Discussions on the Read Paper by Girolami and Calderhead “Riemann manifold Langevin and Hamiltonian Monte Carlo methods” read to the Society on October 13th, 2010

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Summary. This is a collection of discussions of ‘Riemann manifold Langevin and Hamiltonian Monte Carlo methods” by Girolami and Calderhead, to appear in the Journal of the Royal Statistical Society, Series B.

1. Connections with optimisation (S. Barthelmé and N. Chopin)

One of the many things we like about this paper is that it forces us to change our perspective on Metropolis-Hastings. We may not the only ones with the toy example of a bivariate, strongly correlated, Gaussian distribution imprinted in our brain. This example explains well why taking correlations into account is important. However, one often forgets that, contrary to the Gaussian example, the curvature of the log target density may be far from constant, which justifies a local calibration of HM strategies. The authors give compelling evidence that local calibration may lead to strong improvements in large-dimensional problems.

There are two ways to understand these results. One of them, put forward in this paper, stems from the information geometry perspective: the parameter space is endowed with a metric defined by $G(θ)$, which turns the posterior distribution into a density over a manifold. The general MMALA algorithm based on a diffusion over that manifold is a beautiful mathematical device, but it is not immediately apparent how this leads to improved (relative) MCMC performance. A different viewpoint proceeds from optimisation: MMALA performs better because it uses a better local model of the posterior density.

As often pointed out, the Langevin proposal is a noisy version of a gradient ascent step. Similarly, the simplified MMALA step is a noisy version of a (quasi-)Newton step, in which the Hessian is replaced with the Fisher information matrix, an idea known as Iteratively Reweighted Least-Squares in the literature on Generalised Linear Models. It is worth emphasising the fact that
the simplified versions, which just relies on these local curvature ideas, but do not require third derivatives, do better in terms of relative efficiency (not to mention in terms of human computation time!).

This suggests two avenues for further research. First, many optimisation methods have been developed that only require evaluating the gradient. This may be more convenient from the practitioner’s point of view, and it also proves more effective whenever computing Hessian matrices is expensive. Methods, such as the BFGS or Barzilai-Borwein, approximate the Hessian locally from the previous \( k \) iterations. Our preliminary experiments indicate that these methods may reduce the correlation in MCMC chains.

The second point is that the auxiliary Gaussian distribution is merely a choice imposed by the physical interpretation of the Hamiltonian. Do the authors have any intuition on what would be the optimal auxiliary distribution?

2. Multiple potentials (M. Beffy and C.P. Robert)

The paper gives a very clear geometric motivation for the use of an Hamiltonian representation. As such, it suggests for an immediate generalisation by extending the Hamiltonian dynamic to a more general dynamic on the level sets of

\[
\mathcal{H}(\theta, p_1, p_2, \ldots, p_k) = -\mathcal{L}(\theta) + \frac{1}{2} \log \{(2\pi)^D |G_1(\theta)|\} + \frac{1}{2} p_1^T G_1(\theta)^{-1} p_1 \\
+ \frac{1}{2} \log \{(2\pi)^D |G_2(\theta)|\} + \frac{1}{2} p_2^T G_2(\theta)^{-1} p_2 + \ldots \\
+ \frac{1}{2} \log \{(2\pi)^D |G_k(\theta)|\} + \frac{1}{2} p_k^T G_k(\theta)^{-1} p_k,
\]

where the \( p_j \)s are auxiliary vectors of the same dimension \( D \) as \( \theta \) and the \( G_j(\theta) \)s are symmetric matrices. This function is then associated with the pde’s

\[
\frac{d\theta_i}{dt} = \frac{\partial}{\partial p_{ij}} \mathcal{H}(\theta, p_1, \ldots, p_k) = \{G_j(\theta)^{-1} p_j\}_i \\
\frac{dp_{ij}}{dt} = -\frac{\partial}{\partial \theta_i} \mathcal{H}_j(\theta, p_1, \ldots, p_k)
\]

in that those moves preserve the potential \( \mathcal{H}(\theta, p_1, \ldots, p_k) \) and hence the target distribution at all times \( t \). This generalisation would allow for using a range of information matrices \( G_j(\theta) \)s in parallel. The corresponding RHMC implementation is to pick one of the indices \( j \) at random and to follow the same moves as in the paper, given the separation between the different energies.

