Lecture Notes for "Stochastic Modeling and Computations"

M. Chertkov (lecturer), S. Belan and V. Parfeneyv (recitation instructors)

M.Sc. and Ph.D. level course at Skoltech

Moscow, March 28 - May 28, 2016

https://sites.google.com/site/mchertkov/courses

The course offers a soft and self-contained introduction to modern applied probability covering theory and application of stochastic models. Emphasis is placed on intuitive explanations of the theoretical concepts, such as random walks, law of large numbers, Markov processes, reversibility, sampling, etc., supplemented by practical/computational implementations of basic algorithms. In the second part of the course, the focus shifts from general concepts and algorithms per se to their applications in science and engineering with examples, aiming to illustrate the models and make the methods of solution, originating from physics, chemistry, machine learning, control and operations research, clear.

Brief Description. Structure. Requirements.

This course is recommended to M.Sc. and Ph.D. students planning to work on the subjects containing elements of uncertainty, irregularity or what is also called 'stochasticity'. The 'stochastic' subjects are prevalent in natural sciences (physics, chemistry, biology) or engineering disciplines (electrical-, mechanical-, chemical-, industrial-, etc). The course introduces students to modeling and computational concepts, approaches, methods and algorithms which require dealing with stochasticity and uncertainty.

This is a general course recommended to Energy, IT and other Skoltech students. The course is recommended as a core course for students who specializes in computations. It can be chosen as elective by students who use computations and algorithms in their work, however not as the prime focus.

There will be 12 lectures, 11 recitations, 2 homework assignments, a special recitation explaining homework solutions, journal club presentations+reports and, finally, the exam.

Lectures. Lecture notes are to be provided (online) before the actual lecture. Lecturer will mainly be using white-board, sometimes supplemented by computer demonstrations in IJulia.

Recitations. Recitation notes are to be provided (online) after the actual recitations. Recitations will be lead by two instructors (alternating) with the use of whiteboard and computer demonstrations (ijulia notebooks). Students in the class will be called to lead solution of some problems.

Homework assignments. Two assignments will be given. Each homework will consist of ~ 6 problems, including multiple ($\sim 2-4$) sub-problems of varying difficulty. First homework will be distributed in the beginning of the first week and will be collected by Wed, Apr 20, 11:59pm Moscow time. Second homework will be distributed in the beginning of the 4th week and will be collected by Wed, May 18, 11:59pm Moscow time. Problems in the homework will be similar in principle, but different in details from these discussed in lectures and recitations (prior to the homework distribution). Solutions from the homework will be discussed at the recitations after the homework collection. It is encouraged to use electronic formats (latex and/or ipython/ijulia) for the homework reports. Submission of the homework(s) is electronic only.

Each student will be required to choose a subject for **journal club presentation and report**. List of suggested subjects will be provided at the first lecture. In terms of picking a subject – the policy is 'first come first served'. The list of suggested subjects is not meant to be complete or exclusive. In particular, the students are encouraged to suggest additional subjects linked to the course material and possibly related to their own research focus/interest. All additional subjects should be discussed with and approved by the lecturer before Apr 28. Subjects should be presented during the presentation session (tentatively) scheduled for May 24. Each presentation is 20 mins. All reports should be submitted by May 28, 11:59pm. Reports are individual, should be at least 10 pages but not longer that 20 pages. Presentations and reports will be graded together.

A written **exam** will be administered. The exam will include 3-4 problems similar to these discussed at the recitations and contained in the homework. Format of the exam (in class or take home) will be decided at later time depending on how the class progresses.

The three **books** referred extensively in lectures, recitations and homework are [1–3]. In addition, many relevant reviews and papers available online are cite in the lecture notes. Students may also find it useful to check [4–7] for related (but often alternative) explanations. (A number of hard copies of all the aforementioned books are available at the edu@skoltech library.

On pre-requisites and requirements. All necessary concepts from statistics, probability theory and statistical mechanics will be introduced in the course self-consistently (no formal pre-requisites in these disciplines are required). However, solid preparation in practical math (ability to solve problems in linear algebra, calculus, and differential equations) will be required from anybody taking this course.

We will mainly be using in lectures and recitations for computations and illustrations Julia http://julialang.org/under IJulia/Ipython-notebook environment https://github.com/JuliaLang/IJulia.jl. Students are encouraged

to self-learn and use Julia and IJulia. However, computations (e.g. for homework and exam) in any other (reasonably common and transparent) programming languages will also be accepted.

