RSCAM Group Projects
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These group projects are meant to open-ended and self-directed. Each group will need to acquire and evaluate literature, explore relevant questions, formulate and prepare numerical experiments, prepare and present a high quality short talk on their work and prepare a high quality report. The initials next to each group project title are those of one of the tutors and indicate the person who has proposed the work. You should not regard these persons as directing your project work - you need to organise your own work amongst yourselves. However you should feel to contact the proposer (or any of the tutors, for that matter) to get suggestions as you perform your work, for example if you hit an impasse.

GP1 Multilevel Monte Carlo for SDEs [DH]

In 2008, Giles published the idea of Multilevel Monte Carlo for improving the efficiency of SDE simulations. This project will involve (a) understanding the basic method, (b) implementing it for Euler-Maruyama and (c) testing it in the context of financial option pricing.

References:
[1] M.B. Giles. Multi-level Monte Carlo path simulation. *Operations Research*, 56(3):607-617, 2008. https://doi.org/10.1287/opre.1070.0496

[2] D. J. Higham, An introduction to multilevel Monte Carlo for option valuation. International Journal of Computer Mathematics (Special Issue on Computational Methods in Finance) **92**, 2347–2360, 2015. https://doi.org/10.1080/00207160.2015.1077236

[3] E.H. Müller , R. Scheichl and T. Shardlow, Improving multilevel Monte Carlo for stochastic differential equations with application to the Langevin equation, Proc. Roy. Soc. A **471**, 2014. https://doi.org/10.1098/rspa.2014.0679

GP2 Mean Hitting Times for SDEs [DH]

This project will look at the Euler-Maruyama plus Monte Carlo for estimating the mean hitting time of an SDE. After performing initial tests, the key task will be to investigate the use of adaptive timestepping.

References
[1] R. Mannella. A gentle introduction to the integration of stochastic differential equations. *Stochastic Processes in Physics, Chemistry, and Biology*, J. A. Freund and T. Poshel, eds., Springer-Verlag, 2000, pp. 353–364. (see relevant discussion of Mean Hitting Times)

[2] *Lecture notes to be provided by Prof. Higham.*

GP3 Sampling methods based on accelerated Brownian dynamics [TP]

In the lab, we have explored the relevance of weak and ergodic accuracy of numerical methods. Here we focus on another highly important feature: the speed of convergence to

equilibrium. In particular, we concentrate on a recent paper introducing a modification of the dynamics that accelerates this convergence. As nothing comes for free the approximation of the new system is more challenging. The goal of the project is to rise to the challenge.

References:
[1] B.Leimkuhler and C.Matthews, Rational construction of stochastic numerical methods for molecular sampling, *Applied Mathematics Research eXpress*, 2013, pp.~34–56, 2012. https://doi.org/10.1093/amrx/abs010 (see also Ch 7 in the *Molecular Dynamics* book used in class).

[2] A.Abdulle, G.Vilmart, and K.C. Zygalakis, High order numerical approximation of the invariant measure of ergodic SDEs, *SIAM J. Numer. Anal.*, 52 pp.~1600–1622, 2014. https://doi.org/10.1137/130935616

[3] A.Abdulle, G.A. Pavliotis, and G.Vilmart, Accelerated convergence to equilibrium and reduced asymptotic variance for Langevin dynamics using Stratonovich perturbations, *Comptes Rendus Mathematique* **357**, pp.~349–354, 2019. https://doi.org/10.1016/j.crma.2019.04.008

GP4 Ensemble sampling methods [BL]

In RSCAM we have studied methods for sampling based on propagating a single stochastic path. Alternatively one can consider having a collection of copies (replicas, particles, walkers) of the system which either individually or collectively facilitate the sampling of the target distribution. This idea becomes interesting when the walkers work together, since the collective information can enhance the convergence to equilibrium. One important concept here is 'affine invariance'. This is a challenging topic which may bring in some connections to ‘interacting particle systems’ and convergence of measures in the large particle number limit, however there is room for numerical study as well. See for example the code linked in ref. [1].

References:
[1] Ensemble preconditioning for Markov chain Monte Carlo simulation, Benedict Leimkuhler, Charles Matthews, and Jonathan Weare, *J. Stat. Comput.*, 28, 277, 2018. https://doi.org/10.1007/s11222-017-9730-1
https://bitbucket.org/c_matthews/ensembleqn/src/master/
[2] Ensemble samplers with affine invariance, Jonathan Goodman and Jonathan Weare, *Comms. in Appl. Math.s and Comput. Sci.*, 5, 65-80, 2010. https://msp.org/camcos/2010/5-1/camcos-v5-n1-p04-p.pdf
[3] Affine invariant interacting Langevin dynamics for Bayesian inference, A. Garbuno-Inigo, N. Nuesken, and S. Reich, 2019. https://arxiv.org/abs/1912.02859
[4] Interacting Langevin Diffusions: Gradient Structure and Ensemble Kalman Sampler, A. Garbuno-Inigo, F. Hoffman, W. Li, and A. Stuart. SIAM App. Dyn. Sys., 19(1), 412–441, 2020. https://epubs.siam.org/doi/abs/10.1137/19M1251655
with regard to [2.4] see also: https://arxiv.org/pdf/1908.10890v1.pdf

GP5 Role of Metropolisation in Sampling Schemes [BL]

We have seen methods based on SDEs (e.g. Langevin) as well as other schemes based on the Metropolis Hastings acceptance test (e.g. MALA). You could ask why one would consider SDE methods since they introduce bias which is not present in MH methods.

However, there are many important consequences of MH tests. First, we throw out a lot of samples. Second, the use of metropolis tests can slow convergence to the target distribution. Third, the MH test costs something (usually equivalent to an additional energy or force evaluation). Thus it is not clear if, in practice, say, MALA is a better choice than un-metropolized Langevin dynamics. This project can explore that issue.

References:
[1] High-dimensional Bayesian inference via the Unadjusted Langevin Algorithm, Alain Durmus and Eric Moulines, 2018. https://arxiv.org/abs/1605.01559
[2] Exponential convergence of Langevin distributions and their discrete approximations, Gareth Roberts and Richard Tweedie, *Bernoulli*, 2, 341-363, 1996. https://projecteuclid.org/download/pdf_1/euclid.bj/1178291835
[3] Langevin diffusions and Metropolis-Hastings algorithms, Gareth Roberts and Osnat Stramer, Methodology And Computing In Applied Probability 4, 337–357. 2002. https://link.springer.com/article/10.1023/A:1023562417138

GP6 Efficient molecular dynamics with high accuracy [BL]

As we saw, molecular dynamics relies on the solution of differential equations (or stochastic differential equations) involving many degrees of freedom. The forces of interaction in molecular dynamics are normally expensive to compute which favours the use of low-order approximation methods which only require one force evaluation per timestep. On the other hand high order is sometimes desirable. Methods like the Takahashi-Imada scheme and Rowland's method mentioned in class can allow higher order integration by using second derivative information. Are such high order methods justified by practical experiments?

References:
[1] A numerical algorithm for Hamiltonian systems, G. Rowlands, J. Comput. Phys., 97 (1991), pp. 235–239.
[2] Explicit Symplectic Integrators Using Hessian--Vector Products, M. A. López-Marcos, J. M. Sanz-Serna, and Robert D. Skeel, SIAM J Sci. Comput., 18, 223-238, 1997. https://doi.org/10.1137/S1064827595288085
[3] On the energy conservation of the simplified Takahashi-Imada method, E. Hairer, R. McLachlan, and R. Skeel, ESAIM: M2AN 43, 631–644, 2009.