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Atmospheric Measurement Techniques Discussions

Interactive comment on "Notably improved inversion of Differential Mobility Particle Sizer data obtained under conditions of fluctuating particle number concentrations" *by* B. Mølgaard et al.

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Referee comments

The authors propose a model for inversion of Differential Mobility Particle Sizer data, where Gaussian process prior is used to include smoothness assumption of the particle number size distribution. This is quite sensible approach as GPs are flexible way to present such assumptions and accurate approximative inference is usually feasible.

The covariance function along the particle size follows the Matern covariance function with 5/2 degrees of freedom and the covariance function along the time domain is exponential. There is no explanation why these specific covariance functions were selected, but I assume that the choice includes use of prior information and some model assessment?

The priors for GP covariance function parameters are almost as recommended in Gel- man (2006) and Vanhatalo et al (2013). Gelman (2006) recommend priors to be defined on sigma not sigma^2. Reason for defining here the prior on sigma^2 instead of sigma is not explained, but I assume that the posterior is not sensitive to this choice?

The approximative posterior inference is made using common Laplace approximation with also previously used stabilized Newton method to handle the non-log-concave likelihood. This approach provides fast computation and the methods have been successfully used before and they seem to produce good results here, too.

The hyperparameter inference is based on type II MAP estimate. It is not mentioned whether the results are insensitive to not integrating over the hyperparameters, but taking into account the small number of hyperparameters compared to the amount f data it is likely that type II MAP estimate is sufficiently accurate.

Overall the model and computation is described with sufficient accuracy and the in- cluded code makes it possible to replicate the experiments. There were couple issues the authors could clarify: 1) how they decided which covariance functions were used, 2) why prior on sigma^2 instead of prior on sigma as recommend in the previous literature, and 3) the sensitivity to using type II MAP.

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Author reply

1) The covariance function was chosen according to prior information and convenience. Traditional covariance functions include squared exponential and Matern class of covariance functions. The former is physically unrealistically smooth since it corresponds to processes that are infinite times mean square differentiable. In Matern class of covariance functions the smoothness is governed by the degrees of freedom so that a process with 5/2 degrees of freedom corresponds to a process that is twice mean square differentiable which was a priori plausible smoothness. For the purposes of sensitivity test we tried also squared exponential and Matern with with 3/2 degrees of freedom. With the square exponential covariance function the obtained particle size distributions were unrealistically smooth, and with Matern 3/2 they were unrealistically rough.

The exponential covariance function leads to a stationary (homogenous) process in time and it corresponds to a continues-time autoregressive model of order one. It is also a common choice for modeling temporal processes e.g. in spatio-temporal statistics.

2) We thank the reviewer for noticing this inconsistency. The prior should have been for σ and not σ^2. We had an error in our manuscript and code on this regard. It has now been corrected. After correcting this error we ran our algorithm again and inspected the results carefully. The difference between the previous results and the new results is negligible.

3) We tested for the sensitivity of the results to the MAP estimate of the hyperparameters by varying them randomly in the vicinity of the MAP. The results were not sensitive to the MAP estimate.

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Changes in document

Page 10291:
Lines 20 and 21: 'σ^2' changed to 'σ'.
Line 23: '10' changed to '3'.
Page 10294 line 18: The word 'inverse' was an error and has been deleted.

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