

A general framework for scalable Gaussian Processes with applications to astronomical time series

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ABSTRACT

In this paper we describe some generalizations to the *celerite* method.

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1. INTRODUCTION

This manuscript was prepared with *showyourwork*¹ (Luger et al. 2021).
(Foreman-Mackey et al. 2017; Foreman-Mackey 2018; Foreman-Mackey et al. 2021).

2. QUASISEPARABLE LINEAR ALGEBRA

There exist a range of definitions for *quasiseparable matrices* in the literature, so to be explicit, let's select the one that we will consider in all that follows. The most suitable definition for our purposes is nearly identical to the one used by Eidelman & Gohberg (1999), with some small modifications that will become clear as we go.

Let's start by considering an $N \times N$ square *quasiseparable matrix* \mathbf{M} with lower quasiseparable order m_l and upper quasiseparable order m_u . In this note, we represent this matrix \mathbf{M} as:²

$$M_{ij} = \begin{cases} d_i & , \quad \text{if } i = j \\ \mathbf{p}_i^T \left(\prod_{k=i-1}^{j+1} \mathbf{A}_k \right) \mathbf{q}_j & , \text{ if } i > j \\ \mathbf{h}_i^T \left(\prod_{k=i+1}^{j-1} \mathbf{B}_k^T \right) \mathbf{g}_j & , \text{ if } i < j \end{cases} \quad (1)$$

where

- i and j both range from 1 to N ,

¹ <https://show-your.work>

² Comparing this definition to the one from Eidelman & Gohberg (1999), you may notice that we have swapped the labels of \mathbf{g}_j and \mathbf{h}_i , and that we've added an explicit transpose to \mathbf{B}_k^T . These changes simplify the notation and implementation for symmetric matrices where, with our definition, $\mathbf{g} = \mathbf{p}$, $\mathbf{h} = \mathbf{q}$, and $\mathbf{B} = \mathbf{A}$.

- d_i is a scalar,
- \mathbf{p}_i and \mathbf{q}_j are both vectors with m_l elements,
- \mathbf{A}_k is an $m_l \times m_l$ matrix,
- \mathbf{g}_j and \mathbf{h}_i are both vectors with m_u elements, and
- \mathbf{B}_k is an $m_u \times m_u$ matrix.

In Equation 1, the product notation is a little sloppy so, to be more explicit, this is how the products expand:

$$\begin{aligned} \prod_{k=i-1}^{j+1} \mathbf{A}_k &\equiv \mathbf{A}_{i-1} \mathbf{A}_{i-2} \cdots \mathbf{A}_{j+2} \mathbf{A}_{j+1} \quad , \text{ and} \\ \prod_{k=i+1}^{j-1} \mathbf{B}_k^T &\equiv \mathbf{B}_{i+1}^T \mathbf{B}_{i+2}^T \cdots \mathbf{B}_{j-2}^T \mathbf{B}_{j-1}^T \quad . \end{aligned} \quad (2)$$

$$\mathbf{M} = \begin{pmatrix} d_1 & \mathbf{h}_1^T \mathbf{g}_2 & \mathbf{h}_1^T \mathbf{B}_2^T \mathbf{g}_3 & \mathbf{h}_1^T \mathbf{B}_2^T \mathbf{B}_3^T \mathbf{g}_4 \\ \mathbf{p}_2^T \mathbf{q}_1 & d_2 & \mathbf{h}_2^T \mathbf{g}_3 & \mathbf{h}_2^T \mathbf{B}_3^T \mathbf{g}_4 \\ \mathbf{p}_3^T \mathbf{A}_2 \mathbf{q}_1 & \mathbf{p}_3^T \mathbf{q}_2 & d_3 & \mathbf{h}_3^T \mathbf{g}_4 \\ \mathbf{p}_4^T \mathbf{A}_3 \mathbf{A}_2 \mathbf{q}_1 & \mathbf{p}_4^T \mathbf{A}_3 \mathbf{q}_2 & \mathbf{p}_4^T \mathbf{q}_3 & d_4 \end{pmatrix} \quad (3)$$

3. THE CELERITE MATRICES

4. COMMON KERNEL FUNCTIONS

SHO, Matern, cosine, CARMA, approximations, etc., sums and products.

5. BANDED OBSERVATION MODELS

For example, how the S+LEAF models are implemented. (Delisle et al. 2020)

6. MULTI-BAND TIME SERIES

With non-simultaneous observations. Generalizing (Gordon et al. 2020).

7. DERIVATIVE MODELS

Generalizing (Delisle et al. 2022).

8. TIME-INTEGRATED MODELS

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Software: `showyourwork` (Luger et al. 2021), JAX (Bradbury et al. 2018)

APPENDIX

A. ALGORITHMS

Should also look at Pernet & Storjohann (2018).

B. PARALLELIZATION

See Särkkä & García-Fernández (2020).

REFERENCES

- Bradbury, J., Frostig, R., Hawkins, P., et al. 2018, JAX: composable transformations of Python+NumPy programs, 0.4.1.
<http://github.com/google/jax>
- Delisle, J. B., Hara, N., & Ségransan, D. 2020, A&A, 638, A95, doi: [10.1051/0004-6361/201936906](https://doi.org/10.1051/0004-6361/201936906)
- Delisle, J. B., Unger, N., Hara, N. C., & Ségransan, D. 2022, A&A, 659, A182, doi: [10.1051/0004-6361/202141949](https://doi.org/10.1051/0004-6361/202141949)
- Eidelman, Y., & Gohberg, I. 1999, Integral Equations and Operator Theory, 34, 293, doi: [10.1007/BF01300581](https://doi.org/10.1007/BF01300581)
- Foreman-Mackey, D. 2018, Research Notes of the American Astronomical Society, 2, 31, doi: [10.3847/2515-5172/aaaf6c](https://doi.org/10.3847/2515-5172/aaaf6c)
- Foreman-Mackey, D., Agol, E., Ambikasaran, S., & Angus, R. 2017, AJ, 154, 220, doi: [10.3847/1538-3881/aa9332](https://doi.org/10.3847/1538-3881/aa9332)
- Foreman-Mackey, D., Luger, R., Agol, E., et al. 2021, The Journal of Open Source Software, 6, 3285, doi: [10.21105/joss.03285](https://doi.org/10.21105/joss.03285)
- Gordon, T. A., Agol, E., & Foreman-Mackey, D. 2020, AJ, 160, 240, doi: [10.3847/1538-3881/abbc16](https://doi.org/10.3847/1538-3881/abbc16)
- Luger, R., Bedell, M., Foreman-Mackey, D., et al. 2021, arXiv e-prints, arXiv:2110.06271.
<https://arxiv.org/abs/2110.06271>
- Pernet, C., & Storjohann, A. 2018, Journal of Symbolic Computation, 85, 224
- Särkkä, S., & García-Fernández, Á. F. 2020, IEEE Transactions on Automatic Control, 66, 299