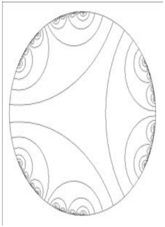
MCMC from Diffusions and Geodesics



- Riemann manifold Langevin and Hamiltonian Monte Carlo Methods
  Girolami, M. & Calderhead, B.
  J.R.Statist. Soc. B, *with discussion*, (2011), **73**, *2*, 123 - 214.

`www.ucl.ac.uk/statistics/research/rmhmc`

Talk Outline

- Motivation to improve MCMC capability for challenging problems

Talk Outline

- Motivation to improve MCMC capability for challenging problems
- Exploring geometric concepts in MCMC methodology

Talk Outline

- Motivation to improve MCMC capability for challenging problems
- Exploring geometric concepts in MCMC methodology
- Diffusions across Riemann manifold as basis for MCMC

Talk Outline

- Motivation to improve MCMC capability for challenging problems
- Exploring geometric concepts in MCMC methodology
- Diffusions across Riemann manifold as basis for MCMC
- Geodesic flows on manifold form basis of MCMC methods

Talk Outline

- Motivation to improve MCMC capability for challenging problems
- Exploring geometric concepts in MCMC methodology
- Diffusions across Riemann manifold as basis for MCMC
- Geodesic flows on manifold form basis of MCMC methods
- Illustrative examples and Hilbert manifolds

Talk Outline

- Motivation to improve MCMC capability for challenging problems
- Exploring geometric concepts in MCMC methodology
- Diffusions across Riemann manifold as basis for MCMC
- Geodesic flows on manifold form basis of MCMC methods
- Illustrative examples and Hilbert manifolds
- Further Work and Conclusions

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum\nolimits_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

- Draw $\boldsymbol{\theta}^n$ from ergodic Markov process with stationary distribution $\pi(\boldsymbol{\theta})$

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

- Draw $\boldsymbol{\theta}^n$ from ergodic Markov process with stationary distribution $\pi(\boldsymbol{\theta})$
- Construct transition kernel as product of two components

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

- Draw $\boldsymbol{\theta}^n$ from ergodic Markov process with stationary distribution $\pi(\boldsymbol{\theta})$
- Construct transition kernel as product of two components
  - Propose a move $\boldsymbol{\theta} \to \boldsymbol{\theta}'$ with probability $p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})$

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum\nolimits_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

- Draw $\boldsymbol{\theta}^n$ from ergodic Markov process with stationary distribution $\pi(\boldsymbol{\theta})$
- Construct transition kernel as product of two components
  - Propose a move $\boldsymbol{\theta} \to \boldsymbol{\theta}'$ with probability $p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})$
  - accept or reject proposal with probability

$$p_a(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \min\left[1, \frac{\pi(\boldsymbol{\theta}')p_p(\boldsymbol{\theta}|\boldsymbol{\theta}')}{\pi(\boldsymbol{\theta})p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})}\right]$$

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

- Draw $\boldsymbol{\theta}^n$ from ergodic Markov process with stationary distribution $\pi(\boldsymbol{\theta})$
- Construct transition kernel as product of two components
  - Propose a move $\boldsymbol{\theta} \to \boldsymbol{\theta}'$ with probability $p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})$
  - accept or reject proposal with probability

$$p_a(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \min\left[1, \frac{\pi(\boldsymbol{\theta}')p_p(\boldsymbol{\theta}|\boldsymbol{\theta}')}{\pi(\boldsymbol{\theta})p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})}\right]$$

- Convergence rate and asymptotic variance dependent on $p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})$

Motivation Simulation Based Inference

- Monte Carlo method employs samples from $\pi(\boldsymbol{\theta})$ to obtain estimate

$$\int \phi(\boldsymbol{\theta})\pi(\boldsymbol{\theta})d\boldsymbol{\theta} = \frac{1}{N}\sum_n \phi(\boldsymbol{\theta}^n) + \mathcal{O}(N^{-\frac{1}{2}})$$

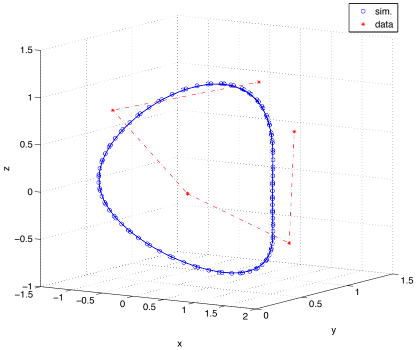
- Draw $\boldsymbol{\theta}^n$ from ergodic Markov process with stationary distribution $\pi(\boldsymbol{\theta})$
- Construct transition kernel as product of two components
  - Propose a move $\boldsymbol{\theta} \to \boldsymbol{\theta}'$ with probability $p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})$
  - accept or reject proposal with probability

$$p_a(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \min\left[1, \frac{\pi(\boldsymbol{\theta}')p_p(\boldsymbol{\theta}|\boldsymbol{\theta}')}{\pi(\boldsymbol{\theta})p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})}\right]$$

