



## Accelerating catalysis simulations using surrogate machine learning models

Vishart, Andreas Lyngø

*Publication date:*  
2023

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*  
Vishart, A. L. (2023). *Accelerating catalysis simulations using surrogate machine learning models*. Technical University of Denmark.

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

**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.

Author: Andreas Lynge Vishart

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	$D_{FB} = \frac{1}{2} + \frac{1}{2} \ln(2\pi) + \frac{1}{2} \ln(\sigma_{*0}(\vec{\theta}_0)) + \frac{1}{2} \ln(\alpha_0^2)$	$D_{FB} = \frac{1}{2} + \frac{1}{2} \ln(2\pi) + \frac{1}{2} \ln(\sigma_{*0}(\vec{\theta}_0)) + \frac{1}{2} \ln(\alpha_0^2)$
15, 4	$\bar{y}_* ==$	$\bar{y}_* =$
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	$\delta_n = \frac{\text{Tr}(\mathbf{K})^2}{c_\epsilon \epsilon_M^{-1} - N_K^2}$	$\delta_n = \frac{\text{Tr}(\mathbf{K}_0)^2}{c_\epsilon \epsilon_M^{-1} - N_K^2}$
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.

