Lectures on Thermodynamic Parameterization at BMS Summer School 2019

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Dear Students

I will be discussing the use of stochastic differential equation-based methods for training neural networks. The starting point here is the previous work we have done in building integration schemes for Langevin dynamics in molecular dynamics.   A good reference for this is our book

Leimkuhler and Matthews, Molecular Dynamics, Springer 2015
https://www.springer.com/gp/book/9783319163741

It should be available to you through your institution via SpringerLink.

Some other useful papers:

Leimkuhler and Matthews, Rational construction of stochastic numerical methods for molecular sampling, Applied Mathematics Research eXpress 2013 (1), 34-56.

Fass, Sivak, Crooks, Beauchamp, Leimkuhler and Chodera, Quantifying configurational sampling error in Langevin simulations of complex molecular systems, Entropy, 20 (5) 318, 2018.

Shang and Leimkuhler, Adaptive thermostats for noisy gradient systems, SIAM J Sci Computing, 38 (2), A712-A736, 2016.

Shang, Zhu, Leimkuhler and Storkey, Covariance controlled adaptive Langevin thermostat for large-scale Bayesian sampling, NIPS, 237-45, 2015.

I will also address other papers from my recent work, especially on the last day. You can find these on google scholar.

We have been using these thermodynamically inspired training methods in many experiments lately involving neural networks. There is a TensorFlow package that implements some of our methods (only the basic ones so far). It is called TATi for Thermodynamic Analytics ToolkIt.   It is available using the pip package manager via

        pip install tati

If you are a tensorflow user you can download this and try some things out using it. There is a draft manuscript on arxiv describing the TATi software and giving a few examples with it: https://arxiv.org/abs/1903.08640

However I appreciate that not everyone is a TensorFlow lover. With my group I have been creating an app "ThermoML" which illustrates the concepts I will discuss in my lectures. I will only be able to make this available on Monday and only in the form of binaries for macintosh Mojave and Linux (ubuntu). The app is very much a development project and the release I will be bringing with me is the "captive beta" version: you are all my captive beta testers!

Looking forward to meeting you next week,
Ben