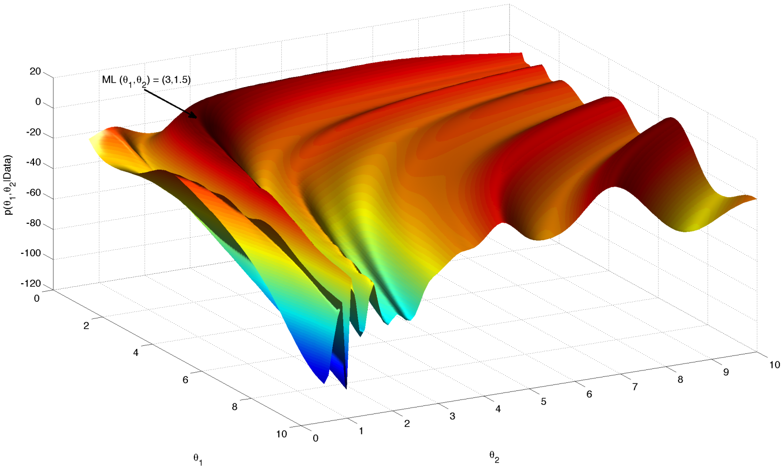
- Convergence rate and asymptotic variance dependent on $p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})$
- Success of MCMC reliant upon appropriate proposal design

Simple Dynamics

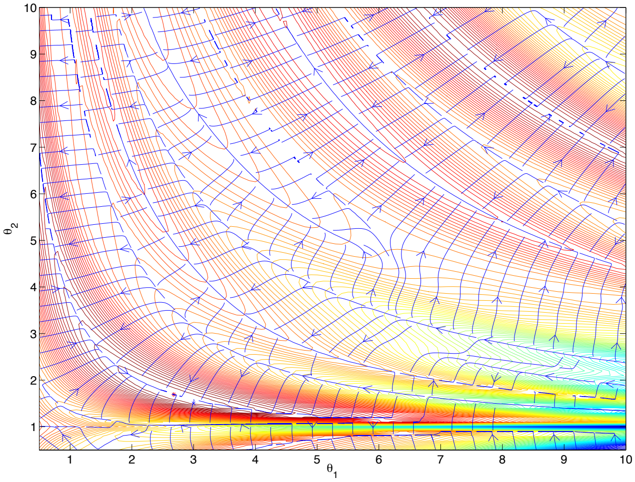
$$\frac{dx}{dt} = \theta_1 yz$$
$$\frac{dy}{dt} = -xz$$
$$\frac{dz}{dt} = -\theta_2 xy$$



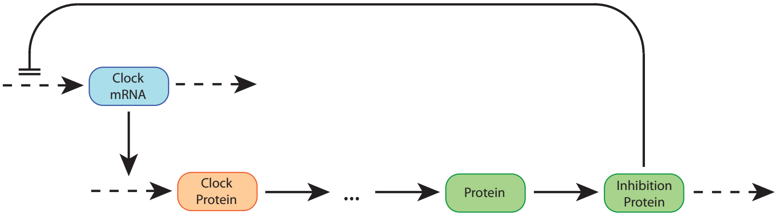
Simple Dynamics



Simple Dynamics

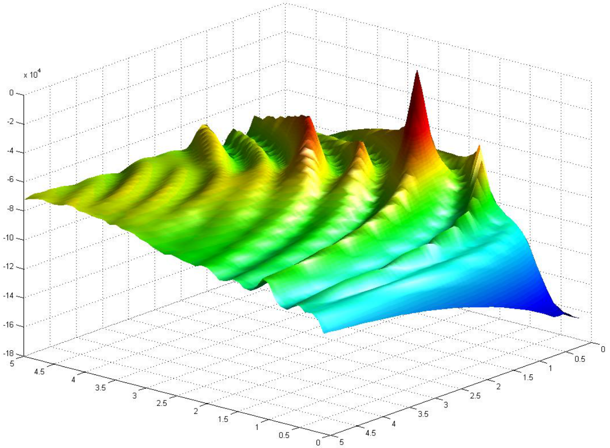


System Identification: Nonlinear ODE Oscillator Model

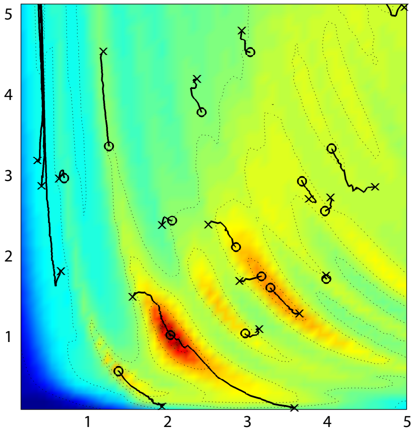


$$
\begin{aligned}
\frac{dx_1}{dt} &= \frac{k_1}{1 + x_n^{\rho}} - m_1 x_1 \\
\frac{dx_2}{dt} &= k_2 x_1 - m_2 x_2 \\
&\vdots \\
\frac{dx_n}{dt} &= k_n x_{n-1} - m_n x_n
\end{aligned}
$$

Systems Identification - Posterior Inference



Mixing of Markov Chains



Geometric Concepts in MCMC

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}))$

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Jeffreys, 1948 to first order

$$D(\boldsymbol{\theta}||\delta\boldsymbol{\theta}) = \int p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) \log \frac{p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T} \mathbf{G}(\boldsymbol{\theta}) \delta\boldsymbol{\theta}$$

