The random walk Metropolis -
linking theory and practice through a case study.

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Much theory on creating efficient random walk Metropolis (RWM) algorithms.

Some applies to special cases, some more generally.

This talk:

1. Compares and contrasts a selection of RWM theory on scaling and shaping.
2. Uses this and other theory to suggest (often incremental) algorithmic improvements.
3. Examines algorithm performance on a non-trivial testing ground (the Markov Modulated Poisson Process).
The **RWM** algorithm explores a $d$-dimensional target density $\pi(x)$ by creating a Markov chain using a $d$-dimensional jump proposal density $\lambda^{-d} \ r(y/\lambda)$ with $r(-y) = r(y)$. 
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From current position $X_i$ propose a jump $Y^*_i$.

Accept with probability $\alpha(x_i, y^*_i) = \min[1, \pi(x_i + y^*_i)/\pi(x_i)]$

If accept $X_{i+1} \leftarrow X + Y^*$ otherwise $X \leftarrow X$. 
The MwG algorithm explores a $d$-dimensional target density $\pi(x)$ by creating a Markov chain.

Jumps are proposed and accepted as for the RWM but have dimension $d^* < d$.

A **deterministic** MwG algorithm updates subsets of the components of $x$ in some predetermined order.

A **random scan** MwG algorithm chooses at random the subset of components of $x$ to be updated.
Integrated Autocorrelation Time

We wish to estimate $\mathbb{E}[f(X)]$ by $n^{-1} \sum_{i=1}^{n} f(x^{(i)})$.

The MCMC sample is correlated and so the standard error of the estimate is $\text{Var}[f(X)] / n_{\text{eff}}$ where $n_{\text{eff}} < n$ is the \textbf{effective sample size}.
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For a stationary chain, let $\gamma_i = \text{Corr}[f(X_k), f(X_{k+i})]$.

The integrated autocorrelation time (ACT) is $\tau_f = 1 + 2 \sum_1^\infty \gamma_i$, and $n_{\text{eff}} = n/\tau$.

We will use ACT to compare the output of the different MCMC algorithms.
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*Finite sample* so use $\tau_f = 1 + 2 \sum_{1}^{l-1} \hat{\gamma}_i$ where $l$ is the first lag such that $\hat{\gamma}_l < 0.05$. 
Squared jumping distances

Could measure theoretical efficiency in terms of expected squared Euclidean jump distance:

\[ S_{d,Euc}^2 := \mathbb{E} \left[ ||X_{i+1} - X_i||^2 \right]. \]

Maximising the Euclidean square jump distance for a component is equivalent to minimising the lag-1 autocorrelation for that component.
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For an elliptical target with contours along lines of constant \( x'\Sigma^{-1}x \) an alternative measure would be the expected square jump distance

\[ S_d^2 := \mathbb{E} \left[ (X_{i+1} - X_i)' \Sigma^{-1} (X_{i+1} - X_i) \right] . \]
Consider a single component (e.g. the first) of the $d$-dimensional chain at iteration $i$ and denote it $X_{1,i}^{(d)}$. 
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(1)

Under certain circumstances it is possible to show that the (weak) limit $\lim_{d \to \infty} W_t^{(d)}$ is a Langevin diffusion.

The speed of this diffusion is another measure of the algorithm’s efficiency.
Roberts and Rosenthal (2001) consider a target with independent components

\[ \pi(x) = \prod_{i=1}^{d} C_i f(C_i x_i), \]

where \( \mathbb{E}[C_i] = 1 \) and \( \mathbb{E}[C_i^2] = b < \infty \). A Gaussian proposal is used: \( \lambda Z \) where \( Z \sim N(0, I) \).

