Spectral Parameterization with Enhanced Model Parsimony and Goodness-of-Fit.

528

529 Our examination of ground-truth data shows that *ms-specparam* is more effective than *specparam*
530 in accurately identifying spectral peaks. It avoids the frequent issue in practice of overfitting the
531 spectral data, which typically overestimates the number of periodic components in power spectra
532 (Figure 2a). In empirical data also, *ms-specparam* consistently generates more parsimonious
533 models (Figure 4). We observed enhanced goodness-of-fit (reduced residual variance) in both
534 synthetic and real-world data (Figures 2b and 4a), particularly at the edges of the frequency
535 spectrum. The implications of these findings are twofold: firstly, *ms-specparam*'s parsimonious
536 approach prevents both overfitting and *underfitting* (see Practical Guidelines below). Secondly,
537 the improved accuracy of aperiodic component estimates is critical for characterizing complex
538 neural dynamics (Donoghue et al., 2020; Gerster et al., 2022).

539

540 The proposed model selection approach features similar benefits for the parameterization of
541 spectrograms, with substantial improvements of the model's positive predictive values and less
542 parameter settings than the ad-hoc post-processing steps proposed by Wilson et al. (2022). We
543 note, however, that combining model selection with post-processing increases dramatically the
544 positive predictive value of detected peaks (83% vs. about 45% for model-selection only), with
545 only a modest reduction (approximately 8%) in peak sensitivity.

546

547 To understand why the benefits of post-processing and model selection are additive, we can
548 consider the mechanism by which they achieve more parsimonious fits. Post-processing removes
549 isolated spectral peaks in time and frequency. Model selection encourages the parsimonious
550 addition of spectral peaks to the model, observing both goodness-of-fit and BIC. When combined,
551 model selection and post-processing remove spectral peaks which either do not substantially
552 improve goodness-of-fit (model selection) or have short durations (post-processing).

553

554

555 Hyperparameter Settings.

556

557 Our empirical investigations emphasize the critical role of hyperparameter settings in spectral
558 modelling. Notably, the choice of spectral parameterization algorithm influenced aperiodic
559 parameter estimates across methods (Figures 5a-c). While deviations were modest, suggesting that
560 default spectral parameterizations may have captured the aperiodic component accurately, our
561 comparative analysis with synthetic data indicates that *ms-specparam* yields improved estimates
562 of the aperiodic exponent and offset (Figure 2b).

563
564 We replicated with the new model selection approach previous observations of changing aperiodic
565 parameters with age (Cellier et al., 2021; Donoghue et al., 2020; Hill et al., 2022). We found that
566 the aperiodic component of the neurophysiological power spectrum flattens with age, which has
567 been discussed as related to increased neural noise and asynchronous neuronal firing, yielding less
568 structured brain dynamics (Usher et al., 1995; Pozzorini et al., 2013; Voytek et al., 2015; Voytek
569 & Knight, 2015). Several empirical observations support this hypothesis (Hanggi and Jung, 1994;
570 Bédard et al., 2006; Sosnoff and Newell, 2011).

571
572 We found, however, that previously reported effects of shifts in the spectral aperiodic exponent
573 and offset with age can be substantially reduced, depending on the spectral parameterization
574 method used and its hyperparameters. This observation encourages the present and further efforts
575 towards more automated and principled parameter selection procedures, promoting robustness and
576 replicability of research results.

577 578 **Practical Guidelines.**

579
580 We provide practical recommendations to adjust the hyperparameters of *ms-specparam*. As with
581 other spectral parameterization methods, we encourage future users to examine their data's power
582 spectra before and after applying *ms-specparam* and verify the model's goodness-of-fit. We refer
583 the reader to the previously published guidelines by Donoghue et al. (2020), Gerster et al. (2022),
584 and Ostlund et al. (2022), which set good foundational principles for neurophysiological spectral
585 parameterization. Here, we highlight more specific considerations for the best possible use of *ms-*
586 *specparam*:

- 587 1. Model selection in *ms-specparam* determines the optimal number of spectral peaks that fit
588 the empirical power spectrum. The setting of other hyperparameters, including peak width
589 limits and aperiodic mode, remain to be defined by the user. The value set for the maximum
590 number of spectral peaks parameter needs to be larger than the number of peaks that are
591 clearly visible in the data's power spectrum. In our investigations, we set this value to 6.
- 592 2. We encourage users to derive measures of model goodness-of-fit, such as Mean-Squared
593 Error, R^2 , and BIC, as in our *Brainstorm* plug-in of the proposed model selection methods.
594 Some of these metrics, like R^2 , may be influenced by the aperiodic component of the
595 spectrum, as demonstrated in previous studies (Donoghue et al., 2020). In the context of
596 model selection, users should choose the spectral model with the lowest BIC (as in the
597 present study).

598
599 These guidelines also apply to time-resolved spectral parameterization with *ms-SPRiNT*. Model
600 selection enhances the positive predictive value of detected spectral peaks and may substitute for

601 post-processing (Wilson et al., 2022). Post-processing requires users to set additional
602 hyperparameters.

603 To conclude, the present report introduced a model selection approach to the parameterization of
604 neurophysiological power spectra and spectrograms. The approach minimizes the requirement for
605 user expertise in the adjustment of hyperparameters, which influences the outcome of analyses. It
606 is grounded in the optimization of parameters that favour model parsimony while maximizing
607 goodness-of-fit. We foresee that this principled approach will contribute to the robust application
608 of spectral parameterization in neuroscience research, further elucidating the roles of rhythmic and
609 arrhythmic brain activity in cognition, health, and disease. We anticipate that the proposed tools,
610 *ms-specparam* and *ms-SPRiNT*, will enhance the reproducibility and robustness of reported
611 findings.

612 **Data and Software Availability**

614 The *ms-specparam* and *ms-SPRiNT* algorithms, as well as simulated power spectra and code used
615 to generate results, are available on GitHub (github.com/lucwilson/model_selection). Simulated
616 neural-like time series used for spectrogram parameterization can be accessed from Wilson et al.
617 (2022). Resting-state MEG recordings were obtained from the CamCAN repository (Shafto et al.,
618 2014; Taylor et al., 2017).

619 **Author Contributions**

620 Conceptualization: LEW, JDSC
621 Data Curation: LEW, JDSC
622 Methodology: LEW, JDSC, BLK
623 Software: LEW, JDSC
624 Visualization: LEW, JDSC, BLK
625 Funding acquisition: SB
626 Writing – original draft: LEW, JDSC, SB
627 Writing – review & editing: LEW, JDSC, BLK, SB

628 **Declaration of Competing Interests**

629 All authors declare no competing conflicts of interest. The listed funding sources in the
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639 NSERC (LEW).

640 Supplemental Materials

641 Algorithm Validation with Alternative Noise Conditions.

642
643 In addition to injecting moderate noise to the synthetic data, we also evaluated *ms-specparam*
644 performance at low (s.d. = 0.05) and high (s.d. = 0.15) noise conditions. In spectra with low
645 noise, *ms-specparam* detected spectral peaks with comparable sensitivity (92%) to *default-*
646 *specparam* (92%). The positive predictive value of peaks detected using *ms-specparam* (97%)
647 was notably higher than that of peaks detected using *default-specparam* (68%). In spectra with
648 high noise, *ms-specparam* detected spectral peaks with lower sensitivity (84%) to *default-*
649 *specparam* (90%). However, the positive predictive value of peaks detected using *ms-specparam*
650 (96%) remained higher than that of peaks detected using *default-specparam* (61%). Taken
651 together, these results support the generalizability of the observed algorithmic performance
652 improvements across noise levels.