- Jeffreys, 1948 to first order

$$D(\boldsymbol{\theta}||\delta\boldsymbol{\theta}) = \int p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) \log \frac{p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T} \mathbf{G}(\boldsymbol{\theta}) \delta\boldsymbol{\theta}$$

- Expected Fisher Information $\mathbf{G}(\boldsymbol{\theta})$ is metric tensor of a Riemann manifold

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Jeffreys, 1948 to first order

$$D(\boldsymbol{\theta}||\delta\boldsymbol{\theta}) = \int p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) \log \frac{p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Expected Fisher Information $\mathbf{G}(\boldsymbol{\theta})$ is metric tensor of a Riemann manifold
- Non-Euclidean geometry - invariants, connections, curvature, geodesics

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Jeffreys, 1948 to first order

$$D(\boldsymbol{\theta}||\delta\boldsymbol{\theta}) = \int p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) \log \frac{p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Expected Fisher Information $\mathbf{G}(\boldsymbol{\theta})$ is metric tensor of a Riemann manifold
- Non-Euclidean geometry - invariants, connections, curvature, geodesics
- Asymptotic statistical analysis. e.g. Amari, 1981; Murray & Rice, 1993; Critchley *et al*, 1993; Kass, 1989; Dawid, 1975; Lauritsen, 1989

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Jeffreys, 1948 to first order

$$D(\boldsymbol{\theta}||\delta\boldsymbol{\theta}) = \int p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) \log \frac{p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Expected Fisher Information $\mathbf{G}(\boldsymbol{\theta})$ is metric tensor of a Riemann manifold
- Non-Euclidean geometry - invariants, connections, curvature, geodesics
- Asymptotic statistical analysis. e.g. Amari, 1981; Murray & Rice, 1993; Critchley *et al*, 1993; Kass, 1989; Dawid, 1975; Lauritsen, 1989
- Statistical shape analysis Kent *et al*, 1996; Dryden & Mardia, 1998

Geometric Concepts in MCMC

- Denote expected Fisher Information as $\mathbf{G}(\boldsymbol{\theta}) = \text{cov}(\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}))$
- Rao, 1945 to first order

$$\chi^2(\delta\boldsymbol{\theta}) = \int \frac{|p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) - p(\mathbf{y};\boldsymbol{\theta})|^2}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Jeffreys, 1948 to first order

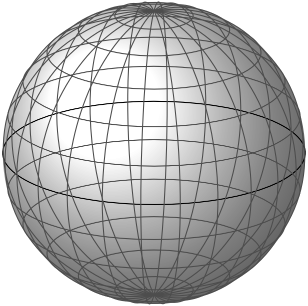
$$D(\boldsymbol{\theta}||\delta\boldsymbol{\theta}) = \int p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta}) \log \frac{p(\mathbf{y};\boldsymbol{\theta}+\delta\boldsymbol{\theta})}{p(\mathbf{y};\boldsymbol{\theta})} d\mathbf{y} \approx \delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$$

- Expected Fisher Information $\mathbf{G}(\boldsymbol{\theta})$ is metric tensor of a Riemann manifold
- Non-Euclidean geometry - invariants, connections, curvature, geodesics
- Asymptotic statistical analysis. e.g. Amari, 1981; Murray & Rice, 1993; Critchley *et al*, 1993; Kass, 1989; Dawid, 1975; Lauritsen, 1989
- Statistical shape analysis Kent *et al*, 1996; Dryden & Mardia, 1998
- Can geometric structure be employed in Monte Carlo methodology?

Manifolds

A manifold is a smooth, curved surface: A set *embedded* in $\mathbb{R}^d$, that locally looks like $\mathbb{R}^n$ ($n < d$).
Example: the unit sphere (2-sphere): $d = 3$, $n = 2$

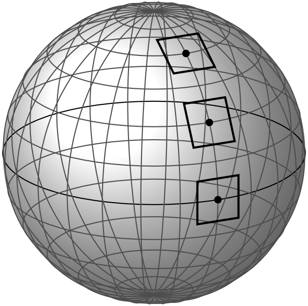
$$\mathcal{S}_2 = \{x \in \mathbb{R}^3 : \sum_i x_i^2 = 1\}$$



Manifolds

A manifold is a smooth, curved surface: A set *embedded* in $\mathbb{R}^d$, that locally looks like $\mathbb{R}^n$ ($n < d$).
Example: the unit sphere (2-sphere): $d = 3$, $n = 2$

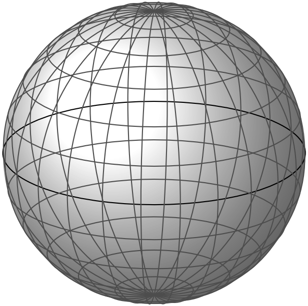
$$\mathcal{S}_2 = \{x \in \mathbb{R}^3 : \sum_i x_i^2 = 1\}$$