It is shown that subject to moment conditions on \( f \), and provided \( \lambda = \mu/d^{1/2} \), for some fixed \( \mu \), then as \( d \to \infty \), \( C_1 W_t^{(d)} \) (from 1) does approach a Langevin diffusion.
Optimal scaling (1)

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The speed of this diffusion is \( \mu^2 \overline{\alpha}_d \times C_1^2 / b \), where

\[ \overline{\alpha}_d := 2\Phi \left( -\frac{1}{2} \mu / 1^{1/2} \right) \]

is the acceptance rate, and \( l \) is a measure of roughness.
Bedard (2007) considers targets with independent components and a triangular sequence of inverse scale coefficients $c_{i,d}$, and shows a similar result provided

$$\max_i c_{i,d}^2 \frac{\sum_{i=1}^{d} c_{i,d}^2}{\sum_{i=1}^{d} c_{i,d}^2} \rightarrow 0.$$

(2)
Optimal scaling (3)

Sherlock and Roberts (2009) consider sequences of elliptically symmetric targets \( \mathbf{X}^{(d)} \) explored by a spherically symmetric proposal \( \lambda \mathbf{Z}^{(d)} \) and use ESJD as a measure of efficiency.

For many spherically symmetric distributions, as \( d \to \infty \) all of the mass converges to a particular radius. It is shown than if

\[
\lambda = \mu / d^{1/2} \times k_x^{(d)} / k_z^{(d)},
\]

and the inverse scale parameters of the axes of the elliptical target satisfy

\[
\frac{|\mathbf{X}^{(d)}|}{k_x^{(d)}} \xrightarrow{p} 1 \quad \text{and} \quad \frac{|\mathbf{Z}^{(d)}|}{k_z^{(d)}} \xrightarrow{m.s.} 1,
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$$\frac{d}{k_x^{(d)} k_x^{(d)}} S_d^2(\mu) \to \mu^2 \alpha_d \quad \text{with} \quad \alpha_d(\mu) := 2\Phi \left( -\frac{1}{2} \mu \right).$$
Optimal scaling (4)

Optimising the efficiency measure w.r.t. $\mu$ and substituting gives

$$\lambda_d = \frac{2.38}{d^{1/2} I^{1/2}} \ (R \text{ and } R) \quad \text{and} \quad \lambda_d = \frac{2.38 \ k_d^{(d)}}{d^{1/2} k_d^{(d)}} \ (S \text{ and } R).$$
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**Algorithm 1**: proposal $\mathbf{Y} \sim N(\mathbf{0}, \lambda^2 I)$ with $\lambda$ chosen so that the acceptance rate is between 0.2 and 0.3.
**NB** The limiting optimal acceptance rate need not be 0.234 - e.g. Bedard (2008), Sherlock and Roberts (2009).
Neal and Roberts (2006) consider the behaviour of the random scan MwG algorithm on a target with iid components.
Neal and Roberts (2006) consider the behaviour of the random scan MwG algorithm on a target with iid components. The optimal scale parameter is larger than for a full update (since the dimension of the update is smaller) but the limiting optimal acceptance rate is still 0.234.
Optimal scaling for MwG (2)

Sherlock (2006) considers a deterministic MwG algorithm on a sequence of elliptical targets (subject to 2) with updates proposed from a spherical distribution, but allowing different scalings for different sub-blocks of principal components of the ellipse.

For equal-sized sub-blocks the limiting relative efficiency (compared the optimal RWM with a single spherical proposal) is shown to be

$$r_{\text{MwG}/\text{RWM}} = \frac{\frac{1}{k} \sum c^2_i}{\left(\frac{1}{k} \sum c^2_i - 1\right)^{-1}}$$

where $c^2_i$ is the mean of the squares of the inverse scale parameters for the $i^{th}$ sub-block.
An optimally tuned MwG algorithm (for orthogonal sub-blocks) will be more efficient than a single block update.

