Accelerating catalysis simulations using surrogate machine learning models

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Corrections sheet *[to be deleted: This is strictly an example. You are welcome to prepare the corrections sheet in a different format if you like. Please remember that the maximum length is 2 pages]*
Thesis title: Accelerating catalysis simulations using surrogate machine learning models.

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Page, line	States	Should state
4, 12	is the second derivative wrt. to the Cartesian coordinates of nucleus or electron *i*	… is the second derivative wrt. the Cartesian coordinates of nucleus or electron *i*
8, 18	The predictive mean is the best prediction of the test target given the training data.	The predictive mean is the most likely prediction of the test target given the training data.
14, 17	$D_{FB} = \frac{1}{2} + \frac{1}{2}\ln(2\pi)) + \frac{1}{2}\ln\left(\sigma_{*0}(\vec{\theta}_0)\right) + \frac{1}{2}\ln(\alpha_0^2)$	$D_{FB} = \frac{1}{2} + \frac{1}{2}\ln(2\pi) + \frac{1}{2}\ln\left(\sigma_{*0}(\vec{\theta}_0)\right) + \frac{1}{2}\ln(\alpha_0^2)$
15, 4	$\bar{\bar{y}}_* ==$	$\bar{\bar{y}}_* =$
17, 20	At last, the FBMGP (see Section 2.5) is compared to the fully Bayesian solution and the MLE solutions.	At last, the FBMGP (see Section 2.5) is compared to the fully Bayesian solution and the MAP solutions.
21, 42	The factorization method uses the analytical solution of the prefactor hyperparameter and performs the eigendecomposition of the covariance matrix with noise as in Eq. 2.33.	The factorization method uses the analytical solution of the prefactor hyperparameter and performs the eigendecomposition of the covariance matrix without noise as in Eq. 2.33.
31, 35	When a larger number of training points is used, the same prediction mean and uncertainty are predicted as for the MLE as expected.	When a larger number of training points is used, the same prediction mean and uncertainty are predicted as for the MAP as expected.
37, 48	Convergence of the algorithm requires five criteria. Firstly, the training set for the ML algorithm has to be greater than or equal to ml_steps.	Convergence of the algorithm requires five criteria. Firstly, the training set for the ML algorithm has to be greater than or equal to min_steps.
44, 14	The GMESs are observed in all the systems considered, and the accelerations of the global searches are significant (see Section ??).	The GMESs are observed in all the systems considered, and the accelerations of the global searches are significant (see Section A.7).
71, 6	$\delta_n = \frac{\mathrm{Tr}(\boldsymbol{K})^2}{c_\epsilon \epsilon_M^{-1} - N_K^2}$	$\delta_n = \frac{\mathrm{Tr}(\boldsymbol{K}_0)^2}{c_\epsilon \epsilon_M^{-1} - N_K^2}$
73, 17	The energy deviation (new method's energy - standard methods' energy) is also shown.	The energy deviation (standard methods' energy - new method's energy) is also shown.