

Simulation and analysis of stochastic processes II

Literature seminar

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1 Introduction

Stochastic processes are relevant to understand all microscopic phenomena in natural sciences, including quantum processes, molecular dynamics and motion of proteins in the cell. They are also useful to quantitatively model many macroscopic processes, such as stock price evolution, evolutionary dynamics and climate changes. In this seminar each of you is assigned a research paper in which a method for the analysis or for the sampling of stochastic processes is described. Starting from this publication, you will become acquainted to the method, and at the end of the semester you will present the method to the other participants of the course. Other purposes of the course are: practice reading scientific literature, practice oral presentations and writing scientific texts.

2 Requirements

- **First meeting with your supervisor.** For this meeting, read the literature, prepare a list of issues which you did not understand or which you want to discuss with your supervisor. Also, you are expected to have an outline of your oral presentation and the paper summary ready to discuss at this meeting.
- **Second meeting with your supervisor.** For this meeting, have the presentation (almost) ready.
- **Oral presentation of your assigned paper.** About 30 minutes presentation + 10-15 minutes discussion. Whether you use the blackboard, a beamer and/or other means of presentation is up to you. I provide a beamer and a laptop (presentation in pdf format), but you can also bring in your own laptop.
- **Written summary of your assigned paper.** About 1 to 3 pages. The goal is to write a summary which can be uploaded to papercore. The summaries will be distributed among the participants of the course.

<http://www.papercore.org/>

"Papercore is a public read-write database, which aims at helping scientists to cope with this development. Papercore collects summaries of scientific papers, in particular in physics, where this database is optimized to. Note that a summary is not just an abstract: A summary should contain the core information of a paper, including a little introduction, basic definitions, outline of methods and key results of a paper, such that a specialist in the field does not have to look into the paper anymore, basically. The rule of thumb is that a summary should be 1/10 of the length of the corresponding paper, the compression factor is automatically computed by Papercore for each summary."

3 How to read a paper

- Structure of research papers:
<http://www.cbcb.umd.edu/confcour/CMSC838K-materials/how-to-read-a-paper.pdf>
- The "three-pass approach" to reading a paper:
http://www.cs.stonybrook.edu/~vyas/teaching/CSE_592/Fall12/papers/howtoread.pdf
- Animated tutorial on reading scientific papers:
<http://www.lib.purdue.edu/phys/assets/SciPaperTutorial.swf>

4 Projects

4.1 Classics: Markov-Chain-Monte-Carlo simulations

Supervisor: Guillermo Pérez-Hernández (guille.perez@fu-berlin.de)

Student: Marcel Schilling

N. Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, E. Teller

"Equation of State Calculations By Fast Computing Machines"

Journal of Chemical Physics, 1953, **21**, 1087-1092

W. K. Hastings

"Monte-carlo Sampling Methods Using Markov Chains and Their Applications "

Biometrika, 1970, **57**, p. 97

4.2 Classics: Information theory and statistical mechanics

Supervisor: Benjamin Trendelkamp-Schroer (benjamin.trendelkamp-schroer@fu-berlin.de)

Student: Han Cheng Lie

E.T. Jaynes

"Information Theory and Statistical Mechanics"

Physical Review, 1957, **106**, pp. 620-630

4.3 Spectral clustering

Supervisor: Jan-Hendrik Prinz (jan.prinz@gmx.de)

Student: Erik Kadikowski

U. von Luxburg

"A tutorial on spectral clustering Statistics and Computing"

Statistics and Computing, 2007, **17**, pp. 395-416

4.4 Markov state models for conformational dynamics

Supervisor: Jan-Hendrik Prinz (jan.prinz@gmx.de)

Student: Markus Mittnenzweig

J.-H. Prinz, H. Wu, M. Sarich, B. Keller, M. Fischbach, M. Held, J.D. Chodera, C. Schütte, F. Noé

"Markov model and molecular kinetics: generation and validation"

Journal of Chemical Physics, 2011, **134**, p. 174105

4.5 Transition path theory

Supervisor: Bettina Keller (bettina.keller@fu-berlin.de)

Student: Lara Kuhnke

E. Weinan, E. Vanden-Eijnden

"Transition Path Theory and Path-Finding Algorithms for the Study of Rare Events"

Annual Reviews of Physical Chemistry, 2010, **61**, pp. 391-421

4.6 Markov models and dynamical fingerprints

not taken

4.7 Hidden Markov models

not taken

4.8 Likelihood functions for the analysis of single-molecule experiments

Supervisor: Bettina Keller (bettina.keller@fu-berlin.de)

Student: Franziska Kreuchwig

I.V. Gopich, A. Szabo

Single-molecule FRET with diffusion and conformational dynamics

Journal Of Physical Chemistry B, 2007, **111**, pp. 12925-12932

4.9 Coarse graining of master equations

Supervisor: Bettina Keller (bettina.keller@fu-berlin.de)

Student: Victor Mireles

S. Pigolotti, A. Vulpiani

Coarse graining of master equations with fast and slow states

Journal Of Chemical Physics, 2008, **128**, pp. 154114

4.10 Localization and tracking of individual fluorescent particles in light microscopes

Supervisor: Frank Noé (frank.noe@fu-berlin.de)

Student: Christoph Schaller

R. E. Thompson, D. R. Larson, W. W. Webb

Precise Nanometer Localization Analysis for Individual Fluorescent Probes

Biophysical Journal, 2002, **62**, pp. 2775-2783

and related literature

5 Schedule

	Date	Lecture plan		
01	17 Oct. 2012	Introduction		
02	24 Oct. 2012			
03	31 Oct. 2012			
04	07 Nov. 2012	1st meeting		
05	14 Nov. 2012	with supervisors		
06	21 Nov. 2012			
07	28 Nov. 2012			
08	05 Dec. 2012	2nd meeting		
09	12 Dec. 2012	with supervisors		
10	19 Dec. 2012	Presentations	M. Mittnenzweig	C. Schaller
		Christmas break		
11	09 Jan. 2013	2nd meeting		
12	16 Jan. 2013	with supervisors		
13	23 Jan. 2013	Presentations	H. C. Lie	V. Mireles
14	30 Jan. 2013	Presentations	L. Kuhnke	E. Kadikowski
15	06 Feb. 2013	Presentations	F. Kreuchwig	M. Schilling
16	13 Feb. 2013	Deadline for summaries		