**Algorithm 2**: MwG with proposed jumps $Y_i \sim N(0, \lambda_i^2)$ optimised along each component ($\alpha \approx 0.4$).
Optimal shaping (1)

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For a sequence where the target with dimension $d$ has elliptical axes with inverse scale parameters $c_{d,1}, \ldots, c_{d,d}$, the limiting ratio of expected squared Euclidean jump distances is

$$r_{sph/ell} = \frac{\lim_{d \to \infty} \left( \frac{1}{d} \sum_{i=1}^{d} c_{d,i}^{-2} \right)^{-1}}{\lim_{d \to \infty} \frac{1}{d} \sum_{i=1}^{d} c_{d,i}^{2}}.$$
Roberts and Rosenthal (2001) examine targets of the form

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and compare the efficiencies of the limiting Langevin diffusions for spherical Gaussian proposals and Gaussian proposals with inverse scale parameter $C_i$ for the $i^{th}$ component.
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The limiting efficiency was found to be

$$r_{id/iid} = \frac{\mathbb{E} [C^2]}{\mathbb{E} [C]^2}$$
We should therefore explore the target using a proposal with a similar shape and orientation to the target.

**Algorithm 3**: use 1000 iterations from Algorithm 1 to estimate the covariance matrix $\hat{\Sigma}$ then propose from $N(0, \lambda \hat{\Sigma})$ with $\lambda$ chosen to give an acceptance rate between 0.2 and 0.3.
Exploring heavy tails

There is evidence (e.g. Roberts, 2003) to suggest that a heavy tailed proposal should better explore a heavy tailed target.

**Algorithm 4** proposes from a Cauchy distribution with modal hessian $\hat{\Sigma}^{-1}$, and scaling chosen so as to minimise the ACT.
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An alternative strategy is to transform the target to one with lighter tails. Dellaportas and Roberts (2003) use a random walk on the posterior for the log of each parameter: the *multiplicative random walk*.

**Algorithm 5** uses a Gaussian proposal on a transformed parameter set $\{\log \theta_1, \ldots, \log \theta_4\}$, with shape matrix estimated as for Algorithm 3 (but on the log parameters!).
Adaptive MCMC (1)

Rather than estimating $\Sigma$ and $\lambda$ from finite tuning runs, we could let a single algorithm learn from its own output.

It is important that changes to the MCMC kernel become vanishingly small as iteration $i \rightarrow \infty$ (e.g. Roberts and Rosenthal, 2007).
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**Algorithm 6** uses a random walk on the posterior for the log parameters. The jump proposal is

$$Y \sim \begin{cases} 
N \left(0, m^2 \hat{\Sigma}_n \right) & \text{w.p. } 1 - \delta \\
N \left(0, \frac{1}{d} \lambda_0^2 I \right) & \text{w.p. } \delta.
\end{cases}$$

Here $\delta = 0.05$, $d = 4$, and $\hat{\Sigma}_n$ is estimated from the logarithms of the posterior sample to date.
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\end{cases}

A few minutes were spent tuning the block multiplicative random walk with proposal variance $\frac{1}{4} \lambda_0^2 I$ to give at least a reasonable value for $\lambda_0$ (acceptance rate $\approx 0.3$), although this is not strictly necessary.
Adaptive MCMC (2)

\[ Y \sim \begin{cases} 
N \left( 0, m^2 \hat{\Sigma}_n \right) & \text{w.p. } 1 - \delta \\
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\end{cases} \]

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\( m \) was updated as follows: if the proposal was rejected then \( m < -m - \Delta / i^{1/2} \), otherwise \( m < -m + 2.3 \Delta / i^{1/2} \). This leads to an equilibrium acceptance rate of \( 1 / 3.3 \) (\( \Delta \) is some small fixed quantity).
The MMPP

A Markov modulated Poisson process (MMPP) is a Poisson process, the intensity of which, $\lambda(X_t)$, depends on the state of a continuous time discrete space Markov chain $X_t$.