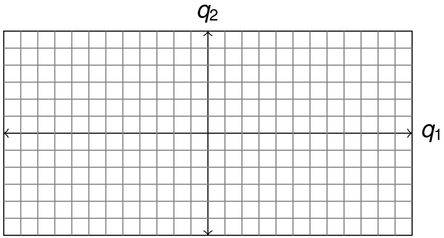


$x \in \mathbb{R}^d$ are the embedded coordinates

Coordinate systems and Riemannian metrics

Can parameterise the manifold with a coordinate system in $q \in \mathbb{R}^n$

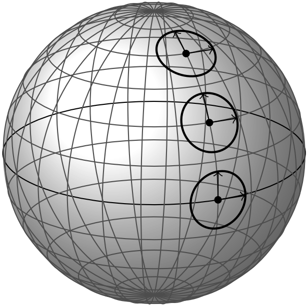


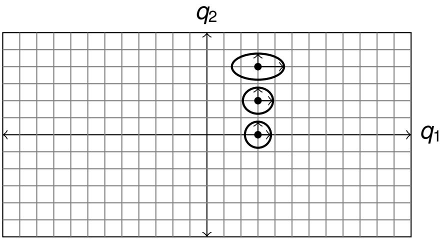


$$(\sin q_1 \sin q_2, \cos q_1 \sin q_2, \cos q_2), \qquad q_1 \in [0, 2\pi], q_2 \in [0, \pi]$$

Coordinate systems and Riemannian metrics

Can parameterise the manifold with a coordinate system in $q \in \mathbb{R}^n$



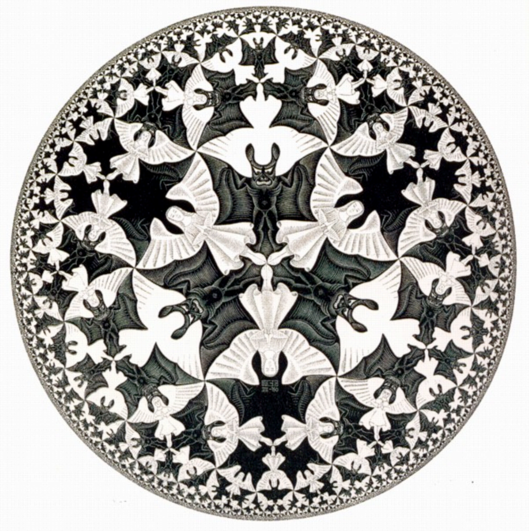


$$(\sin q_1 \sin q_2, \cos q_1 \sin q_2, \cos q_2), \qquad q_1 \in [0, 2\pi], q_2 \in [0, \pi]$$

The Euclidean metric $\|\cdot\|$ induces a Riemannian metric G in the coordinate system:

$$\|\mathrm{d}x\|^2 = \sum_{i,j} G(q)\mathrm{d}q_i\mathrm{d}q_j$$

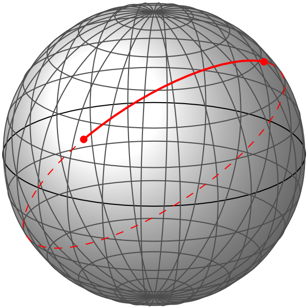
M.C. Escher, Heaven and Hell, 1960

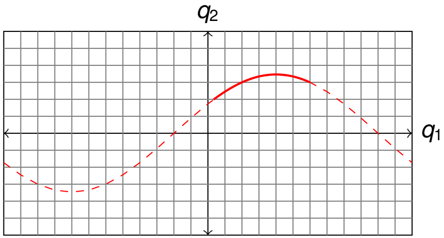


Geodesics

Geodesics are the paths of shortest distance.

- On a sphere, these are the *great circles*

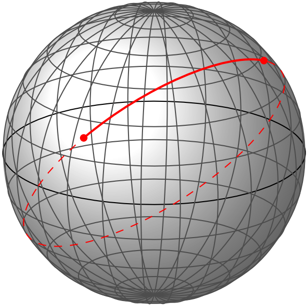


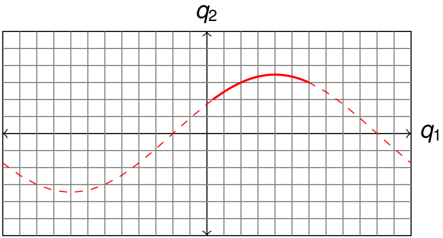


Geodesics

Geodesics are the paths of shortest distance.

- On a sphere, these are the *great circles*



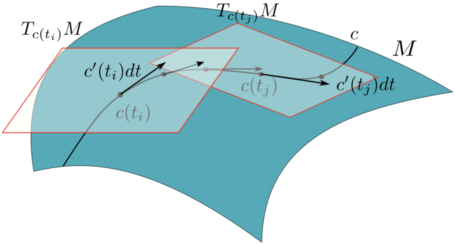


Given an initial velocity $v(0) \perp x(0)$, we have a nice explicit form

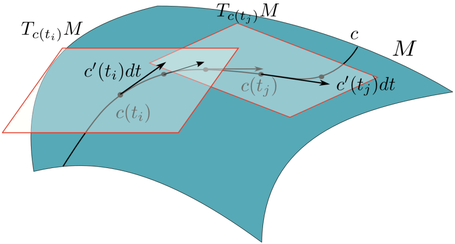
$$\begin{bmatrix} x(t) & v(t) \end{bmatrix} = \begin{bmatrix} x(0) & v(0) \end{bmatrix} \begin{bmatrix} 1 & \\ & \alpha^{-1} \end{bmatrix} \begin{bmatrix} \cos(\alpha t) & -\sin(\alpha t) \\ \sin(\alpha t) & \cos(\alpha t) \end{bmatrix} \begin{bmatrix} 1 & \\ & \alpha \end{bmatrix}$$

where $\alpha = \|v(0)\|$.

