Errata

for

"Prediction of contact residue pairs based on co-substitution between sites in protein structures",

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1. Eqs. 3 and 4 on page 2,

$$P(\mathcal{A}_i|T,\Theta,\theta_\alpha) = \sum_\kappa \sum_\lambda P(\mathcal{A}_i|v_{bL}=\kappa, v_{bR}=\lambda, T,\Theta,\theta_\alpha) \tag{3}$$

$$\begin{aligned} &P(\mathcal{A}_i|v_{bL}=\kappa, v_{bR}=\lambda, T,\Theta,\theta_\alpha) \equiv \\ &\quad P_{bL}(\mathcal{A}_i|v_{bL}=\kappa, T,\Theta,\theta_\alpha) f_\kappa P(\lambda|\kappa, t_b,\Theta,\theta_\alpha) P_{bR}(\mathcal{A}_i|v_{bR}=\lambda, T,\Theta,\theta_\alpha) \end{aligned} \tag{4}$$

   and Eq. 6 on page 3,

$$\Delta_{ib}(\mathcal{A}_i,\hat{T},\hat{\Theta},\theta_\alpha) \equiv \sum_{\kappa,\lambda} \frac{\Delta_{\kappa,\lambda} P(\mathcal{A}_i|v_{bL}=\kappa, v_{bR}=\lambda,\hat{T},\hat{\Theta},\theta_\alpha)}{P(\mathcal{A}_i|\hat{T},\hat{\Theta},\theta_\alpha)} \tag{6}$$

   should be

$$P(\mathcal{A}_i|T,\Theta,\theta_\alpha) = \sum_\kappa \sum_\lambda P(\mathcal{A}_i, v_{bL}=\kappa, v_{bR}=\lambda \mid T,\Theta,\theta_\alpha) \tag{3}$$

$$\begin{aligned} &P(\mathcal{A}_i, v_{bL}=\kappa, v_{bR}=\lambda \mid T,\Theta,\theta_\alpha) = \\ &\quad P_{bL}(\mathcal{A}_i|v_{bL}=\kappa, T,\Theta,\theta_\alpha) f_\kappa P(\lambda|\kappa, t_b,\Theta,\theta_\alpha) P_{bR}(\mathcal{A}_i|v_{bR}=\lambda, T,\Theta,\theta_\alpha) \end{aligned} \tag{4}$$

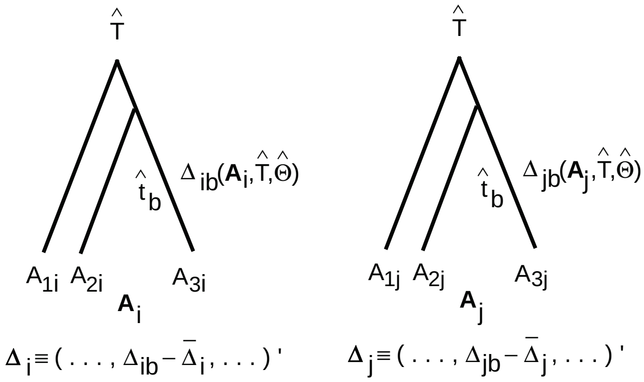
   and

$$\Delta_{ib}(\mathcal{A}_i,\hat{T},\hat{\Theta},\theta_\alpha) \equiv \sum_{\kappa,\lambda} \frac{\Delta_{\kappa,\lambda} P(\mathcal{A}_i, v_{bL}=\kappa, v_{bR}=\lambda \mid \hat{T},\hat{\Theta},\theta_\alpha)}{P(\mathcal{A}_i|\hat{T},\hat{\Theta},\theta_\alpha)} \tag{6}$$

2. Figure 1 should be replaced by the figure shown on the next page; the edge of the lefthand side in the original is too much trimmed by one character.

Topology: Pfam reference tree

Branch lengths: by a ML method in a mechanistic codon substitution model



Correlation coefficient matrix of feature vectors between sites:

$$C_{ij} \equiv r_{\Delta_i \Delta_j} = \frac{(\boldsymbol{\Delta}_i, \boldsymbol{\Delta}_j)}{\|\boldsymbol{\Delta}_i\| \|\boldsymbol{\Delta}_j\|}$$

Partial correlation coefficients of feature vectors between sites:

$$\mathcal{C}_{ij} \equiv \frac{(\Pi_{\perp\{\Delta_{k \neq i,j}\}} \boldsymbol{\Delta}_i \ , \ \Pi_{\perp\{\Delta_{k \neq i,j}\}} \boldsymbol{\Delta}_j)}{\|\Pi_{\perp\{\Delta_{k \neq i,j}\}} \boldsymbol{\Delta}_i\| \ \|\Pi_{\perp\{\Delta_{k \neq i,j}\}} \boldsymbol{\Delta}_j\|} = - \frac{(C^{-1})_{ij}}{((C^{-1})_{ii} (C^{-1})_{jj})^{1/2}}$$

Co-evolution score based on partial correlation coefficients:

$$\rho_{ij} \equiv \max[\rho^s_{ij}, \max(-\rho^v_{ij}, 0), \max(-\rho^c_{ij}, 0), \max(-\rho^{hb}_{ij}, 0), |\rho^h_{ij}|, \ldots]$$

$$\rho^s_{ij} \equiv \max \, (\mathcal{C}^s_{ij}, \ 0) \ , \ \rho^x_{ij} \equiv \operatorname{sgn} \mathcal{C}^x_{ij} \ (|\rho^s_{ij} \mathcal{C}^x_{ij}|)^{1/2} \quad (x \in \{v, c, hb, h, \ldots\})$$