

Appendix

This appendix gives a more formal account of the estimators implemented in the algorithm.

1 Peak alpha frequency

Peak alpha frequency (PAF) can be formalised in terms of the local maximum within the alpha band:

$$\text{PAF} = \begin{cases} \arg \max_{f \in \text{alpha band}} \text{PSD}(f), & \text{PSD}(f) - \text{PSD}(f') \geq \varphi \forall f' \neq f \\ \text{undefined}, & \text{otherwise} \end{cases}$$

where $\arg \max$ returns the frequency bin (or subset of bins) f containing the maximal power value $\max \text{PSD}(f)$ registered within the set of frequency bins spanning the alpha band. Note that, for the output of $\arg \max$ to qualify as an estimate of PAF, it must return a single frequency bin f with a corresponding power spectral density $\geq \varphi$, where φ defines the minimum threshold value differentiating a substantive spectral peak from background noise.

2 First- and second-derivative tests

Derivatives describe the relative rate of change in the dependent variable or function $g(x)$ given some value of the independent variable x . The first derivative of a vector of PSD estimates thus provides point estimates of the (instantaneous) rate of change in the amount of spectral power estimated for each frequency bin resolved in the analysis. This relationship can be formalised as

$$g'(x) = \lim_{\Delta x \rightarrow 0} \frac{\Delta g(x)}{\Delta x},$$

where $g'(x)$ is the first derivative of the relative change in the power estimate $g(x)$ at frequency bin x .

Another way to conceptualise this relationship is to construe the derivative as describing the slope of the tangent line to the PSD function $g(x)$ at any given frequency bin x . From this perspective, it becomes clear that the first derivative will be zero (i.e. the slope of the tangent will be horizontal) at any point in the function corresponding to a peak or trough. In the case of the former, the derivative will change from a positive value (as the function ascends towards its peak) to a negative value (once the function begins to descend) as the tangent traverses the local maximum. As such, positive to negative sign changes (i.e. downward going zero crossings) within the first derivative offer a convenient index of local maxima. Conversely, sign changes in the opposite direction (i.e. upward going zero crossings) can likewise be used to identify local minima.¹

The second derivative of the PSD is derived by differentiating the first derivative:

$$g''(x) = \lim_{\Delta x \rightarrow 0} \frac{\Delta g'(x)}{\Delta x},$$

where $g''(x)$ is the derivative of the first derivative $g'(x)$ at frequency bin x . In other words, the second derivative is simply the rate of change of the first derivative of some function $g(x)$. Second derivatives are useful for evaluating whether the curvature of a function is concave up (i.e. convex) or concave down at any given value of x . The transition of a curve's direction between concave up and concave down is characterised

¹A lack of sign change – e.g., a positive derivative going to zero and then becoming strictly positive again – corresponds to a plateau.

by an inflection point, which registers a second derivative value of zero. Consequently, inflection points can be identified by applying the same zero-crossing procedure described for locating optima in the first derivative.

3 Quantifying peak quality

Having defined both the height and width of the putative alpha peak by means of the first- and second-derivative test, relative peak quality is quantified as

$$Q = \frac{\int_{i_1}^{i_2} \text{PSD}(f) df}{i_2 - i_1},$$

where Q is the scaled average power within the peak interval $[i_1, i_2]$.² (In a very strict sense, Q is the mean value of the power spectral density function on the peak interval as given by the Mean Value Theorem.) Note that the inclusion of the denominator ensures that spectral width is taken into account when calculating Q .

4 Centre of gravity

The centre of gravity (CoG) is the PSD-weighted mean alpha frequency, which can be expressed as

$$\text{CoG} = \frac{\int_{f_1}^{f_2} \text{PSD}(f) \cdot f df}{\int_{f_1}^{f_2} \text{PSD}(f) df},$$

where f_1 and f_2 index the frequency bins bounding the alpha-band interval.

CoG calculation follows the standard procedure described by Klimesch and colleagues (1993; 1990), with the exception that the bounds of each channel's alpha interval are detected automatically. The analysis routine derives these bounds by taking the left- and right-most peaks within W_α (i.e. those peaks in the lowest and highest frequency bins, respectively; these may coincide with the PAF), and searching the first derivative for evidence of the nearest local minimum (1) prior to the left-most peak (f_1), and (2) following the right-most peak (f_2).³ Since some spectra show a relatively shallow roll-off as the edges of the alpha peak diminish, and thus do not culminate in a local minimum several frequency bins away from the main body of the component structure, we relaxed the requirement for an upward going zero crossing (i.e. evidence of a local minimum) such that the transition into a prolonged shallow gradient is taken as sufficient evidence of the individual alpha bounds f_1 or f_2 . This criterion was formalised as

$$f_1 = \arg \max_{f < \text{PAF}} |\text{PSD}'(f)| < 1,$$

$$f_2 = \arg \min_{f > \text{PAF}} |\text{PSD}'(f)| < 1.$$

f_1 and f_2 estimates from each eligible channel are averaged to yield the individualised alpha-band window. This window defines the index of summation (i.e. frequency band coverage) used to calculate the CoG across all available channels.

²Notice that the interval bounded by $[i_1, i_2]$ is distinct from that bounded by $[f_1, f_2]$, the estimated span of the individualised alpha-band window. The former yields a narrower frequency range than the latter, and does not take into account secondary peaks within the alpha band.

³This contingency allows for the individualised alpha-band window, and thus the CoG, to be estimated even in cases where there is no clear PAF; e.g., in the presence of split-peaks.

5 Summary statistics

If a sufficient number of channels (as stipulated by *cMin*) furnish PAF and individualised alpha window estimates, channel PAF and CoG estimates are averaged to generate IAF summary statistics. Mean PAF (PAF_M) is a weighted average that takes into account the Q values associated with each peak estimate:

$$\text{PAF}_M = \frac{\sum_{c=1}^C \text{PAF}_c \cdot \lambda_c}{\sum_{c=1}^C \lambda_c},$$

where c identifies the channel drawn from the set of all available channels C , and λ_c is the channel weighting derived by dividing Q_c by the maximum Q_c in C (such that $\sum \lambda_c = 1$). In contrast to PAF_M , all CoG channel estimates contribute equally to the calculation of mean CoG (CoG_M). If there are an insufficient number of channel estimates to satisfy *cMin*, no PAF_M or CoG_M estimates are returned (in some cases, *cMin* will be satisfied for CoG_M , but not PAF_M , on account of the latter's more stringent criteria).

Since pre/post-experiment recordings may not be equivalent in terms of quantity of information rendered, grand averaged IAF estimates (IAF_{GA}) are calculated using a weighted mean which takes into account the proportion of channels that contributed to each constituent summary statistic:

$$\text{IAF}_{GA} = \frac{\text{IAF}_1\beta_1 + \text{IAF}_2\beta_2}{\beta_1 + \beta_2},$$

where either PAF or CoG are substituted in place of IAF, β constitutes the weighting afforded to the channel-wise mean estimates derived from each recording, and subscript indices indicate the identity of the EEG recording. For PAF estimates, β is the number of channels used to estimate PAF_M divided by total number of channels included in the analysis. For CoG estimates, β is the number of channels used to estimate the mean individualised alpha-band window divided by total number of channels included in the analysis.

References

- Klimesch, W., Schimke, H., & Pfurtscheller, G. (1993). Alpha frequency, cognitive load and memory performance. *Brain Topography*, 5(3), 241–251.
- Klimesch, W., Schimke, H., Ladurner, G., & Pfurtscheller, G. (1990). Alpha frequency and memory performance. *Journal of Psychophysiology*, 4, 381–390.