PCCP

ROYAL SOCIETY OF CHEMISTRY

CORRECTION

View Article Online
View Journal | View Issue

Cite this: *Phys. Chem. Chem. Phys.*, 2020, **22**, 27914

Correction: A critical comparison of neural network potentials for molecular reaction dynamics with exact permutation symmetry

Jun Li, *[ab] Kaisheng Song[a] and Jörg Behler *[b]

DOI: 10.1039/d0cp90265a

rsc.li/pccp

Correction for 'A critical comparison of neural network potentials for molecular reaction dynamics with exact permutation symmetry' by Jun Li *et al.*, *Phys. Chem. Chem. Phys.*, 2019, **21**, 9672–9682, DOI: 10.1039/C8CP06919K.

We have discovered an error in the published paper for the discussion on the significance of inclusion of the angular symmetry functions. As a result, the paragraph below eqn (14) needs be modified. All other conclusions are not affected by this correction.

For consistency and clarity, the following equations are given without relabeling. They provide descriptions for the local chemical environments of the central atom i being 1, 2, 3, and 4.

$$G_{1,t}\begin{cases} G_{1,tr}{}^{2}\begin{cases} = G_{12,tr}{}^{2}, \mathrm{AA} \\ = G_{13,tr}{}^{2}, \mathrm{AB} \\ = G_{14,tr}{}^{2}, \mathrm{AC} \end{cases} \\ G_{1,ta}{}^{3}\begin{cases} = G_{123,ta}{}^{3}, \mathrm{AAB} \\ = G_{124,ta}{}^{3}, \mathrm{AAC} \\ = G_{134,ta}{}^{2}, \mathrm{ABC} \end{cases} \end{cases}, \tag{9}$$

$$G_{2,t}\begin{cases} G_{2,tr}{}^{2}\begin{cases} = G_{21,tr}{}^{2}, \mathrm{AA} \\ = G_{23,tr}{}^{2}, \mathrm{AB} \\ = G_{24,tr}{}^{2}, \mathrm{AC} \end{cases} \\ G_{2,ta}{}^{3}\begin{cases} = G_{213,ta}{}^{3}, \mathrm{AAB} \\ = G_{214,ta}{}^{3}, \mathrm{AAC} \\ = G_{234,ta}{}^{2}, \mathrm{ABC} \end{cases} \end{cases}, \tag{10}$$

$$G_{3,t}\begin{cases} G_{3,tr}{}^{2}\begin{cases} = G_{31,tr}{}^{2} + G_{32,tr}{}^{2}, \mathrm{BA} \\ = G_{34,tr}{}^{2}, \mathrm{BC} \end{cases} \\ G_{3,ta}{}^{3}\begin{cases} = G_{312,ta}{}^{3}, \mathrm{BAA} \\ = G_{314,ta}{}^{3} + G_{324,ta}{}^{3}, \mathrm{BAC} \end{cases} \end{cases}, \tag{11}$$

[a] *School of Chemistry and Chemical Engineering, Chongqing University, Chongqing 401331, China. E-mail: jli15@cqu.edu.cn*
[b] *Universität Göttingen, Institut für Physikalische Chemie, Theoretische Chemie, Tammannstr. 6, 37077 Göttingen, Germany. E-mail: joerg.behler@uni-goettingen.de*

$$G_{4,t}\begin{cases} {G_{4,tr}}^2\begin{cases} = {G_{41,tr}}^2 + {G_{42,tr}}^2, \mathrm{CA} \\ = {G_{43,tr}}^2, \mathrm{CB} \end{cases} \\ {G_{4,ta}}^3\begin{cases} = {G_{412,ta}}^3, \mathrm{CAA} \\ = {G_{413,ta}}^3 + {G_{423,ta}}^3, \mathrm{CAB} \end{cases} \end{cases}, \tag{12}$$

If only radial symmetry functions would be included, eqn (9)–(12) would only have ${G_{i,tr}}^2$ (i = 1–4) left. Explicitly, they read,

$$G_{1,t} = {G_{1,tr}}^2\begin{cases} = {G_{12,tr}}^2, \mathrm{AA} \\ = {G_{13,tr}}^2, \mathrm{AB} \\ = {G_{14,tr}}^2, \mathrm{AC} \end{cases}, \tag{9a}$$

$$G_{2,t} = {G_{2,tr}}^2\begin{cases} = {G_{21,tr}}^2, \mathrm{AA} \\ = {G_{23,tr}}^2, \mathrm{AB} \\ = {G_{24,tr}}^2, \mathrm{AC} \end{cases}, \tag{10a}$$

$$G_{3,t} = {G_{3,tr}}^2\begin{cases} = {G_{31,tr}}^2 + {G_{32,tr}}^2, \mathrm{BA} \\ = {G_{34,tr}}^2, \mathrm{BC} \end{cases},$$

$$G_{4,t} = {G_{4,tr}}^2\begin{cases} = {G_{41,tr}}^2 + {G_{42,tr}}^2, \mathrm{CA} \\ = {G_{43,tr}}^2, \mathrm{CB} \end{cases},$$

The exchange of the two identical atoms 1 and 2 results in the permutation of the characterizations $\{G_{1,t}\}$ and $\{G_{2,t}\}$, and has no effect on $\{G_{3,t}\}$ and $\{G_{4,t}\}$. Explicitly,

$$G_{2,t} = {G_{2,tr}}^2\begin{cases} = {G_{12,tr}}^2, \mathrm{AA} \\ = {G_{23,tr}}^2, \mathrm{AB} \\ = {G_{24,tr}}^2, \mathrm{AC} \end{cases}, \tag{9b}$$

$$G_{1,t} = {G_{1,tr}}^2\begin{cases} = {G_{21,tr}}^2, \mathrm{AA} \\ = {G_{13,tr}}^2, \mathrm{AB} \\ = {G_{14,tr}}^2, \mathrm{AC} \end{cases}, \tag{10b}$$

$$G_{3,t} = {G_{3,tr}}^2\begin{cases} = {G_{31,tr}}^2 + {G_{32,tr}}^2, \mathrm{BA} \\ = {G_{34,tr}}^2, \mathrm{BC} \end{cases}, \tag{11a}$$

$$G_{4,t} = {G_{4,tr}}^2\begin{cases} = {G_{41,tr}}^2 + {G_{42,tr}}^2, \mathrm{CA} \\ = {G_{43,tr}}^2, \mathrm{CB} \end{cases}, \tag{12a}$$

However, if only (r_{13}, r_{23}) or (r_{14}, r_{24}) exchange, the resulting configurations are different generally. Taking the exchange of (r_{13}, r_{23}) as an example, the original $\{r_{12}, r_{13}, r_{14}, r_{23}, r_{24}, r_{34}\}$ becomes $\{r_{12}, r_{23}, r_{14}, r_{13}, r_{24}, r_{34}\}$,[1] whose configuration and the corresponding characterizations have been changed. In other words, in the special A_2BC case without angular symmetry functions, the resulting fingerprints do not introduce "false symmetry" properties with respect to the exchange of the artificial bond pair, either (r_{13}, r_{23}) or (r_{14}, r_{24}). However, the number of the fingerprints needs to be increased significantly to provide sufficient environment information. In other words, in some cases one can only use radial symmetry functions in the high-dimensional neural network potentials (HD-NNPs).

Prof. Bin Jiang is thanked for detailed discussion on this correction.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

References

1 J. Li, B. Jiang and H. Guo, *J. Chem. Phys.*, 2013, **139**, 204103.