ORTHOGONAL PROCRUSTES PROBLEM FOR SPD MATRICES

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May 3, 2021

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Procrustes problem

For that hero punished those who offered him violence in the manner in which they had plotted to serve him.

Given A and B two matrices and $\mathbb O$ the space of orthogonal matrices, the classical Procrustes problem ask to find a matrix R such that

$$R = \operatorname*{argmin}_{\Omega \in \mathbb{O}} \|\Omega A - B\|_{F}$$

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The solution to this problem is known

$$R = UV^{\mathsf{T}}$$

$$BA^{\mathsf{T}} = UDV^{\mathsf{T}}$$

Multiple differences:

■ The Frobenius norm is not appropriate: use of Affine-Invariant norm

$$\|\Sigma_1 - \Sigma_2\|_{AI} = \|\text{Log}\left[\Sigma_1^{-1/2}\Sigma_2\Sigma_1^{-1/2}\right]\|_{F}$$

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■ Orthogonal matrices don't preserve symmetry or positive definiteness: use an appropriate transformation

$$T_{\Omega} \colon \mathcal{S}^+ \to \mathcal{S}^+$$

$$\Sigma \mapsto T_{\Omega}(\Sigma) = \Omega \Sigma \Omega^{\mathsf{T}}$$

(if $\Omega \in \mathbb{O}$ this preserve also the determinant thus behaves as an orthogonal transformation)

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A proof for this result is in Bhatia and Congedo 2019 and the solution is

$$R = \Gamma_1 \Gamma_2^{\mathsf{T}}$$

$$\Sigma_i = \Gamma_i \Lambda_i \Gamma_i^{\mathsf{T}}$$

Multiple matrices

In general one might want to extend this analysis to a set of K matrices (K > 2) X_i (generalized Procrustes problem)

$$\underset{\Omega_1...\Omega_K \in \mathbb{O}}{\operatorname{argmin}} \sum_{i>j} \|\Omega_i X_i - \Omega_j X_j\|_F$$

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In general one might want to extend this analysis to a set of K matrices (K > 2) X_i (generalized Procrustes problem)

$$\underset{\Omega_{1}...\Omega_{K}\in\mathbb{O}}{\operatorname{argmin}} \sum_{i>j} \|\Omega_{i}X_{i} - \Omega_{j}X_{j}\|_{F}$$

In this case one uses this identity

$$\sum_{i>j} \|\Omega_i X_i - \Omega_j X_j\|_F = K \sum_i \|\Omega_i X_i - G\|_F \qquad G = K^{-1} \sum_j \Omega_j X_j$$

to build a two step algorithm (start with a random initialization of the Ω_i)

- 1 Compute G
- **2** Decouple the problem in K simple Procrustes problem and obtain the new Ω_i

Repeat until convergence

The identity of before **most probably** does not hold. We decide to focus on a slightly different version of the right hand side:

1 Solve the K independent Procrustes

$$\underset{\Omega_1...\Omega_K \in \mathbb{O}}{\operatorname{argmin}} \sum_{i} \|M - T_{\Omega_i}(\Sigma_i)\|_{AI}$$

given a known reference M

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1 Solve the *K* independent Procrustes

$$\underset{\Omega_1...\Omega_K \in \mathbb{O}}{\operatorname{argmin}} \sum_{i} \|M - T_{\Omega_i}(\Sigma_i)\|_{AI}$$

given a known reference M

2 Compute the optimal reference *M* that satisfies

$$\underset{M \in \mathcal{S}^{+}}{\operatorname{argmin}} \sum_{i} \|M - T_{\Omega_{i}}(\Sigma_{i})\|_{AI}$$

with Ω_i known from step 1.

Solution to step 1 is simple (and analytical)

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There is an analytical solution also for step 2, but it provides only the eigenvalues

$$\lambda_h^{(M)} = \left[\prod_i^K \lambda_h^{(i)}\right]^{\frac{1}{K}}$$

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There are infinite solutions $M = \Gamma_M \Lambda_M \Gamma_M^T$ depending on the choice Γ_M : how to choose it?

Minimization of a **rotational effort**: the matrix Γ_M that provides the *smallest* total rotation

$$\Gamma_{M} = \operatorname*{argmin}_{\Gamma \in \mathbb{O}} \sum_{i} \left\| \Gamma \Gamma_{i}^{\intercal} - \mathbb{I} \right\|_{F}$$

This can be seen as a special case of the generalized Procrustes problem and has solution

$$\Gamma_{\mathit{M}} = \mathit{UV}^{\intercal}$$

$$\sum_{i} \Gamma_{i} = \mathit{UDV}^{\intercal}$$

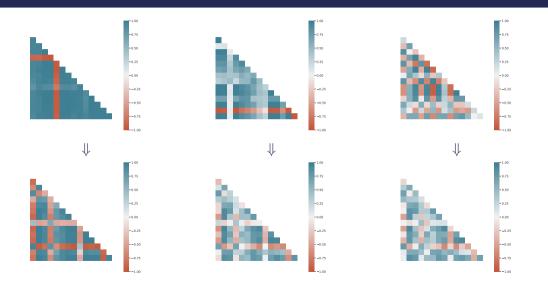
Applications

In EEG data one might be interested in observing the empirical covariance matrix between signal recorded from different point of the skull of an individual, as this is a proxy for the connections between various regions of the brain.

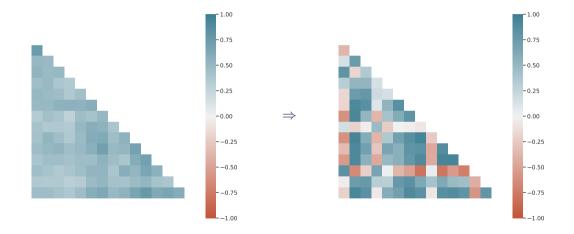
One obtains one SPD matrix for each individual in the study and might be interested to compare them (for instance to detect anomalies due to various diseases).

But there are various slight differences between each individual data that are not related to the actual connections between brain regions (for instance, the position of the electrodes on the scalp): this add artifacts to the data that hide the actual differences between individuals.

Applications



Applications



References I

- Bhatia, Rajendra (2007). Positive definite matrices. Princeton University Press.
- Bhatia, Rajendra and Marco Congedo (2019). "Procrustes problems in Riemannian manifolds of positive definite matrices". In: *Linear Algebra and its Applications* 563, pp. 440–445.
- Cattan, Grégoire, Pedro L. C. Rodrigues, and Marco Congedo (2018). *EEG Alpha Waves dataset*. Zenodo.
- Gower, John C. and Garmt B. Dijksterhuis (2004). *Procrustes Problems*. Oxford University Press.