Geometric Concepts in MCMC

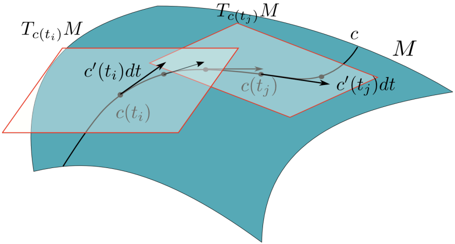


Geometric Concepts in MCMC



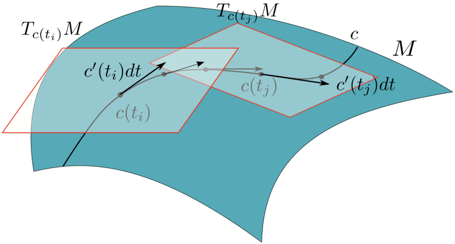
- Tangent space - local metric defined by $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = g_{kl}\delta\theta_k\delta\theta_l$

Geometric Concepts in MCMC



- Tangent space - local metric defined by $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = g_{kl}\delta\theta_k\delta\theta_l$
- Christoffel symbols - characterise Levi-Civita connection on manifold

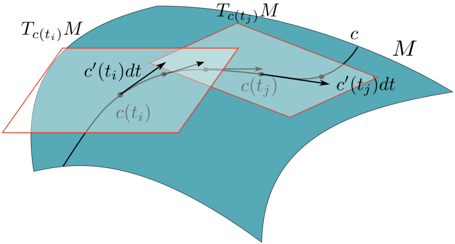
Geometric Concepts in MCMC



- Tangent space - local metric defined by $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = g_{kl}\delta\theta_k\delta\theta_l$
- Christoffel symbols - characterise Levi-Civita connection on manifold

$$\Gamma^i_{kl} = \frac{1}{2}\sum_m g^{im}\left(\frac{\partial g_{mk}}{\partial\theta^l} + \frac{\partial g_{ml}}{\partial\theta^k} - \frac{\partial g_{kl}}{\partial\theta^m}\right)$$

Geometric Concepts in MCMC

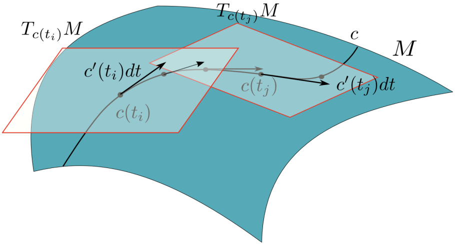


- Tangent space - local metric defined by $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = g_{kl}\delta\theta_k\delta\theta_l$
- Christoffel symbols - characterise Levi-Civita connection on manifold

$$\Gamma^i_{kl} = \frac{1}{2}\sum_m g^{im}\left(\frac{\partial g_{mk}}{\partial\theta^l} + \frac{\partial g_{ml}}{\partial\theta^k} - \frac{\partial g_{kl}}{\partial\theta^m}\right)$$

- Geodesics - shortest path between two points on manifold

Geometric Concepts in MCMC



- Tangent space - local metric defined by $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = g_{kl}\delta\theta_k\delta\theta_l$
- Christoffel symbols - characterise Levi-Civita connection on manifold

$$\Gamma^i_{kl} = \frac{1}{2}\sum_m g^{im}\left(\frac{\partial g_{mk}}{\partial\theta^l} + \frac{\partial g_{ml}}{\partial\theta^k} - \frac{\partial g_{kl}}{\partial\theta^m}\right)$$

- Geodesics - shortest path between two points on manifold

$$\frac{d^2\theta^i}{dt^2} + \sum_{k,l}\Gamma^i_{kl}\frac{d\theta^k}{dt}\frac{d\theta^l}{dt} = 0$$

Fisher–Rao metric

A family of probability densities $\{p(\cdot \mid \theta) : \theta \in \Theta\}$, the Fisher information forms a natural Riemannian metric, known as Fisher–Rao metric:

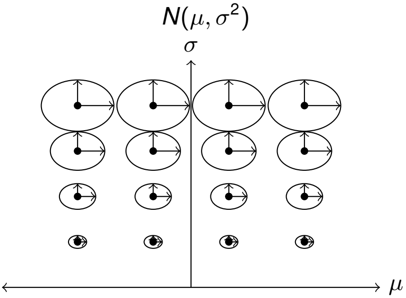
$$g_{ij} = E_{Y|\theta}\left[-\frac{\partial^2}{\partial\theta_i\partial\theta_j}\log p(Y \mid \theta)\right]$$

Fisher–Rao metric

A family of probability densities $\{p(\cdot \mid \theta) : \theta \in \Theta\}$, the Fisher information forms a natural Riemannian metric, known as Fisher–Rao metric:

$$g_{ij} = E_{Y|\theta}\left[-\frac{\partial^2}{\partial\theta_i\partial\theta_j}\log p(Y \mid \theta)\right]$$

Examples:

