

CVM functional, jacobian and hessian

$$G = \sum_i^{\text{maxclus}} m_i J_i \xi_i + k_B T \sum_i^{\text{maxclus}} k_i \left[ \sum_j^{\text{config}} \alpha_{ij} \left( \sum_c^{\text{corrs}} v_{ijc} \xi_c \right) \log \left( \sum_c^{\text{corrs}} v_{ijc} \xi_c \right) \right]$$

$$\begin{aligned} \therefore \frac{dG}{d\xi_k} &= m_k J_k + k_B T \sum_i^{\text{maxclus}} k_i \left[ \sum_j^{\text{config}} \alpha_{ij} v_{ijk} \log \left( \sum_c^{\text{corrs}} v_{ijc} \xi_c \right) + a_{ij} \sum_c^{\text{corrs}} v_{ijc} \xi_c \frac{v_{ijk}}{\sum_c^{\text{corrs}} v_{ijc} \xi_c} \right] \\ \Rightarrow &= m_k J_k + k_B T \sum_i^{\text{maxclus}} k_i \left[ \sum_j^{\text{config}} a_{ij} v_{ijk} \left\{ 1 + \log \left( \sum_c^{\text{corrs}} v_{ijc} \xi_c \right) \right\} \right] \end{aligned}$$

$$\frac{d^2 G}{d\xi_k d\xi_{k'}} = k_B T \sum_i^{\text{maxclus}} k_i \sum_j^{\text{config}} \frac{a_{ij} v_{ijk} v_{ijk'}}{(\sum_c^{\text{corrs}} v_{ijc} \xi_c)}$$