Have unpleasant expression:

$$\sum_{\substack{ijkl\\mnop}}\sum_{J}\langle I|ijk^{\dagger}l^{\dagger}m^{\dagger}n^{\dagger}op|J\rangle c_J^N H^{\dagger}_{ijkl}G_{mnop} \tag{1}$$

where $a_i^{\dagger}=i$. Reorder to normal ordering to ensuer no non-active indexes in BraKet.

$$\sum_{\substack{ijkl\\mnop}}\sum_{J}\langle I|k^{\dagger}l^{\dagger}m^{\dagger}n^{\dagger}ijop|J\rangle c_J^N H^{\dagger}_{ijkl}G_{mnop} \tag{2}$$

Reorder back to ordering where indexes corresponding to like operators are grouped:

$$\sum_{\substack{ijkl\\mnop}}\sum_{J}\langle I|ijk^{\dagger}l^{\dagger}m^{\dagger}n^{\dagger}op|J\rangle c_J^N H^{\dagger}_{ijkl}G_{mnop} \tag{3}$$

If no contractions between operators, perform the contractions between operator representation and rdms/rdms derivatives seperately:

$$\sum_{ijkl}H^{\dagger}_{ijkl}\sum_{K}\langle I|ijk^{\dagger}l^{\dagger}|K\rangle\sum_{mnop}\sum_{J}G_{mnop}\langle K|m^{\dagger}n^{\dagger}op|J\rangle c_J^N \tag{4}$$

If there are some contractions between different operators can use a similar approach

$$\sum_{ijkl}H^{\dagger}_{ijkl}\sum_{K}\langle I|ijk^{\dagger}|K\rangle\sum_{nop}\sum_{J}G_{lnop}\langle K|n^{\dagger}op|J\rangle c_J^N \tag{5}$$

Can evaluate this using the following sequence of operations:

- $\sum_J\langle K|n^{\dagger}op|J\rangle c_J^N=\sigma^K_{n^{\dagger}op}$
- $\sum_{nop}G_{lnop}\sigma^K_{n^{\dagger}op}=\tilde{x}^K_l$
- $\sum_l H^{\dagger}_{ijkl}\tilde{x}^K_l=\tilde{w}^K_{ijk}$
- $\sum_{ijk}\sum_K\langle I|ijk^{\dagger}|K\rangle\tilde{w}^K_{ijk}=\tilde{c}^I$

This avoids the need to perform the contractions or perform index shuffling on large combined operators, e.g., shuffling on $A_{ijkmno}=\sum_l H^{\dagger}_{ijkl}G_{lnop}$, and also eliminate the need to store rdms/rdm derivatives with more than 4 indexes. However, it is worth noting that the contracted index, l in the above example, is often not active, and hence $\tilde{x}^K_l$ is usually either $n_{core}n_{det}$ or $n_{virt}n_{det}$, which is typically $>>n_{act}n_{det}$. However, so long as $n_{virt}<n_{act}^4$ the size of $\tilde{x}^K_l<\sigma^K_{ijkl}$, so $\tilde{x}^K_l$ is still unlikely to be the largest matrix we have to deal with.

A disadvantage is that it requires repeated performance of the operations of the sort $a_i^\dagger a_j a_k |J\rangle$. And the fact that the determinant used in the RI ($|K\rangle$ in the above example are not the same as the active determinants.