PAO LNV for arbitrary A and B matrices

The LNV energy functional is:

$$\Omega = 3\,\text{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\,\text{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}]$$

The tilded variables are in the smaller PAO-basis. The transformations between the larger primary basis and the PAO-basis are:

$$\tilde{P} = A^T P A \qquad\qquad \tilde{H} = B^T H B \qquad\qquad \tilde{S} = B^T S B$$

Notice that: $A^T B = B^T A = \tilde{I}$, where $\tilde{I}$ is the identity matrix in the smaller PAO basis.

The relationship between A and B is defined via the Moore-Penrose pseudo-inverse:

$$B = S^{-1}A(A^T S^{-1}A)^{-1} = NNA(A^T NNA)^{-1}$$

1. Derivative

$$\frac{d\Omega}{dA_{ij}} = \sum_{ab} \frac{\partial \Omega}{\partial \tilde{P}_{ab}} \frac{\partial \tilde{P}_{ab}}{\partial A_{ij}} + \sum_{ab} \frac{\partial \Omega}{\partial \tilde{H}_{ab}} \frac{\partial \tilde{H}_{ab}}{\partial A_{ij}} + \sum_{ab} \frac{\partial \Omega}{\partial \tilde{S}_{ab}} \frac{\partial \tilde{S}_{ab}}{\partial A_{ij}}$$

$$= \sum_{ab} M^1_{ab} \frac{\partial \tilde{P}_{ab}}{\partial A_{ij}} + \sum_{ab} M^2_{ab} \frac{\partial \tilde{H}_{ab}}{\partial A_{ij}} + \sum_{ab} M^3_{ab} \frac{\partial \tilde{S}_{ab}}{\partial A_{ij}}$$

$$= T^1_{ij} + T^2_{ij} + T^3_{ij}$$

$$T^1_{ij} = \sum_{ab} M^1_{ab} \frac{\partial \tilde{P}_{ab}}{\partial A_{ij}}$$

$$= \sum_{ablk} M^1_{ab} \frac{\partial}{\partial A_{ij}} A_{la} P_{lk} A_{kb}$$

$$= \sum_{ablk} M^1_{ab} \left[\delta_{li}\delta_{aj} P_{lk} A_{kb} + A_{la} P_{lk} \delta_{ki}\delta_{bj} \right]$$

$$= \left[PAM^{1T} \right]_{ij} + \left[P^T A M^1 \right]_{ij}$$

$$= 2 \left[PAM^1 \right]_{ij}$$

$$T^2_{ij} = \sum_{ab} R^2_{ab} \frac{\partial B_{ab}}{\partial A_{ij}}$$

$$T^3_{ij} = \sum_{ab} R^3_{ab} \frac{\partial B_{ab}}{\partial A_{ij}}$$

$$R_{ij}^2 = \sum_{ab} M_{ab}^2 \frac{\partial \tilde{H}_{ab}}{\partial B_{ij}}$$

$$= \sum_{ablk} M_{ab}^2 \frac{\partial}{\partial B_{ij}} B_{la} H_{lk} B_{kb}$$

$$= \sum_{ablk} M_{ab}^2 \left[\delta_{li} \delta_{aj} H_{lk} B_{kb} + \delta_{ki} \delta_{bj} B_{la} H_{lk} \right]$$

$$= \left[HBM^{2T} \right]_{ij} + \left[H^T BM^2 \right]_{ij}$$

$$= 2 \left[HBM^2 \right]_{ij}$$

Educated guess:

$$R_{ij}^3 = \sum_{ab} M_{ab}^3 \frac{\partial \tilde{S}_{ab}}{\partial B_{ij}}$$

$$= 2 \left[SBM^3 \right]_{ij}$$

$$M^1_{ab} = \frac{\partial \Omega}{\partial \tilde{P}_{ab}}$$
$$= \frac{\partial}{\partial \tilde{P}_{ab}} \left(3\operatorname{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\operatorname{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}] \right)$$
$$= 3\tilde{H}\tilde{P}\tilde{S} + 3\tilde{S}\tilde{P}\tilde{H} - 2\tilde{H}\tilde{P}\tilde{S}\tilde{P}\tilde{S} - 2\tilde{S}\tilde{P}\tilde{H}\tilde{P}\tilde{S} - 2\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}$$