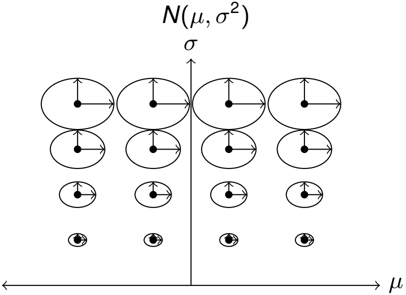


Fisher–Rao metric

A family of probability densities $\{p(\cdot \mid \theta) : \theta \in \Theta\}$, the Fisher information forms a natural Riemannian metric, known as Fisher–Rao metric:

$$g_{ij} = E_{Y|\theta}\left[-\frac{\partial^2}{\partial\theta_i\partial\theta_j}\log p(Y \mid \theta)\right]$$

Examples:



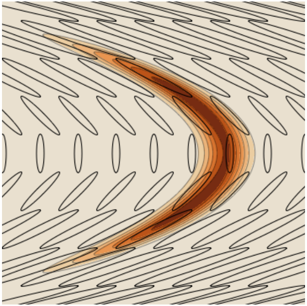


Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu, \sigma) = \mathcal{N}_x(\mu, \sigma)$

Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu, \sigma) = \mathcal{N}_x(\mu, \sigma)$
- Local inner product on tangent space defined by metric tensor, i.e. $\delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\mu, \sigma)^\mathsf{T}$

Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu, \sigma) = \mathcal{N}_x(\mu, \sigma)$
- Local inner product on tangent space defined by metric tensor, i.e. $\delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\mu, \sigma)^\mathsf{T}$
- Metric is Expected Fisher Information

$$\mathbf{G}(\mu, \sigma) = \begin{bmatrix} \sigma^{-2} & 0 \\ 0 & 2\sigma^{-2} \end{bmatrix}$$

Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu,\sigma) = \mathcal{N}_x(\mu,\sigma)$
- Local inner product on tangent space defined by metric tensor, i.e. $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\mu,\sigma)^{\mathsf{T}}$
- Metric is Expected Fisher Information

$$\mathbf{G}(\mu,\sigma) = \left[\begin{array}{cc} \sigma^{-2} & 0 \\ 0 & 2\sigma^{-2} \end{array}\right]$$

- Components of connection $\partial_\mu \mathbf{G} = \mathbf{0}$ and $\partial_\sigma \mathbf{G} = -\operatorname{diag}(2\sigma^{-3}, 4\sigma^{-3})$

Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu,\sigma) = \mathcal{N}_x(\mu,\sigma)$
- Local inner product on tangent space defined by metric tensor, i.e. $\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\mu,\sigma)^{\mathsf{T}}$
- Metric is Expected Fisher Information

$$\mathbf{G}(\mu,\sigma) = \left[\begin{array}{cc} \sigma^{-2} & 0 \\ 0 & 2\sigma^{-2} \end{array}\right]$$

- Components of connection $\partial_\mu \mathbf{G} = \mathbf{0}$ and $\partial_\sigma \mathbf{G} = -\,\mathrm{diag}(2\sigma^{-3}, 4\sigma^{-3})$
- Metric on tangent space

$$\delta\boldsymbol{\theta}^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = \frac{(\delta\mu^2 + 2\delta\sigma^2)}{\sigma^2}$$

Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu, \sigma) = \mathcal{N}_x(\mu, \sigma)$

- Local inner product on tangent space defined by metric tensor, i.e. $\delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\mu, \sigma)^\mathsf{T}$

- Metric is Expected Fisher Information

$$\mathbf{G}(\mu, \sigma) = \begin{bmatrix} \sigma^{-2} & 0 \\ 0 & 2\sigma^{-2} \end{bmatrix}$$

- Components of connection $\partial_\mu \mathbf{G} = \mathbf{0}$ and $\partial_\sigma \mathbf{G} = -\operatorname{diag}(2\sigma^{-3}, 4\sigma^{-3})$
- Metric on tangent space

$$\delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = \frac{(\delta\mu^2 + 2\delta\sigma^2)}{\sigma^2}$$

- Metric tensor for univariate Normal defines a Hyperbolic Space

Illustration of Geometric Concepts

- Consider Normal density $p(x|\mu,\sigma) = \mathcal{N}_x(\mu,\sigma)$
- Local inner product on tangent space defined by metric tensor, i.e. $\delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\mu,\sigma)^\mathsf{T}$
- Metric is Expected Fisher Information

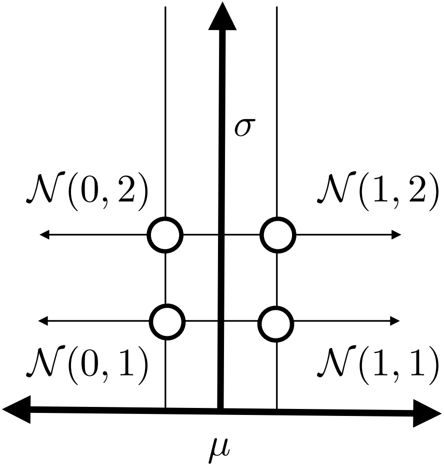
$$\mathbf{G}(\mu,\sigma) = \begin{bmatrix} \sigma^{-2} & 0 \\ 0 & 2\sigma^{-2} \end{bmatrix}$$

- Components of connection $\partial_\mu \mathbf{G} = \mathbf{0}$ and $\partial_\sigma \mathbf{G} = -\operatorname{diag}(2\sigma^{-3}, 4\sigma^{-3})$
- Metric on tangent space