3. Information approximations (A. Doucet, P. Jacob and A.M. Johansen)

Congratulations to the authors for their elegant contribution.
Consider those situations in which one does not have direct access to an appropriate metric but can obtain pointwise, simulation-based estimates of its values. For example, we might be interested in performing Bayesian inference in general state-space Hidden Markov Models (HMM) using particle MCMC methods (Andrieu et al. 2010). In this context, we integrate out numerically the latent variables of the model using a Sequential Monte Carlo (SMC) scheme. A sensible metric to use is the observed information matrix which can also be estimated using SMC (Poyadjis et al. 2010). We discuss here the use of such estimates in an MCMC context.

Assume we want to sample from a target \( \pi(x) \) on \( \mathcal{X} \) using the Metropolis-Hastings (M-H) algorithm. Denote the proposal’s parameters (e.g. scale) \( r \in \mathcal{R} \). Defining an extended target over \( \mathcal{X} \times \mathcal{R} \), as \( \tilde{\pi}(x,r) = \pi(x)q(r|x) \) an algorithm may be defined on \( \mathcal{X} \times \mathcal{R} \) in which both \( \mathcal{R} \) and \( \mathcal{X} \) are sampled.

At iteration \( n + 1 \) draw \( X^* \sim s(\cdot|x_n,r_n) \) and \( R^* \sim q(\cdot|x^*) \). Accept this proposal with the standard M-H acceptance probability on the extended space

\[
\alpha(x_n,r_n;x^*,r^*) = 1 \wedge \frac{\tilde{\pi}(x^*,r^*)}{\tilde{\pi}(x_n,r_n)} \cdot \frac{s(x_n|x^*,r^*)q(r_n|x_n)}{s(x^*|x_n,r_n)q(r^*|x^*)} = 1 \wedge \frac{\pi(x^*)}{\pi(x_n)} \cdot \frac{s(x^*|x_n,r_n)q(r^*|x^*)}{s(x^*|x_n,r_n)}.
\]

Hence it is not necessary to be able to evaluate \( q \), even pointwise, provided that it can be sampled from. The resulting transition is reversible on the extended space and admits \( \pi \) as a marginal of its invariant distribution. This simple result is well-known: see Besag (1995, Appendix 1).

The MMALA, with metric tensor obtained by sampling, may be justified using precisely the same argument: A proposal of the form of (10), may be implemented with a sampled estimate of the metric tensor and such gradients as are required (objects which can be obtained readily in settings of interest, such as HMMs); the extended space construction above holds with \( x = \theta; r = (G, \nabla G) \) and the acceptance probability remains of the same form; the constant curvature proposal may be implemented without the need for estimates of \( \nabla G \) with \( x = \theta \) and \( r = G \).

The HMC variant of the same is not trivial. As each step of the implicit integrator requires access to the value of the metric at several (implicitly-defined) points, direct application of the above principles does not appear possible. However, more subtle approaches can be employed. In particular one could consider trying to approximate the metric using the expectation of a function with respect to a probability measure independent of \( x \) and using common random variates from this measure during an HMC update.

4. On some examples (J.-M. Marin and C.P. Robert)

This paper is a welcome addition to the recent MCMC literature and the authors are to be congratulated for linking together the two threads that are the
Langevin modification of the random walk Metropolis–Hastings algorithm and the Hamiltonian acceleration. Overall, trying to take advantage of second order properties of the target density $\pi(\theta)$, just like the Langevin improvement takes advantage of the first order (Roberts and Tweedie, 1995, Stramer and Tweedie, 1999a,b) is a natural idea which, when implementable, can obviously speed up convergence. This is the Langevin part, which may use a fixed metric $M$ or a local metric defining a Riemann manifold, $G(\theta)$. Obviously, this requires that the derivation of an appropriate (observed or expected) information matrix $G(\theta)$ is feasible up to some approximation level. Or else that authoritative enough directions are given about the choice of an alternative $G(\theta)$.

While the logistic example used in the paper mostly is a toy problem (where importance sampling works extremely well, as shown in Marin and Robert, 2010), the stochastic volatility model is more challenging and the fact that the Hamiltonian scheme applies to the missing data (volatility) as well as to the three parameters of the model is quite interesting. We would thus welcome more details on the implementation of the algorithm in such a large dimension space. We however wonder at the appeal of this involved scheme when considering that the full conditional distribution of the volatility can be simulated exactly.

