
fMRI-Based Inter-Subject Cortical Alignment Using Functional Connectivity Supplementary Material

1 Efficient Computation of the Registration Objective

Here we derive the efficient computation of the similarity portion of the registration objective, $\|\tilde{C}_F - C_R\|_f^2$. Making the substitution $\tilde{A} = W_F B W_R^T$, we obtain:

$$\|\tilde{C}_F - C_R\|_f^2 = \|W_R B^T W_F^T C_F W_F B W_R^T - C_R\|_f^2 \quad (1)$$

$$= \left\| W_R B^T \begin{bmatrix} \Sigma_F & 0 \\ 0 & 0 \end{bmatrix} B W_R^T - C_R \right\|_f^2 \quad (2)$$

$$= \left\| W_R \left(\begin{bmatrix} B_1^T \Sigma_F B_1 & B_1^T \Sigma_F B_2 \\ B_2^T \Sigma_F B_1 & B_2^T \Sigma_F B_2 \end{bmatrix} - \begin{bmatrix} \Sigma_R & 0 \\ 0 & 0 \end{bmatrix} \right) W_R^T \right\|_f^2 \quad (3)$$

$$= \|B_1^T \Sigma_F B_1 - \Sigma_R\|_f^2 + 2 \|B_1^T \Sigma_F B_2\|_f^2 + \|B_2^T \Sigma_F B_2\|_f^2 \quad (4)$$

where we made use of the fact that $\|OX\|_f^2 = \|XO\|_f^2 = \|X\|_f^2$ for an orthogonal matrix O .

2 Partial Derivative of Registration Objective

The partial derivative of the registration objective with respect to $\tilde{\phi}_j$ is given by:

$$\frac{\partial S(g)}{\partial \tilde{\phi}_j} = \sum_{i=1}^{N_v} \frac{\partial \|\tilde{C}_F - C_R\|_f^2}{\partial \tilde{a}_{ij}} \frac{\partial \tilde{a}_{ij}}{\partial \tilde{\phi}_j} + \lambda \frac{\partial \text{Reg}(g)}{\partial \tilde{\phi}_j} \quad (5)$$

where

$$\frac{\partial \tilde{a}_{ij}}{\partial \tilde{\phi}_j} = d_j \frac{\partial a_{ij}}{\partial \tilde{\phi}_j} + a_{ij} \frac{\partial d_j}{\partial \tilde{\phi}_j} \quad (6)$$

A similar expression is obtained for $\partial S(g) / \partial \tilde{\theta}_j$.

First, we focus on the term $\partial \|\tilde{C} - C_R\|_f^2 / \partial \tilde{a}_{ij}$. Given that the Frobenius norm of a matrix A can be expressed as $\|A\|_f^2 = \text{tr}(A^T A)$, where $\text{tr}(\cdot)$ is the matrix trace, we have:

$$\|\tilde{C}_F - C_R\|_f^2 = \text{tr} \left((\tilde{C}_F - C_R) (\tilde{C}_F - C_R) \right) \quad (7)$$

We will now take derivatives of the expression above. Since the trace operator is linear, the derivative can be pulled inside the trace to obtain:

$$\frac{\partial \|\tilde{C}_F - C_R\|_f^2}{\partial \tilde{a}_{ij}} = 2 \text{tr} \left((\tilde{C}_F - C_R) \frac{\partial \tilde{C}_F}{\partial \tilde{a}_{ij}} \right) \quad (8)$$

where $\frac{\partial \tilde{C}_F}{\partial \tilde{a}_{ij}}$ is the matrix whose $(i, j)^{th}$ entry is given by $\partial \left[\tilde{C}_F \right]_{i,j} / \partial \tilde{a}_{ij}$. This matrix can be computed as:

$$\frac{\partial \tilde{C}_F}{\partial \tilde{a}_{ij}} = \frac{\partial \left(\tilde{A}^T C_F \tilde{A} \right)}{\partial \tilde{a}_{ij}} \quad (9)$$

$$= E_{ji} C_F \tilde{A} + \tilde{A}^T C_F E_{ij} \quad (10)$$

$$= \left(\tilde{A}^T C_F E_{ij} \right)^T + \tilde{A}^T C_F E_{ij} \quad (11)$$

where $E_{ij} = e_i e_j^T$ is the matrix with all zeros except for a one in the $(i, j)^{th}$ entry. Substituting (11) into (8), we obtain:

$$\frac{\partial \left\| \tilde{C}_F - C_R \right\|_f^2}{\partial \tilde{a}_{ij}} = 4tr \left(\left(\tilde{C}_F - C_R \right) \tilde{A}^T C_F E_{ij} \right) \quad (12)$$

$$= 4tr \left(\left(\tilde{C}_F - C_R \right) \tilde{A}^T C_F e_i e_j^T \right) \quad (13)$$

$$= 4tr \left(e_j^T \left(\tilde{C}_F - C_R \right) \tilde{A}^T C_F e_i \right) \quad (14)$$

$$= 4 \left[C_F \tilde{A} \left(\tilde{C}_F - C_R \right) \right]_{i,j} \quad (15)$$

