Homework 624 Probilistic Numerics Paper Reading *

10-424/10-624 BAYESIAN METHODS IN ML https://www.cs.cmu.edu/~hchai2/courses/10624

OUT: 03/20/25 DUE: 04/24/25

1 Paper Presentation

For the course project in this course, you will be doing a deep dive into Bayesian optimization, which falls under the broader umbrella of *probabilistic numerics*. Broadly speaking, probabilistic numerics is the application of Bayesian inference to numerical analysis tasks, where the goal is to compute or estimate some intractable/incomputable quantity. Black-box optimization is perhaps the most accessible task from this field, but there are lots of other applications, including quadrature and solving differential equations.

For this assignment you will read a recent paper on probabilistic numerics and record a (short, 10-15 minute) video presentation about your findings.

We will follow the role-playing methodology from Collin Raffel and Alec Jacobson.

https://colinraffel.com/blog/role-playing-seminar.html

Specifically, for this assignment, you will select *two* of the following roles and present your paper in that format. (The instructions below were copied and adapted from 10-719's use of the role-playing paper presentation approach.)

- 1. Scientific Peer Reviewer: Complete a full review of the paper as if it were submitted to a conference. Follow the guidelines for NeurIPS reviewers to produce your review. In particular, please answer Questions 1 to 10 under "Review Form", including assigning an overall score.
- 2. Archaeologist: Determine where this paper sits in the context of previous and subsequent work. Find and briefly report on both: (1) a prior paper that substantially influenced the current paper, and (2) a more recent paper that cites this current paper.
- 3. Academic Researcher: You're an academic researcher working on a new project in this area. Propose an imaginary follow-up project that builds on the current paper. Pretend that this new project has been successful, and write up a brief introduction for a paper about your project using the five-point structure provided here (under "The Introduction"). You do not need to actually write the introduction, but instead should present in the style of an introduction to this new project.

^{*}Compiled on Thursday 20th March, 2025 at 20:04

- 4. **Industry Practitioner:** You work at a company or organization developing an application or product of your choice (one that has not already been suggested in a prior session). Describe the application/product in detail, and bring a convincing pitch for why you should be paid to implement the method in the paper for this particular application.
- 5. **Private Investigator:** You are a detective who needs to run a background check on one of the paper's authors. Where have they worked? What did they study? What previous projects might have led to working on this one? What motivated them to work on this project?
- 6. **Social Impact Assessor:** Identify how this paper self-assesses its positive or negative impact on the world. Have any additional positive social impacts been left out? What are possible negative social impacts that were overlooked or omitted? Please read this short paper to see examples.

A few notes:

- Regardless of which roles you choose, your presentation must start with a summary of the paper.
- After the summary, you must clearly state which roles you are presenting as.
- You are welcome to record with your webcam turned off (Khan Academy style).
- After submitting your recordings, we will share all the HW624 video presentations with the rest of class via our course Panopto folder so others can learn from you as well; we will set the permissions on these videos such that only students enrolled in this course this semester can view them.
- You must make slides to complement your recording and submit them alongside the video.

2 Select a paper

We encourage you to pick of the papers from the list below for this homework. If you would like to present a probabilistic numerics paper not on this list, send a direct message on Slack to the instructors with the paper and 1-2 sentences about why you are interested in it.

- [1] Michael Osborne et al. "Active Learning of Model Evidence Using Bayesian Quadrature". In: Advances in Neural Information Processing Systems. Ed. by F. Pereira, C.J. Burges, L. Bottou, and K.Q. Weinberger. Vol. 25. Curran Associates, Inc., 2012. URL: https://proceedings.neurips.cc/paper_files/paper/2012/file/6364d3f0f495b6ab9dcf8d3b5c6e0b01-Paper.pdf.
- [2] Michael Osborne et al. "Bayesian Quadrature for Ratios". In: Proceedings of the Fifteenth International Conference on Artificial Intelligence and Statistics. Ed. by Neil D. Lawrence and Mark Girolami. Vol. 22. Proceedings of Machine Learning Research. La Palma, Canary Islands: PMLR, Apr. 2012, pp. 832–840. URL: https://proceedings.mlr.press/v22/osborne12.html.
- [3] Roman Garnett, Michael A. Osborne, and Philipp Hennig. Active Learning of Linear Embeddings for Gaussian Processes. 2013. arXiv: 1310.6740 [stat.ML]. URL: https://arxiv.org/abs/1310.6740.
- [4] Philipp Hennig. "Fast Probabilistic Optimization from Noisy Gradients". In: *Proceedings* of the 30th International Conference on Machine Learning. Ed. by Sanjoy Dasgupta and David McAllester. Vol. 28. Proceedings of Machine Learning Research 1. Atlanta, Georgia, USA: PMLR, June 2013, pp. 62–70. URL: https://proceedings.mlr.press/v28/hennig13.html.
- [5] David Barber. On solving Ordinary Differential Equations using Gaussian Processes. 2014. arXiv: 1408.3807 [stat.ME]. URL: https://arxiv.org/abs/1408.3807.
- [6] Tom Gunter, Michael A. Osborne, Roman Garnett, Philipp Hennig, and Stephen J. Roberts. Sampling for Inference in Probabilistic Models with Fast Bayesian Quadrature. 2014. arXiv: 1411.0439 [stat.ML]. URL: https://arxiv.org/abs/1411.0439.
- [7] Michael Schober, David Duvenaud, and Philipp Hennig. *Probabilistic ODE Solvers with Runge-Kutta Means*. 2014. arXiv: 1406.2582 [stat.ML]. URL: https://arxiv.org/abs/1406.2582.
- [8] Sebastian Dorn and Torsten A. Enßlin. "Stochastic determination of matrix determinants". In: *Phys. Rev. E* 92 (1 July 2015), p. 013302. DOI: 10.1103/PhysRevE.92.013302. URL: https://link.aps.org/doi/10.1103/PhysRevE.92.013302.
- [9] Maren Mahsereci and Philipp Hennig. "Probabilistic Line Searches for Stochastic Optimization". In: Advances in Neural Information Processing Systems. Ed. by C. Cortes, N. Lawrence, D. Lee, M. Sugiyama, and R. Garnett. Vol. 28. Curran Associates, Inc., 2015. URL: https://proceedings.neurips.cc/paper_files/paper/2015/file/812b4ba287f5ee0bc9d43bbf5bbe87fb-Paper.pdf.
- [10] Simon Bartels and Philipp Hennig. "Probabilistic Approximate Least-Squares". In: Proceedings of the 19th International Conference on Artificial Intelligence and Statistics. Ed. by Arthur Gretton and Christian C. Robert. Vol. 51. Proceedings of Machine Learning Research. Cadiz, Spain: PMLR, May 2016, pp. 676–684. URL: https://proceedings.mlr.press/v51/bartels16.html.
- [11] Oksana A. Chkrebtii, David A. Campbell, Ben Calderhead, and Mark A. Girolami. Bayesian Solution Uncertainty Quantification for Differential Equations. 2016. arXiv: 1306.2365 [stat.ME]. URL: https://arxiv.org/abs/1306.2365.