Grading:

- Homework 35%
- Exam 35%
- Journal Club Presentation & Report 20%
- Participation 10%

(Tentative) Schedule

Mon, Tue, Thu 9:00–10:30 + 10:30–12:00 (two periods 1.5 hours each) l=lecture, r=recitation

First week:

March 28, Mon

9:00–10:30 1#1 Random Variables: Characterization and Description

10:30-12:00 free period

March 29, Tue

9:00–10:30 1#2 Random Variables: Operations & Transformations

10:30-12:00 free period

March 31, Thu

9:00–10:30 r#1 Moments/Averages/Cumulants/Generation Function on Examples

10:30–12:00 r#2 Example of Gaussian Variables: Matrix Inversion, Normalization, Moments

Second week:

Apr 4, Mon

9:00–10:30 1#3 Information-Theoretic View on Randomness

10:30–12:00 r#3 Entropy, Mutual Information and Probabilistic Inequalities on Example (Communication over Noisy Channel)

Apr 5, Tue

9:00–10:30 1#4 Markov Chains [discrete space, discrete time]

10:30–12:00 1#5 From Bernoulli Processes to Poisson Processes [discrete space, discrete & continuous time]

Apr 7, Thu

free day

Third week:

Apr 11, Mon

9:00–10:30 r#4 Markov Chains: Detailed Balance. Mixing time.

10:30–12:00 r#5 Examples of Bernoulli & Poisson Processes

Apr 12, Tue

9:00–10:30 free period

10:30–12:00 1#6 Monte-Carlo Algorithms: General Concepts and Direct Sampling

Apr 14, Thu

9:00-10:30 1#7 Markov-Chain Monte-Carlo

10:30-12:00 r#6 MC and MCMC on example of the Ising model

Fourth week:

Apr 18, Mon

9:00-10:30 1#8 Exact & Approximate Inference

10:30–12:00 1#9 Inference & Learning with Belief Propagation

Apr 19, Tue

9:00–10:30 r#7 Inference & Learning on Trees

10:30-12:00 1#10 Space-time Continuous Stochastic Processes

Apr 21, Thu

free day

Fifth week:

Apr 25, Mon

9:00-10:30 r#8 Homogeneous and Forced Brownian Motion

10:30-12:00 r#9 First Passage Problem and Effects of Boundaries

Apr 26, Tue
9:00–10:30 free period
10:30-12:00 l#11 Queuing Systems
Apr 28, Thu
9:00–10:30 free period 10:30–12:00 l#12 Markov Decision Processes & Stochastic Optimal Control

Sixth week:

May 16, Mon
9:00–10:30 r#10 Queuing Systems
10:30–12:00 r#11 Markov Decision Processes & Stochastic Optimal Control
May 17, Tue
free day
May 19, Thu
9:00–10:30 solution of homework (#1 & #2)
10:30–12:00 consultation for exam (questions-answers with TAs)
Seventh week:

May 23, Mon nothing is scheduled (reserve) May 24, Tue 9:00–12:00 & 14:00-17:00 Project presentations May 26, Thu 9:00-13:00 exam

IV. PROJECTS: (INCOMPLETE) POOL OF OPTIONS

1. Large Deviation for Multiplicative Processes

Stretching and Rotations of clouds and particles, ordered exponentials, long time statistics of Lyapunov exponents. Cramer/entropy function. http://arxiv.org/abs/cond-mat/0105199

2. The Noisy Channel Coding (Shannon) Theorem

Sec. 9.3 and 10 of [2]

3. Compressed Sensing and its many uses (How l_1 norm promotes sparcity?)

Pick a review from the extended list available at https://en.wikipedia.org/wiki/Compressed_sensing An original option is http://statweb.stanford.edu/~candes/papers/DecodingLP.pdf

4. Slice Sampling MCMC

See https://en.wikipedia.org/wiki/Slice_sampling. Recommended review is Neal, Radford M. (2003). "Slice Sampling". Annals of Statistics 31 (3): 705767.

5. Simulated Annealing Sampling

Important idea and algorithm allowing to explore seriously non-convex problems – rugged landscape with multiple valleys, saddle points, minima and peaks. The original paper is Kirkpatrick, S.; Gelatt Jr, C. D.; Vecchi, M. P. (1983). "Optimization by Simulated Annealing". Science 220 (4598): 671680. See also https://en.wikipedia.org/wiki/Simulated_annealing and references there in.

6. Hamiltonian MCMC

MCMC which is capable to accelerate sampling by adding additional degrees of freedom - related to controlled inertia/momenta expressed through a Hamiltonian description (from physics) — thus the name. Recommended review http://www.cs.utoronto.ca/~radford/ftp/ham-mcmc.pdf

7. Irreversible Monte Carlo algorithms for efficient sampling

The original paper is http://arxiv.org/abs/0809.0916.