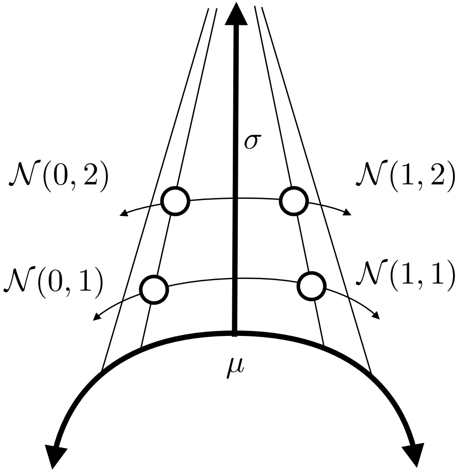
$$\delta\boldsymbol{\theta}^\mathsf{T}\mathbf{G}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = \frac{(\delta\mu^2 + 2\delta\sigma^2)}{\sigma^2}$$

- Metric tensor for univariate Normal defines a Hyperbolic Space
- Consider densities $\mathcal{N}(0,1)$ & $\mathcal{N}(1,1)$ and $\mathcal{N}(0,2)$ & $\mathcal{N}(1,2)$

Normal Density - Euclidean Parameter space



Normal Density - Riemannian Functional space



Langevin Diffusion on Riemannian manifold

- Discretised Langevin diffusion on manifold defines proposal mechanism

$$\boldsymbol{\theta}'_d = \boldsymbol{\theta}_d + \frac{\epsilon^2}{2}\left(\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta})\right)_d - \epsilon^2 \sum_{i,j}^{D} \boldsymbol{G}(\boldsymbol{\theta})^{-1}_{ij}\Gamma^d_{ij} + \epsilon\left(\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}\right)_d$$

Langevin Diffusion on Riemannian manifold

- Discretised Langevin diffusion on manifold defines proposal mechanism

$$\boldsymbol{\theta}'_d = \boldsymbol{\theta}_d + \frac{\epsilon^2}{2}\left(\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta})\right)_d - \epsilon^2 \sum_{i,j}^{D} \boldsymbol{G}(\boldsymbol{\theta})^{-1}_{ij}\Gamma^d_{ij} + \epsilon\left(\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}\right)_d$$

- Manifold with constant curvature then proposal mechanism reduces to

$$\boldsymbol{\theta}' = \boldsymbol{\theta} + \frac{\epsilon^2}{2}\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}) + \epsilon\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}$$

Langevin Diffusion on Riemannian manifold

- Discretised Langevin diffusion on manifold defines proposal mechanism

$$\boldsymbol{\theta}'_d = \boldsymbol{\theta}_d + \frac{\epsilon^2}{2}\left(\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta})\right)_d - \epsilon^2 \sum_{i,j}^{D} \boldsymbol{G}(\boldsymbol{\theta})^{-1}_{ij}\Gamma^d_{ij} + \epsilon\left(\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}\right)_d$$

- Manifold with constant curvature then proposal mechanism reduces to

$$\boldsymbol{\theta}' = \boldsymbol{\theta} + \frac{\epsilon^2}{2}\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}) + \epsilon\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}$$

- MALA proposal with preconditioning

$$\boldsymbol{\theta}' = \boldsymbol{\theta} + \frac{\epsilon^2}{2}\mathbf{M}\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}) + \epsilon\sqrt{\mathbf{M}}\mathbf{z}$$

Langevin Diffusion on Riemannian manifold

- Discretised Langevin diffusion on manifold defines proposal mechanism

$$\boldsymbol{\theta}'_d = \boldsymbol{\theta}_d + \frac{\epsilon^2}{2}\left(\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta})\right)_d - \epsilon^2 \sum_{i,j}^{D} \boldsymbol{G}(\boldsymbol{\theta})^{-1}_{ij}\Gamma^d_{ij} + \epsilon\left(\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}\right)_d$$

- Manifold with constant curvature then proposal mechanism reduces to

$$\boldsymbol{\theta}' = \boldsymbol{\theta} + \frac{\epsilon^2}{2}\boldsymbol{G}^{-1}(\boldsymbol{\theta})\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}) + \epsilon\sqrt{\mathbf{G}^{-1}(\boldsymbol{\theta})}\mathbf{z}$$

- MALA proposal with preconditioning

$$\boldsymbol{\theta}' = \boldsymbol{\theta} + \frac{\epsilon^2}{2}\mathbf{M}\nabla_{\boldsymbol{\theta}}\mathcal{L}(\boldsymbol{\theta}) + \epsilon\sqrt{\mathbf{M}}\mathbf{z}$$

- Proposal and acceptance probability

$$p_p(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}'|\boldsymbol{\mu}(\boldsymbol{\theta}, \epsilon), \epsilon^2\mathbf{G}^{-1}(\boldsymbol{\theta}))$$

$$p_a(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \min\left[1, \frac{\pi(\boldsymbol{\theta}')p_p(\boldsymbol{\theta}|\boldsymbol{\theta}')}{\pi(\boldsymbol{\theta})p_p(\boldsymbol{\theta}'|\boldsymbol{\theta})}\right]$$