- [12] Motonobu Kanagawa, Bharath K. Sriperumbudur, and Kenji Fukumizu. "Convergence guarantees for kernel-based quadrature rules in misspecified settings". In: Advances in Neural Information Processing Systems. Ed. by D. Lee, M. Sugiyama, U. Luxburg, I. Guyon, and R. Garnett. Vol. 29. Curran Associates, Inc., 2016. URL: https://proceedings.neurips.cc/paper_files/paper/2016/file/81c650caac28cdefce4de5ddc18befa0-Paper.pdf.
- [13] Jack Fitzsimons, Kurt Cutajar, Michael Osborne, Stephen Roberts, and Maurizio Filippone. Bayesian Inference of Log Determinants. 2017. arXiv: 1704.01445 [stat.ML]. URL: https://arxiv.org/abs/1704.01445.
- [14] Toni Karvonen and Simo Särkkä. "Classical quadrature rules via Gaussian processes". In: 2017 IEEE 27th International Workshop on Machine Learning for Signal Processing (MLSP). 2017, pp. 1-6. DOI: 10.1109/MLSP.2017.8168195. URL: https://ieeexplore.ieee.org/stamp/stamp.jsp?tp=&arnumber=8168195.
- [15] Michael Schober, Simo Särkkä, and Philipp Hennig. A probabilistic model for the numerical solution of initial value problems. 2017. arXiv: 1610.05261 [math.NA]. URL: https://arxiv.org/abs/1610.05261.
- [16] Hans Kersting and Philipp Hennig. Active Uncertainty Calibration in Bayesian ODE Solvers. 2018. arXiv: 1605.03364 [cs.NA]. URL: https://arxiv.org/abs/1605.03364.
- [17] Xiaoyue Xi, François-Xavier Briol, and Mark Girolami. Bayesian Quadrature for Multiple Related Integrals. 2018. arXiv: 1801.04153 [stat.CO]. URL: https://arxiv.org/abs/1801.04153.
- [18] Jonathan Wenger and Philipp Hennig. *Probabilistic Linear Solvers for Machine Learning*. 2020. arXiv: 2010.09691 [cs.LG]. URL: https://arxiv.org/abs/2010.09691.
- [19] Jon Cockayne, Ilse C. F. Ipsen, Chris J. Oates, and Tim W. Reid. *Probabilistic Iterative Methods for Linear Systems*. 2021. arXiv: 2012.12615 [stat.ME]. URL: https://arxiv.org/abs/2012.12615.
- [20] Tim W. Reid, Ilse C. F. Ipsen, Jon Cockayne, and Chris J. Oates. BayesCG As An Uncertainty Aware Version of CG. 2022. arXiv: 2008.03225 [math.NA]. URL: https://arxiv.org/abs/2008.03225.

3 Video Recording and Submission

Video Recording For the presentation, you will record yourself and then send us the link to the recording. Here are the steps you should take:

- 1. Open Zoom and start your "Personal Meeting". Be sure to turn on your microphone.
- 2. Click "Record" and then "Record to the Cloud".
- 3. Introduce yourself by name. Then go ahead and present for 10-15 minutes.
- 4. Extremely important: Now click "End the Meeting". Your recording will be uploaded to the cloud and processed.
- 5. Go to https://cmu.zoom.us/recording and wait (~ 15 minutes) for your recording to finish processing.
- 6. Click the "Share..." button on the left of the recording, then click "Copy Sharing Information" and paste the clipboard text into Gradescope.

Submitting to Gradescope You will submit your presentation video and slides to Gradescope.

- 7. Open the HW624 assignment in Gradescope.
- 8. Paste the video recording information that you copy/pasted above into the free-text field on the assignment.
- 9. Then upload your slides as a PDF on the file-upload question.
- 10. In Gradescope, save and submit this assignment.