Bayesian experimental design for the active nitridation of graphite by atomic nitrogen

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(Submitted on 7 Jul 2011)

The problem of optimal data collection to efficiently learn the model parameters of a graphite nitridation experiment is studied in the context of Bayesian analysis using both synthetic and real experimental data. The paper emphasizes that the optimal design can be obtained as a result of an information theoretic sensitivity analysis. Thus, the preferred design is where the statistical dependence between the model parameters and observables is the highest possible. In this paper, the statistical dependence between random variables is quantified by mutual information and estimated using a k-nearest neighbor based approximation. It is shown, that by monitoring the inference process via measures such as entropy or Kullback-Leibler divergence, one can determine when to stop the data collection process. The methodology is applied to select the most informative designs on both a simulated data set and on an experimental data set, previously published in the literature. It is also shown that the sequential Bayesian analysis used in the experimental design can also be useful in detecting conflicting information between measurements and model predictions.

Comments:	Preprint submitted to Experimental Thermal and Fluid Science, February 2011
Subjects:	**Data Analysis, Statistics and Probability (physics.data-an)**; Information Theory (cs.IT); Applications (stat.AP)
Cite as:	**arXiv:1107.1445 [physics.data-an]**
	(or **arXiv:1107.1445v1 [physics.data-an]** for this version)

Submission history

From: Gabriel Terejanu [view email]

[v1] Thu, 7 Jul 2011 16:46:43 GMT (517kb,D)