$$M^2_{ab} = \frac{\partial \Omega}{\partial \tilde{H}_{ab}}$$
$$= \frac{\partial}{\partial \tilde{H}_{ab}} \left(3\operatorname{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\operatorname{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}] \right)$$
$$= 3\tilde{P}\tilde{S}\tilde{P} - 2\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}$$

$$M^3_{ab} = \frac{\partial \Omega}{\partial \tilde{S}_{ab}}$$
$$= \frac{\partial}{\partial \tilde{S}_{ab}} \left(3\operatorname{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{H}] - 2\operatorname{tr}[\tilde{P}\tilde{S}\tilde{P}\tilde{S}\tilde{P}\tilde{H}] \right)$$
$$= 3\tilde{P}\tilde{H}\tilde{P} - 2\tilde{P}\tilde{H}\tilde{P}\tilde{S}\tilde{P} - 2\tilde{P}\tilde{S}\tilde{P}\tilde{H}\tilde{P}$$

direct param

$$T = NN = S^{-1}$$
$$Z = (A^T S^{-1} A)^{-1}$$

$$B = S^{-1} A (A^T S^{-1} A)^{-1}$$
$$= TAZ$$

$$FOO_{ij} = \sum_{ab} M_{ab} \frac{\partial B_{ab}}{\partial A_{ij}}$$

$$= \sum_{ablk} M_{ab} \frac{\partial}{\partial A_{ij}} T_{al} A_{lk} Z_{kb}$$

$$= \sum_{ablk} M_{ab} T_{al} \frac{\partial A_{lk}}{\partial A_{ij}} Z_{kb} + \sum_{ablk} M_{ab} T_{al} A_{lk} \frac{\partial Z_{kb}}{\partial A_{ij}}$$

$$= \sum_{ablk} M_{ab} T_{al} \delta_{li} \delta_{kj} Z_{kb} + \sum_{ablk} M_{ab} T_{al} A_{lk} \frac{\partial Z_{kb}}{\partial A_{ij}}$$

$$= \sum_{ab} M_{ab} T_{ai} Z_{jb} + \sum_{abk} (A^T T^T M)_{kb} \frac{\partial Z_{kb}}{\partial A_{ij}}$$

$$= (T^T M Z^T)_{ij} + \sum_{abk} (A^T T^T M)_{kb} \frac{\partial Z_{kb}}{\partial A_{ij}}$$

$$= (T M Z^T)_{ij} + \sum_{abk} (A^T T M)_{kb} \frac{\partial Z_{kb}}{\partial A_{ij}}$$

$$
\begin{aligned}
BAR_{ij} &= \sum_{ab} M_{ab} \frac{\partial (A^T T A)_{ab}}{\partial A_{ij}} \\
&= \sum_{ablk} M_{ab} \frac{\partial}{\partial A_{ij}} A_{la} T_{lk} A_{kb} \\
&= \sum_{ablk} M_{ab} \frac{\partial A_{la}}{\partial A_{ij}} T_{lk} A_{kb} + \sum_{ablk} M_{ab} A_{la} T_{lk} \frac{\partial A_{kb}}{\partial A_{ij}} \\
&= \sum_{ablk} M_{ab} \delta_{li} \delta_{aj} T_{lk} A_{kb} + \sum_{ablk} M_{ab} A_{la} T_{lk} \delta_{ki} \delta_{bj} \\
&= \sum_{bk} M_{jb} T_{ik} A_{kb} + \sum_{al} M_{aj} A_{la} T_{li} \\
&= (TAM^T)_{ij} + (T^T A M)_{ij} \\
&= 2(TAM)_{ij}
\end{aligned}
$$