The matrix $C_F \tilde{A} \left(\tilde{C}_F - C_R \right)$ can be simplified further using the matrix decomposition $\tilde{A} = W_F B W_R^T$. First, note that:

$$C_F \tilde{A} = V_F \Sigma_F V_F^T W_F B W_R^T \quad (16)$$

$$= V_F \Sigma_F [B_1 \ B_2] W_R^T \quad (17)$$

and:

$$\left(\tilde{C}_F - C_R \right) = W_R \left(\begin{bmatrix} B_1^T \\ B_2^T \end{bmatrix} \Sigma_F V_F^T \tilde{A} - \begin{bmatrix} \Sigma_R \\ 0 \end{bmatrix} V_R^T \right) \quad (18)$$

Multiplying the two, we obtain:

$$C_F \tilde{A} \left(\tilde{C}_F - C_R \right) = V_F \Sigma_F \left[\left(B_1 B_1^T + B_2 B_2^T \right) \Sigma_F V_F^T \tilde{A} - B_1 \Sigma_R V_R^T \right] \quad (19)$$

In practice, only select entries of the $N_v \times N_v$ matrix $C_F \tilde{A} \left(\tilde{C}_F - C_R \right)$ need to be computed, since the interpolation kernel is locally supported. These entries can be computed from (19), by taking inner products of rows of the $N_v \times d$ matrix $V_F \Sigma_F$ with columns of the $d \times N_v$ matrix $\left[\left(B_1 B_1^T + B_2 B_2^T \right) \Sigma_F V_F^T \tilde{A} - B_1 \Sigma_R V_R^T \right]$.

Now, we turn to partial derivatives of $a_{ij} = \Phi_i \left(x \left(\tilde{\phi}_j, \tilde{\theta}_j \right) \right)$ with respect to $\tilde{\phi}_j$ and $\tilde{\theta}_j$. Since $\Phi_i \left(x \left(\tilde{\phi}_j, \tilde{\theta}_j \right) \right) = \varphi(s)$, where $s = d \left(x \left(\tilde{\phi}_j, \tilde{\theta}_j \right), p_i \right)$ is the geodesic distance between $g(p_j)$ and p_i , we can compute partials using the chain rule: $\frac{\partial a_{ij}}{\partial \tilde{\phi}_j} = \frac{\partial \varphi}{\partial s} \frac{\partial s}{\partial \tilde{\phi}_j}$ and $\frac{\partial a_{ij}}{\partial \tilde{\theta}_j} = \frac{\partial \varphi}{\partial s} \frac{\partial s}{\partial \tilde{\theta}_j}$. Let $p_i = x(\phi_i, \theta_i)$, and assume a particular form for x : $x(\phi, \theta) = (\cos(\phi), \sin(\phi) \sin(\theta), \sin(\phi) \cos(\theta))$. Then $\partial s / \partial \tilde{\phi}_j$ and $\partial s / \partial \tilde{\theta}_j$ can be computed using the identity:

$$\cos s = \left\langle x \left(\tilde{\phi}_j, \tilde{\theta}_j \right), p_i \right\rangle \quad (20)$$

$$= \sin \tilde{\phi}_j \sin \phi_i \left(\cos \tilde{\theta}_j \cos \theta_i + \sin \tilde{\theta}_j \sin \theta_i \right) + \cos \tilde{\phi}_j \cos \phi_i \quad (21)$$

$$= \sin \tilde{\phi}_j \sin \phi_i \cos \left(\tilde{\theta}_j - \theta_i \right) + \cos \tilde{\phi}_j \cos \phi_i \quad (22)$$

Taking derivatives with respect to $\tilde{\phi}_j$:

$$\frac{\partial}{\partial \tilde{\phi}_j} \cos s = \frac{\partial}{\partial \tilde{\phi}_j} \left(\sin \tilde{\phi}_j \sin \phi_i \cos (\tilde{\theta}_j - \theta_i) + \cos \tilde{\phi}_j \cos \phi_i \right) \quad (23)$$

$$- \sin s \frac{\partial s}{\partial \tilde{\phi}_j} = \cos \tilde{\phi}_j \sin \phi_i \cos (\tilde{\theta}_j - \theta_i) - \sin \tilde{\phi}_j \cos \phi_i \quad (24)$$

$$\frac{\partial s}{\partial \tilde{\phi}_j} = \frac{\sin \tilde{\phi}_j \cos \phi_i - \cos \tilde{\phi}_j \sin \phi_i \cos (\tilde{\theta}_j - \theta_i)}{\sin s} \quad (25)$$