5. Moving away from continuous time (C.P. Robert)

This paper is an interesting addition to recent MCMC literature and I am eager to see how the community is going to react to this potential addition to the MCMC toolbox. I am however wondering about the impact of the paper on MCMC practice. Indeed, while the dynamic on the level sets of

$$H(\theta, p) = -L(\theta) + \frac{1}{2} \log \left\{ (2\pi)^D |G(\theta)| \right\} + \frac{1}{2} p^T G(\theta)^{-1} p,$$

where $p$ is an auxiliary vector of dimension $D$, is associated with Hamilton’s equations, in that those moves preserve the potential $H(\theta, p)$ and hence the target distribution at all times $t$, I argue that the transfer to the simulation side, i.e. the discretisation part, is not necessarily useful, or at least that it does not need to be so painstakingly reproducing the continuous phenomenon.

In a continuous time-frame, the purpose of the auxiliary vector $p$ is clearly to speed up the exploration of the posterior surface by taking advantage of the additional energy it provides. In the discrete-time universe of simulation, on the one hand, the fact that the discretised (Euler) approximation to Hamilton’s equations are not exact nor available in closed form does not present such a challenge in that approximations can be corrected by a Metropolis-Hastings step, provided of course all terms in the Metropolis-Hastings ratio are available. On the other hand, the continuous-time (physical or geometric) analogy at the core of the Hamiltonian may be unnecessary costly when trying to carry a physical pattern in a discrete (algorithmic) time. MCMC algorithms are not set to work in continuous time and therefore the invariance and stability properties
of the continuous-time process that motivates the method do not carry to the
discretised version of the process. For one thing, the (continuous) time unit has
no equivalent in discrete time. Therefore, the dynamics of the Hamiltonian do
not tell us how long the discretised version should run, as illustrated on Figure
1. As a result, convergence issues (of the MCMC algorithm) should not be im-
acted by inexact renderings of the continuous-time process in discrete time. For
instance, when considering the Langevin diffusion, the corresponding Langevin
algorithm could as well use another scale $\eta$ for the gradient than the one $\tau$
used for the noise, i.e.

$$y = x^t + \eta \nabla \pi(x) + \tau \epsilon^t$$

rather than a strict Euler discretisation where $\eta = \tau^2/2$. A few experiments
run in [Robert and Casella] (1999, Chapter 6, Section 6.5) showed that using
a different scale $\eta$ could actually lead to improvements, even though we never
pursued the matter any further.

References

Andrieu, C., Doucet, A. and Holenstein, R. (2010). Particle Markov
Chain Monte Carlo Methods. *J Royal Stat. Soc. B* (with discussion), 72 (3),
269–342.

Besag, J., Green, P.J., Higdon, D. and Mengersen, K. (1995). Bayesian
Computation and Stochastic Systems. *Statistical Science*, 10 (1), 3–66.

Poyiadjis, G., Doucet, A. and Singh, S.S. (2010). Particle Approximations
of the Score and Observed Information Matrix in State-Space Models with
Application to Parameter Estimation. *Biometrika*. To appear.

Marin, J. and Robert, C. (2010). Importance sampling methods for Bayesian
discrimination between embedded models. In *Frontiers of Statistical Decision
Making and Bayesian Analysis* (M.-H. Chen, D. Dey, P. Müller, D. Sun and
K. Ye, eds.). Springer-Verlag, New York. To appear.

Robert, C. and Casella, G. (1999). *Monte Carlo Statistical Methods*. 1st ed.
Springer-Verlag, New York.

Roberts, G. and Tweedie, R. (1995). Exponential convergence for Langevin
diffusions and their discrete approximations. Tech. rep., Statistics Laboratory,
Univ. of Cambridge.

Stramer, O. and Tweedie, R. (1999a). Langevin-type models I: diffusions
with given stationary distributions, and their discretizations. *Methodology and
Computing in Applied Probability*, 1 283–306.

Stramer, O. and Tweedie, R. (1999b). Langevin-type models II: Self-
targeting candidates for Hastings-Metropolis algorithms. *Methodology and
Computing in Applied Probability*, 1 307–328.
Fig. 1. Comparison of the fits of discretised Langevin diffusions to the target $f(x) \propto \exp(-x^4)$ when using a discretisation step $\sigma^2 = .01$ (left) and $\sigma^2 = .0001$ (right), after $T = 10^7$ steps. This comparison illustrates the need for more time steps when using a smaller discretisation step.