Figure: Two 2-state cts time MCs simulated from generator $Q$ with $q_{12} = q_{21} = 1$; rug plots show events from MMPPs simulated from these chains, with intensity $\psi = (10, 30)$ (upper) and $\psi = (10, 17)$ (lower).
The MMPP Test Data

Simulated test data was from 100 secs of MMPPs with $q_{12} = q_{21} = 1$ and either $\psi = (10, 30)$ (D1 - 3 replicates) or $\psi = (10, 17)$ (D2 - 3 replicates).
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D1 - more events + easier to distinguish the state of the underlying chain $\Rightarrow$ lighter tails + parameters $(\psi_1, \psi_2, q_{12}, q_{21})$ closer to orthogonal.
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D1 - more events + easier to distinguish the state of the underlying chain $\Rightarrow$ lighter tails + parameters $(\psi_1, \psi_2, q_{12}, q_{21})$ closer to orthogonal.

D2 - fewer events + harder to distinguish the state of the underlying chain $\Rightarrow$ heavier tails + parameters far from orthogonal.
Using problem specific information

When \( \psi_1 \approx \psi_2 \) can Taylor expand likelihood in \( \psi \) about \( \bar{\psi}_1 \).

Leads to a new reparamterisation with new parameters approximately orthogonal (when \( \psi_2 \approx \psi_1 \)).

**Algorithm 7**: MwG updates on the new parameters, multiplicative where possible (3/4).
Priors: Exponential, with mean the known “true” parameter value.

Runs of 10 000 iterations (+ burn in of 1000)

Accuracy? Compared with 100 000 iterations of a Gibbs sampler (Sherlock and Fearnhead, 2006). All OK.

Efficiency: ACT (multiplied by 4 for MwG).
All algorithms performed better on D1 than D2 because D1 has lighter tails.
ACT Results (1)

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Alg2 (MwG, \( N(0, \chi_i^2 I) \)) 2-3 times better than Alg1 for D1 but only 1.5 times better than Alg1 for D2, as parameters closer to orthogonal for D1.
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Alg3 ($N(0, \hat{\Sigma})$) 4-6 times better than Alg1 ($N(0, \lambda^2 I)$).
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**Alg2** (MwG, $N(0, \lambda^2 I)$) 2-3 times better than **Alg1** for D1 but only 1.5 times better than Alg1 for D2, as parameters closer to orthogonal for D1.

**Alg3** ($N(0, \hat{\Sigma})$) 4-6 times better than Alg1 ($N(0, \lambda^2 I)$).

Improvements in Alg2 and Alg3 best for $\psi$ as Alg1 limited by variance of $q$. 

ACT Results (1)
**ACT Results (2)**

**Alg4** (Cauchy, $\hat{\Sigma}$) performs $\approx 1.5$ times **worse** than **Alg3** (Normal, $\hat{\Sigma}$) for **both** algorithms!

More negative proposals? $\hat{\Sigma}$ not representative away from the modes?
ACT Results (2)

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**Alg5** (Multiplicative, Normal, $\hat{\Sigma}_*$) performs the same as Alg3 for D1 and $\approx 1.5 - 2$ times better than Alg3 for D2.

Heavier tails.
**ACT Results (2)**

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Heavier tails.

**Alg6** (Adap, mult; Normal, \( \hat{\Sigma}_* \)) performs the same as **Alg5** for **D1** and \( 1-1.5 \) times better than **Alg5** for **D2**.

Takes \( > 1000 \) iterations to estimate \( \hat{\Sigma} \)?
**ACT Results (3)**

Alg7 (Reparameterisation; MwG, mult. where possible, Normal) performs $\approx 2$ times worse than Alg6 (Adap, mult; Normal, $\hat{\Sigma}$) for D1 **but** performance is very similar to Alg6 for D2.

Alg7 was designed for cases such as D2.
Summary

- Two different approaches to optimising RWM.
- Apply to different distributions (independent components / elliptical contours).
- Use different measures (diffusion speed / ESJD)
- Suggest similar methods for producing efficient algorithms.
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- Two different approaches to optimising RWM.
- Apply to different distributions (independent components / elliptical contours).
- Use different measures (diffusion speed / ESJD)
- Suggest similar methods for producing efficient algorithms.
- Algorithms perform as might be expected, except for the Cauchy proposal - worse.
- On the heavier tailed data set, the adaptive algorithm performs as well as the algorithm which uses problem specific knowledge.
References