Peter Challenor, Ph.D. and Sebastian Reich, Ph.D., SIAM/ASA Journal on Uncertainty Quantification

December 4, 2024

Dear Drs. Challenor and Reich,

Please see attached for our revised manuscript and below for our responses to the referees.

Sincerely,

Dr. Florian Schäfer Assistant Professor fts@gatech.edu https://f-t-s.github.io/

Johns Malik

# 1 Responses to Referees

We thank the referees for their valuable feedback. Please find our responses and clarifications below. Unless otherwise mentioned, all references to citations, lines, and sections in our response are with respect to the revised draft.

## 1.1 Responses to Referee #1

Thank you for appreciating the relevance of our results and for providing suggestions for improving our work. Please see below for our responses to your comments, in the order in which they were raised.

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## **Major comments**

"1) The manuscript cites 74 references, which seems a bit exaggerated. Unfortunately, several key references addressing similar topics are missing:..."

In our original submission, the discussion of related work was more narrowly scoped, but we are happy to include a discussion of a broader class of alternative methods for computing with dense covariance matrices and appreciate your pointers to relevant related works. We have added add numbers discussing add description.

"2) With regard to the references mentioned above, which cover Nystrom approximation, fast multipole method and sparse Cholesky factorization, the advantages of and drawbacks of the presented method should be clearly stated, particularly in terms of the (overall) computational cost."

We have included such a discussion in add section.

"3) The numerical results all with less than  $10^5$  data points are way behind the state of the art and it should be justified why no larger problems, which actually require sparsification, have been considered."

We have included results on larger problems in add section.

"4) In Subsection 6.3, it would be informative to also consider the spectral error  $||I - \Theta LL^T||_2$ , which gives an indication on the quality of the approximate precision matrix."

We have included plots of these quantities in add section.

#### **Minor comments**

"l 68. Define the term precision matrix."

We have added the definition in where?

"l 127. What is the covariance matrix of a Gaussian process?"

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We have changed this to "covariance matrix of a multivariate Gaussian. do!

"l 144. What information does the formula  $\Theta_{Tr,Tr}^{-1}$ ... convey?"

### address

"l 188. Is the reverse-maximin ordering the same as the maximin ordering?"

It is the reverse of the maximin ordering, meaning if the maximin ordering is  $1, \ldots, N$ , the reverse maximin ordering is  $N \ldots 1$ . We have clarified this in where?.

"Figure 9. (and later) Remove  $log_10$  from the x/y axis label (or actually use the exponents as ticks)."

Done! do!

"Figure 11. (and later) The compression rate  $nnz/N^2$  might be a better measure here."

Good point, we have made this change. Do!

"Subsection 6.3. The cost of the matrix-vector product by the covariance matrix is  $O(N^2)$ . It should be mentioned how this can be mitigated. Otherwise, the example seems to be very academic."

Good point, we have addressed this by how?.

## 1.2 Responses to Referee # 2

Thank you for your detailed comments and suggestions. We are glad to learn that you find our method interesting and dealing with a relevant problem. In the following, we address your comments in the order in which they were raised.

"In [54], the authors have shown that the minimization problem has an explicit solution, i.e. there is an explicit formula for the sparse Cholesky matrix, given the sparsity pattern, see formula (2.1). The new content of this paper, when compared to [54], is that the authors provide a closed solution formula of the iterated minimization problem, see formula (2.2) and its proof in Appendix A.1."

We admit we are slightly confused what the referee means here. Formulas (2.1) and (2.2) in the

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first version of our submission are, as we indicate, the standard formulas for the conditional mean and covariance of a multivariate Gaussian. The closed form solution of the KL optimization was, as we indicate in line 215 (in the first version of our submission), derived by the prior work [54] (numbering as in first submission). Appendix A.1 computes the loss attained by this minimizer.

"to stay computational competitive, the possible candidates of indices have to be artificially restricted, see the last paragraph before Section 5. Here, the authors only say that they proceed as in [54], which is reasonable, but as the index selection is the key topic in this paper, a more elaborate discussion would have been useful."

We have added a more detailed discussion in add where?.

"Next, there is no discussion of or comparison to other popular methods for computing with covariance matrices such as far field and multipole expansions and H-matrices. At least a numerical comparison would be important."

We have added a more detailed discussion to methods other than sparse inverse Cholesky factorization in where?. We have also added a numerical comparison against Cholesky factorization in hierarchical matrix format in where?.

"The numerical examples are interesting but I miss (or might have missed) a more sophisticated discussion of the accuracy of the approximate Cholesky factorization not only in the Kullback-Leibler divergence but a standard matrix norm."

We have added plots of operator norms of the error in where? In the setting of the rigorous results [54] (numbering with respect to first submitted version), a small error in KL divergence implies a small operator norm error, we have added a brief discussion of this in where?.

"The title of the paper seems to be too generic and should reflect that precision matrices of Gaussian processes are considered. The literature should be updated. Finally, the paper is obviously an extension of [54]; I have some doubts that the extension is scientifically significant enough to grant publication."

Shall we add anything here? Shall we change the title of the paper?

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