Some notes on extending the SOAP kernel to multi-component systems

Jonathan Vandermause

(Dated: September 17, 2018)

I. REVIEW OF THE SINGLE-COMPONENT SOAP KERNEL

A. SOAP as a dot product of normalized rotational power spectra

In the SOAP scheme, an atomic environment is represented by an atomic neighbor density function $\rho(\vec{r})$, where

$$\rho(\vec{r}) = \sum_i \exp\left(-\alpha|\vec{r} - \vec{r}_i|^2\right), \tag{1}$$

α is a hyperparameter, and $\vec{r}_i$ is the position of atom i in the environment of the central atom. The single-component SOAP kernel between two atomic neighbor densities ρ and ρ' is defined by Eq. (36) of [1] as:

$$K(\rho, \rho') = \left(\frac{k(\rho, \rho')}{\sqrt{k(\rho, \rho)k(\rho', \rho')}}\right)^{\xi}, \tag{2}$$

where $k(\rho, \rho')$ is a rotationally invariant symmetry kernel given by

$$k(\rho, \rho') = \int d\hat{R} \left| \int \rho(\vec{r})\rho'(\hat{R}\vec{r})d\vec{r} \right|^n, \tag{3}$$

and $\hat{R}$ is a 3-D rotation. The integral is over all rotations and ensures that the kernel is rotationally symmetric.

In Section IV(B) of [1], it is shown that $k(\rho, \rho')$ is equal to the dot product of the "rotational power spectra" of densities ρ and ρ', which is efficient to compute. I will review this derivation here, since a similar argument can be applied to multi-component systems.

Letting $g_n(r)$ be an orthonormal set of radial basis functions, so that

$$\int dr r^2 g_n(r) g_{n'}(r) = \delta_{nn'}, \tag{4}$$

an atomic neighbor density $\rho(\vec{r})$ may be expanded into spherical harmonics as

$$\rho(\vec{r}) = \sum_{nlm} c_{nlm} g_n(r) Y_{lm}(\vec{r}). \tag{5}$$

We first compute that

$$\begin{aligned}
S(\rho, \hat{R}\rho') &\equiv \int d\vec{r}\rho(\vec{r})\rho'(\hat{R}\vec{r}) \\
&= \int d\vec{r} \left(\sum_{nlm} c^*_{nlm} g_n(r) Y^*_{lm}(\hat{r}) \right) \left(\sum_{n'l'm'} c'_{n'l'm'} g_{n'}(r) Y_{l'm'}(\hat{R}\vec{r}) \right) \\
&= \sum_{nlmn'l'm'} c^*_{nlm} c'_{n'l'm'} \int dr g_n(r) g_{n'}(r) \int d\hat{r} Y^*_{lm}(\hat{r}) Y_{l'm'}(\hat{R}\vec{r}) \\
&= \sum_{nlml'm'} c^*_{nlm} c'_{nl'm'} \int d\hat{r} Y^*_{lm}(\hat{r}) Y_{l'm'}(\hat{R}\vec{r}).
\end{aligned} \tag{6}$$

Note that

$$\begin{aligned}
Y_{l'm'}(\vec{R}\hat{r}) &= \langle \vec{r} | \hat{R}^\dagger | Y_{l'm'} \rangle \\
&= \sum_{m''} \langle \vec{r} | Y_{l'm''} \rangle \langle Y_{l'm''} | \hat{R}^\dagger | Y_{l'm'} \rangle \\
&= \sum_{m''} \langle \vec{r} | Y_{l'm''} \rangle \langle Y_{l'm'} | \hat{R} | Y_{l'm''} \rangle^* \\
&= \sum_{m''} Y_{l'm''}(\hat{r}) D^*(\hat{R})^{l'}_{m'm''},
\end{aligned} \tag{7}$$

where the Wigner function $D(\hat{R})^l_{mm'}$ is defined as

$$D(\hat{R})^l_{mm'} = \langle Y_{lm} | \hat{R} | Y_{lm'} \rangle . \tag{8}$$

Plugging into Eq. (6) gives

$$\begin{aligned}
S(\rho, \hat{R}\rho') &= \sum_{nlml'm'm''} c^*_{nlm} c'_{nl'm'} D^*(\hat{R})^{l'}_{m'm''} \int d\hat{r} Y^*_{lm}(\hat{r}) Y_{l'm''}(\hat{r}) \\
&= \sum_{nlmm'} c^*_{nlm} c'_{nlm'} D^*(\hat{R})^l_{m'm}.
\end{aligned} \tag{9}$$

The symmetry kernel $k(\rho, \rho')$ with $n = 2$ then takes the form

$$\begin{aligned}
k(\rho, \rho') &= \int d\hat{R} S(\rho, \hat{R}\rho') S^*(\rho, \hat{R}\rho') \\
&= \sum_{nlmm'n'\lambda\mu\mu'} c^*_{nlm} c'_{nlm'} c_{n'\lambda\mu} (c'_{n'\lambda\mu'})^* \int d\hat{R} D^*(\hat{R})^l_{m'm} D(\hat{R})^\lambda_{\mu'\mu} \\
&= \sum_{nlmm'n'} c^*_{nlm} c'_{nlm'} c_{n'lm} (c'_{n'lm'})^* \\
&= \sum_{nn'l} \left(\sum_m c^*_{nlm} c_{n'lm} \right) \left(\sum_{m'} c'_{nlm'} (c'_{n'lm'})^* \right) \\
&= \sum_{nn'l} p_{n'nl} p'_{nn'l}.
\end{aligned} \tag{10}$$

Because the atomic densities ρ and ρ' are real-valued functions, $p_{n'nl} = p_{nn'l}$, so $k(\rho, \rho')$ may be expressed as the dot product of the power spectra $\vec{p}$ and $\vec{p'}$:

$$k(\rho, \rho') = \vec{p} \cdot \vec{p'}. \tag{11}$$

The full SOAP kernel $K(\rho, \rho')$ is

$$K(\rho, \rho') = \left(\frac{\vec{p}}{|\vec{p}|} \cdot \frac{\vec{p'}}{|\vec{p'}|} \right)^{\xi}. \tag{12}$$

B. Computing the SOAP kernel

The key step in compuing $K(\rho, \rho')$ is determining the coefficients $c_{nlm}(r, \{\vec{r_i}\})$, which depend on the radial distance r, the positions $\vec{r_i}$ of the environment atoms, and the radial basis set.

---

[1] A. P. Bartók, R. Kondor, and G. Csányi, Physical Review B **87**, 184115 (2013).