653

654

Parameter estimation error	exponent		offset		cent. freq.		amplitude		st. dev.	
	Mean	SE	Mean	SE	Mean	SE	Mean	SE	Mean	SE
<i>SPRiNT</i>	0.16	5x10 ⁻⁴	0.21	5x10 ⁻⁴	0.59	9x10 ⁻⁴	0.24	8x10 ⁻⁴	0.24	5x10 ⁻⁴
<i>SPRiNT</i> with post-processing	0.13	5x10 ⁻⁴	0.16	5x10 ⁻⁴	0.49	9x10 ⁻⁴	0.24	8x10 ⁻⁴	0.24	5x10 ⁻⁴
<i>ms-SPRiNT</i>	0.15	5x10 ⁻⁴	0.19	5x10 ⁻⁴	0.49	9x10 ⁻⁴	0.24	8x10 ⁻⁴	0.24	5x10 ⁻⁴
<i>ms-SPRiNT</i> with post-processing	0.12	5x10 ⁻⁴	0.15	5x10 ⁻⁴	0.41	9x10 ⁻⁴	0.23	9x10 ⁻⁴	0.23	5x10 ⁻⁴

655 Table S1. Parameter estimation error for spectrograms with and without model selection.

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<i>Predictors</i>	<i>Estimates</i>	exponent	
		<i>CI</i>	<i>p</i>
(Intercept)	0.00	-0.07 – 0.08	0.944
algorithm [default vs ms-specparam]	-0.01	-0.03 – 0.01	0.610
age (continuous)	-0.44	-0.51 – -0.37	< 0.001
algorithm [default vs ms-specparam] × age (continuous)	0.04	0.02 – 0.06	< 0.001
Random Effects			
σ^2	0.03		
$\tau_{00 \text{ subID}}$	0.80		
ICC	0.96		
N_{subID}	606		
Observations	1212		
Marginal R^2 / Conditional R^2	0.174 / 0.969		

662 Table S2. Hyperparameter choice impacts the age's effect on the aperiodic exponent: default
663 hyperparameter setting vs *ms-specparam*.

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<i>Predictors</i>	<i>Estimates</i>	exponent	
		<i>CI</i>	<i>p</i>
(Intercept)	-0.12	-0.19 – -0.05	0.001
algorithm [conservative vs ms-specparam]	0.24	0.21 – 0.26	<0.001
age (continuous)	-0.50	-0.57 – -0.43	<0.001
algorithm [conservative vs ms-specparam] × age (continuous)	0.12	0.09 – 0.14	<0.001
Random Effects			
σ^2	0.06		
$\tau_{00 \text{ subID}}$	0.73		
ICC	0.93		
N_{subID}	606		
Observations	1212		
Marginal R^2 / Conditional R^2	0.209 / 0.942		

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675 Table S3. Hyperparameter choice impacts the age's effect on the aperiodic exponent:

676 conservative hyperparameter setting vs *ms-specparam*.

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<i>Predictors</i>	offset		
	<i>Estimates</i>	<i>CI</i>	<i>p</i>
(Intercept)	0.19	0.13 – 0.26	<0.001
algorithm [default vs ms-specparam]	-0.39	-0.41 – -0.36	<0.001
age raw	-0.52	-0.59 – -0.46	<0.001
algorithm [default vs ms-specparam] × age raw	0.04	0.01 – 0.06	0.002
Random Effects			
σ^2	0.04		
$\tau_{00 \text{ subID}}$	0.67		
ICC	0.94		
N_{subID}	606		
Observations	1212		
Marginal R^2 / Conditional R^2	0.294 / 0.960		

697 Table S4. Hyperparameter choice impacts the age's effect on the aperiodic offset: default
698 hyperparameter setting vs *ms-specparam*.

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<i>Predictors</i>	offset		
	<i>Estimates</i>	<i>CI</i>	<i>p</i>
(Intercept)	0.12	0.05 – 0.19	<0.001
algorithm [conservative vs ms-specparam]	-0.24	-0.27 – -0.22	<0.001
age raw	-0.58	-0.65 – -0.52	<0.001
algorithm [conservative vs ms-specparam] × age raw	0.11	0.09 – 0.14	<0.001
Random Effects			
σ^2	0.05		
$\tau_{00 \text{ subID}}$	0.66		
ICC	0.93		
N_{subID}	606		
Observations	1212		
Marginal R^2 / Conditional R^2	0.294 / 0.948		

719 Table S5. Hyperparameter choice impacts the age's effect on the aperiodic offset: conservative
720 hyperparameter setting vs *ms-specparam*.

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