ERRATUM

Erratum: Improving the generative performance of chemical autoencoders through transfer learning (2020 Mach. Learn.: Sci. Technol. 1 045010)

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The following error was introduced during the production process. Figures 3 and 4 were printed incorrectly; the correct figures are reproduced here.

![Correct Figures](image-url)

Figure 3. Distribution of $U_0$ for structures for the training set (a) compared with structures generated from extrapolation along the first principal component of models trained on (b) encoding and decoding alone, (c) an ancillary $U_0$ prediction task, (d) $U_0$ and ZPVE prediction tasks, and (e) $U_0$, ZPVE, and $E_g$ prediction tasks. For each paradigm, 3000 unique structures are generated across the ten duplicate models for a total of 30 000 structures. The mean of each distribution is denoted with a dashed red line and the largest $|U_0|$ value in the training data is indicated by the dashed green line. The percentage of generated compounds with $|U_0|$ greater than observed in the training data is shown on the right.
Figure 4. Distribution of $E_g$ for the training data (a) and structures generated from models trained to predict $E_g$ by targeting (b) 1.5–2.0 eV, (c) 5.5–6.0 eV, and (d) 9.5–10.0 eV. While (c) and (d) show good specificity, the model is unable to resolve structures in the 1.5–2.0 eV range (b). For each target, 3000 unique structures are generated across the ten duplicate models for a total of 30,000 structures. The median of each distribution is indicated by a dashed red line. Targeted regions are highlighted in blue.

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