

CVM functional, jacobian and hessian

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

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

$$= m_k J_k + k_B T \sum_i^{\text{maxclus}} k_i \left[ \sum_j^{\text{config}} \alpha_{ij} v_{ijk} \left\{ 1 + \log \left( \left| \sum_c^{\text{corrs}} v_{ijc} \xi_c \right| \right) \right\} \right]$$

$$\begin{aligned} \Rightarrow \frac{d^2 G}{d\xi_k d\xi_{k'}} &= k_B T \sum_i^{\text{maxclus}} k_i \sum_j^{\text{config}} a_{ij} v_{ijk} \left( \frac{1}{\left| \sum_c^{\text{corrs}} v_{ijc} \xi_c \right|} \frac{\sum_c^{\text{corrs}} v_{ijc} \xi_c}{\sum_c^{\text{corrs}} v_{ijc} \xi_c} v_{ijk'} \right) \\ &= k_B T \sum_i^{\text{maxclus}} k_i \sum_j^{\text{config}} \frac{a_{ij} v_{ijk} v_{ijk'}}{\sum_c^{\text{corrs}} v_{ijc} \xi_c} \end{aligned}$$