Taking derivatives with respect to $\tilde{\theta}_j$:

$$\frac{\partial}{\partial \tilde{\theta}_j} \cos s = \frac{\partial}{\partial \tilde{\theta}_j} \left(\sin \tilde{\phi}_j \sin \phi_i \cos (\tilde{\theta}_j - \theta_i) + \cos \tilde{\phi}_j \cos \phi_i \right) \quad (26)$$

$$- \sin s \frac{\partial s}{\partial \tilde{\theta}_j} = - \sin \tilde{\phi}_j \sin \phi_i \sin (\tilde{\theta}_j - \theta_i) \quad (27)$$

$$\frac{\partial s}{\partial \tilde{\theta}_j} = \frac{\sin \tilde{\phi}_j \sin \phi_i \sin (\tilde{\theta}_j - \theta_i)}{\sin s} \quad (28)$$

Using the radial basis function φ given in the main paper, we have:

$$\varphi(s) = \left(1 - \frac{2}{r} \sin \left(\frac{s}{2} \right) \right)_+^4 \left(\frac{8}{r} \sin \left(\frac{s}{2} \right) + 1 \right) \quad (29)$$

$$\frac{\partial \varphi(s)}{\partial s} = - \frac{40}{r^2} \left(1 - \frac{2}{r} \sin \left(\frac{s}{2} \right) \right)_+^3 \cos \left(\frac{s}{2} \right) \sin \left(\frac{s}{2} \right) \quad (30)$$

$$= - \frac{20}{r^2} \left(1 - \frac{2}{r} \sin \left(\frac{s}{2} \right) \right)_+^3 \sin(s) \quad (31)$$

Thus, combining (31) with (25) and (28), we obtain:

$$\frac{\partial a_{ij}}{\partial \tilde{\phi}_j} = \frac{20}{r^2} \left(1 - \frac{2}{r} \sin \left(\frac{s}{2} \right) \right)_+^3 \left(\cos \tilde{\phi}_j \sin \phi_i \cos (\tilde{\theta}_j - \theta_i) - \sin \tilde{\phi}_j \cos \phi_i \right) \quad (32)$$

$$\frac{\partial a_{ij}}{\partial \tilde{\theta}_j} = \frac{20}{r^2} \left(1 - \frac{2}{r} \sin \left(\frac{s}{2} \right) \right)_+^3 \sin \tilde{\phi}_j \sin \phi_i \sin (\tilde{\theta}_j - \theta_i) \quad (33)$$

which are nonzero only for $s < 2 \sin^{-1}(r/2)$.

Now we look at d_j and its partial derivatives.

$$d_j = \|T_F a(g(p_j))\|^{-1}. \quad (34)$$

$$= (a_j^T C_F a_j)^{-1/2} \quad (35)$$

where a_j is the j^{th} column of the matrix A . Then

$$\frac{\partial d_j}{\partial \tilde{\phi}_j} = - \frac{1}{2} d_j^3 \frac{\partial (a_j^T C_F a_j)}{\partial \tilde{\phi}_j} \quad (36)$$

$$= - d_j^3 a_j^T V_F \Sigma_F V_F^T \frac{\partial a_j}{\partial \tilde{\phi}_j} \quad (37)$$

Since a_j and $\partial a_j / \partial \tilde{\phi}_j$ are sparse vectors, the expression above can be computed efficiently by sparse multiplication.

3 Computing Leave-one-out Templates

The leave-one-out template \bar{C}_k for subject $k \in 1, \dots, N_s$ is given by:

$$\bar{C}_k = \frac{1}{N_s - 1} \sum_{j \neq k} \tilde{C}_j \quad (38)$$

where $\tilde{C}_j = \tilde{V}_j \tilde{\Sigma}_j \tilde{V}_j^T$ and $\bar{C}_k = \bar{V}_k \bar{\Sigma}_k \bar{V}_k^T$. Here we prove that $\text{range}(\tilde{V}_n) \subseteq \text{range}(\bar{V}_k)$ for $n \neq k$.

Proof. Select $n \neq k$ and pick $x \in \text{range}(\tilde{V}_n)$. Then

$$x^T \bar{C}_k x = \frac{1}{N_s - 1} \left(x^T \left[\sum_{j \neq k} \tilde{C}_j \right] x \right) \quad (39a)$$

$$= \frac{1}{N_s - 1} \left(x^T \tilde{C}_n x + \sum_{j \notin \{k, n\}} x^T \tilde{C}_j x \right) \quad (39b)$$

The first term in (39b) is greater than zero since $x \in \text{range}(\tilde{V}_n)$. The second term in (39b) is greater than or equal to zero since each \tilde{C}_j is positive semi-definite. Thus, $x^T \bar{C}_k x > 0$, which implies that $x \in \text{range}(\bar{V}_k)$. \square