University of Göttingen Seminar on numerical methods for sampling and SDEs Summer semester 2025

Prof. Dr. Anja Sturm and Dr. Alex Lewis

Version: April 8, 2025

In this seminar we consider numerical methods for sampling probability distributions and estimating expectations, as well as for approximating stochastic differential equations (SDE). Sampling from probability distributions and computing integrals with respect to them has important applications in many areas, such as for calculating posterior distributions in Bayesian statistics, determining stationary states in statistical physics and molecular dynamics, and stochastic optimization and deep learning algorithms.

In the seminar, we shall focus on Markov chain Monte Carlo techniques for sampling. Here, a suitable Markov chain is chosen that converges to a target probability distribution, regardless of the initial state of the chain. In order to employ Markov chain convergence for efficient sampling from the stationary distribution or for numerical integration with respect to this distribution, it is essential to select a Markov chain that is easy to simulate and converges quickly to the stationary distribution. Therefore, we will investigate the choice of the Markov chain as well as the the rate of convergence to the stationary distribution.

We will consider sampling from both discrete and continuous distributions, which entails the study of Markov processes with discrete (the focus of [LPW]) and continuous (the focus of [BE]) state spaces. In the latter case, we draw our attention to diffusion processes that solve SDEs, such as the Langevin diffusion, whose stationary distribution is the target distribution. In this context, the numerical approximation of these SDEs by a time discretization, which is again usually a Markov chain, plays a role and will also be studied in this seminar, see [MT] and [C].

Times: The seminar will take place on Tuesdays at 14:15-15:45 in the seminar room of the Institute of Mathematical Stochastics (SR IMS 5.101). There will be a first meeting on

April 15, 2025 at 14:15

in the seminar room of the Institute of Mathematical Stochastics. A tentative list of presentation topics can be found below. You will be asked to submit a list of three seminar topics that you are interested in alongside your background in probability theory and stochastic processes. After this meeting topics will be distributed. If you cannot attend the meeting or if you have further questions please contact me directly at

asturm@math.uni-goettingen.de

Prerequisites: For participation in the seminar knowledge of probability theory and stochastic processes is needed such as is acquired in the lecture *Mass- und Wahr-scheinlichkeitstheorie* and *Stochastik*" as well as the introductory lecture of the cycle *Stochastic Processes* or equivalent. The seminar is meant to accompany the second part of this cycle (which takes place in the summer semester Mondays and Thursdays from 10-12).

Language: The language of the seminar will be English.

Literature: The main sources for the seminar are the following:

- [BE] Markov Chain Monte Carlo methods, N. Bou-Rabee and A. Eberle, Lecture notes, Version of January 31, 2024.
- [LPW] Markov chains and mixing times, D. Levin, Y. Peres and E. Wilmer, American Mathematical Society, 2008. Choose second edition!
 - [C] Log-concave sampling, S. Chewi, Lecture notes, Version of November 23, 2024.
 - [MT] Stochastic Numerics for Mathematical Physics, G. Milstein and M. Tretyakov, Springer 2021. Choose second edition!
 - [G] Multilevel Monte Carlo Path Simulation, M.B. Giles, Operations Research 56 (3), 607-617

Tentative list of presentations:

- 1. Total variation distance, coupling, mixing times and conductance [BE]1.3
- 2. Eigenvalue and conductance lower bounds on mixing times [BE] 1.3 and 1.4
- 3. Couplings of Markov processes and upper bounds for mixing times and convergence rates [BE] 2.1
- 4. Wasserstein distance and couplings [BE] 2.2
- 5. Wasserstein contractions and geometric convergence [BE] 2.3
- 6. Convergence of the Gibbs sampler [BE] 2.4
- 7. Couplings and convergence bounds for diffusions [BE] 2.6, see also 4.1 in [C]
- 8. General Markov processes and f-divergences [BE] 3 and 3.1 until page 73
- 9. Relaxation times, mixing times and functional inequalities [BE] 3.1 from page 73
- 10. Poincaré inequalities, L^2 relaxation and conductance [BE] 3.2
- 11. Hamiltonian Monte Carlo [C] 5.2 and [BE] 5.3
- 12. Mean Square Convergence of SDEs [MT] 1.1.1, 1.1.2 and 1.1.5
- 13. Multilevel Monte Carlo [G]

General information on seminars: Before your seminar talk please make an appointment with me which should take place approximately one week before your presentation. Before this meeting you have read and worked through the material on which your presentation will be based. You should have come up with a structure for your talk and you should be ready to ask questions on details that still need to be clarified.

In structuring your talk keep in mind that you will generally not be able to present every detail of the source text. Preference should be given to presenting results and proofs as well as your own thoughts and ideas such as worked out examples and pictures that add to the intuitive understanding of the subject. Sometimes it is sufficient and in fact more instructive to give only an overview of the idea of the proof and to skip technical and lengthy calculations in the presentation (which you yourself should have gone through nonetheless!).

You will need to make your own notes from the source text. Hereby it is crucial to think about which parts of your notes you will put on the black board. (In order to gauge how many pages of hand written notes you can cover on the board think about how many you produce during a 90 minute lecture. This is most definitely an upper bound.) Practicing the talk beforehand -preferably using a black board- is also recommended in order to check that your timing is right.

Some more pointers regarding a good seminar talk: In order to give a good seminar talk you must have understood and thought through the material very well yourself and you should be able to place it into the larger context (of the seminar). Only then can you motivate the topic and explain the results well to your audience. You should be able answer questions on details of your presentation precisely or you should know that a precise answer would go beyond the scope of the seminar. This means that you need to fill in little gaps and unclear points in the proofs of the source text as needed. Sometimes presenting the solutions to exercises of the text are helpful. However, if something has remained unclear in the end it is most constructive to say so. This gives us the chance to clarify this point for everybody.

Naturally, your talk needs to be well structured (in general and also on the blackboard) in order to be comprehensible. You should start your talk by giving us a short overview over the main topic and goals of the talk as well as over the structure of the talk. You need to introduce all the notation and concepts that you use (maybe only briefly if they have been encountered before). I strongly recommend that you prepare a short handout with the most important notation, definitions and results. You can also add reminders of previous notation and results to your handout that you may only review orally. (Nonetheless, the main results of your talk should be written down in precise form on the black board.)