8. Warm Algorithm in Classical and Quantum Statistical Physics

The original paper is http://scholarworks.umass.edu/cgi/viewcontent.cgi?article=2194&context=physics_faculty_pubs. See also http://wiki.phys.ethz.ch/quantumsimulations/_media/lecture_101007.pdf.

9. Gillespie algorithm

Sampling from stochastic equations (Langevin type) which proceeds by jumps. See the original paper Gillespie, Daniel T. (1977). "Exact Stochastic Simulation of Coupled Chemical Reactions". The Journal of Physical Chemistry 81 (25): 23402361 and also check https://en.wikipedia.org/wiki/Gillespie_algorithm.

10. Sequential Monte Carlo for Importance Sampling & Inference

Recommended paper https://www.irisa.fr/aspi/legland/ensta/ref/doucet00b.pdf.

11. Ising models and Other Graphical Models in Image Analysis

Recommended tutorial https://www.math.ntnu.no/~joeid/TMA4250/image_ana.pdf.

12. Efficient Exact Inference in Planar Ising Model

Recommended paper http://arxiv.org/pdf/0810.4401.pdf.

13. Stochastic Resonances

Curious physics phenomena important in optics & communications which explains how noise/randomness allows to amplify signal and observe what otherwise would be difficult to detect. Recommended paper is Benzi, R.; Sutera, A.; and Vulpiani, A. "The Mechanism of Stochastic Resonance." J. Phys. A 14, L453-L457, 1981.

14. Decoding of Low Density Parity Check Codes

Section 47 of [2].

15. Analytic and Algorithmic Solution of Satisfiability Problem

The original paper is http://cacs.usc.edu/education/cs653/Mezard-RSAT-Science02.pdf See the book of Mezard and Montanari + papers/reviews of Parisi, Mezard and Zechina.

16. Neural Network Learning

Part V of [2].

17. Jackson Networks of Queues

Recommended paper is Kelly, F. P. (Jun 1976). "Networks of Queues". Advances in Applied Probability 8 (2): 416432. See alos https://en.wikipedia.org/wiki/Jackson_network and references there in.

18. Path Integral Control & Reinforcement Learning

Recommended review http://www.snn.ru.nl/~bertk/kappen_granada2006.pdf

- [1] N. van Kampen, *Stochastic Processes in Physics and Chemistry (Third Edition)*, third edition ed. Amsterdam: Elsevier, 2007. [Online]. Available: http://www.sciencedirect.com/science/article/pii/B9780444529657500003
- [2] D. J. C. Mackay, *Information theory, inference, and learning algorithms*. Cambridge: Cambridge University Press, 2003. [Online]. Available: http://www.inference.phy.cam.ac.uk/itprnn/book.html
- [3] C. Moore and S. Mertens, *The Nature of Computation*. New York, NY, USA: Oxford University Press, Inc., 2011. [Online]. Available: http://www.nature-of-computation.org/
- [4] H. E. Taylor and S. Karlin, *An Introduction to Stochastic Modeling*, 3rd ed. Academic Press, Feb. 1998. [Online]. Available: http://www.ime.usp.br/~fmachado/MAE5709/KarlinTaylorIntrodStochModeling.pdf
- [5] C. W. Gardiner, *Handbook of stochastic methods for physics, chemistry and the natural sciences*, 3rd ed., ser. Springer Series in Synergetics. Berlin: Springer-Verlag, 2004, vol. 13.
- [6] B. L. Nelson, Stochastic modeling analysis and simulation (reprint from 1995). Dover Publications, 2002.
- [7] E. Cinclar, *Introduction to stochastic processes*. Prentice-Hall, 1975. [Online]. Available: http://gso.gbv.de/DB=2.1/CMD?ACT= SRCHA&SRT=YOP&IKT=1016&TRM=ppn+021423008&sourceid=fbw_bibsonomy
- [8] T. Richardson and R. Urbanke, Modern Coding Theory. Cambridge University Press, 2008.
- [9] J. S. Yedidia, W. T. Freeman, and Y. Weiss, "Constructing free-energy approximations and generalized belief propagation algorithms," *Information Theory, IEEE Transactions on*, vol. 51, no. 7, pp. 2282–2312, 2005.
- [10] M. J. Wainwright and M. I. Jordan, "Graphical models, exponential families, and variational inference," *Found. Trends Mach. Learn.*, vol. 1, no. 1-2, pp. 1–305, Jan. 2008. [Online]. Available: https://www.eecs.berkeley.edu/~wainwrig/Papers/WaiJor08_FTML.pdf