Langevin Diffusion on Riemannian manifold

- Discretised Langevin diffusion on manifold defines proposal mechanism

$$\theta'_d = \theta_d + \frac{\epsilon^2}{2}\left(\boldsymbol{G}^{-1}(\theta)\nabla_\theta \mathcal{L}(\theta)\right)_d - \epsilon^2 \sum_{i,j}^{D} \boldsymbol{G}(\theta)^{-1}_{ij}\Gamma^d_{ij} + \epsilon\left(\sqrt{\mathbf{G}^{-1}(\theta)}\mathbf{z}\right)_d$$

- Manifold with constant curvature then proposal mechanism reduces to

$$\theta' = \theta + \frac{\epsilon^2}{2}\boldsymbol{G}^{-1}(\theta)\nabla_\theta \mathcal{L}(\theta) + \epsilon\sqrt{\mathbf{G}^{-1}(\theta)}\mathbf{z}$$

- MALA proposal with preconditioning

$$\theta' = \theta + \frac{\epsilon^2}{2}\mathbf{M}\nabla_\theta \mathcal{L}(\theta) + \epsilon\sqrt{\mathbf{M}}\mathbf{z}$$

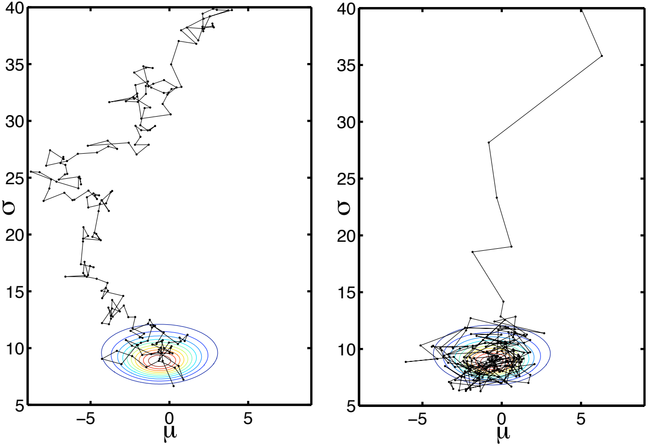
- Proposal and acceptance probability

$$p_p(\theta'|\theta) = \mathcal{N}(\theta'|\mu(\theta,\epsilon), \epsilon^2\mathbf{G}^{-1}(\theta))$$

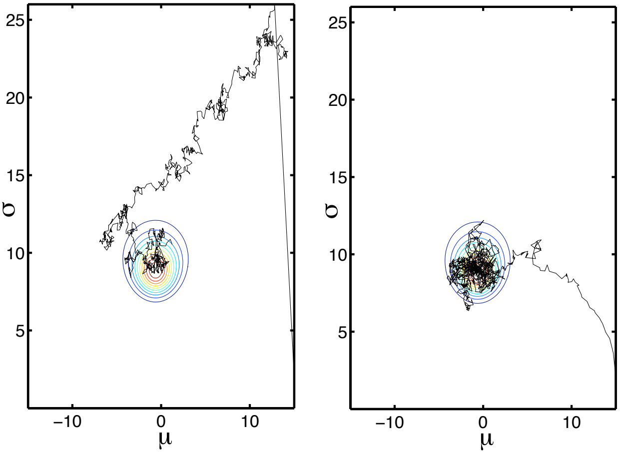
$$p_a(\theta'|\theta) = \min\left[1, \frac{\pi(\theta')p_p(\theta|\theta')}{\pi(\theta)p_p(\theta'|\theta)}\right]$$

- Proposal mechanism diffuses approximately along the manifold

Langevin Diffusion on Riemannian manifold



Langevin Diffusion on Riemannian manifold



Second-Order Diffusions

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field **v** to obtain

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Vector function γ has components $\gamma_k = \sum_{i,j}\Gamma^k_{ij}v^i v^j$

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Vector function γ has components $\gamma_k = \sum_{i,j} \Gamma_{ij}^k v^i v^j$
- Each $\Gamma_{i,j}^k$ being the Christofell symbols of the Levi-Civita connection corresponding to the metric tensor $\mathbf{G}(\mathbf{x}_t)$

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Vector function γ has components $\gamma_k = \sum_{i,j} \Gamma_{ij}^k v^i v^j$
- Each $\Gamma_{i,j}^k$ being the Christofell symbols of the Levi-Civita connection corresponding to the metric tensor $\mathbf{G}(\mathbf{x}_t)$
- Note $d\mathbf{v}_t + \gamma(\mathbf{x}_t, \mathbf{v}_t)dt$ is the covariant time derivative of velocity and the contravariant form of the potential gradient is simply $\mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)$

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Vector function γ has components $\gamma_k = \sum_{i,j} \Gamma^k_{ij} v^i v^j$
- Each $\Gamma^k_{i,j}$ being the Christofell symbols of the Levi-Civita connection corresponding to the metric tensor $\mathbf{G}(\mathbf{x}_t)$
- Note $d\mathbf{v}_t + \gamma(\mathbf{x}_t, \mathbf{v}_t)dt$ is the covariant time derivative of velocity and the contravariant form of the potential gradient is simply $\mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)$
- Physically defines acceleration of a particle across manifold under the influence of potential field

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Vector function γ has components $\gamma_k = \sum_{i,j} \Gamma^k_{ij} v^i v^j$
- Each $\Gamma^k_{i,j}$ being the Christofell symbols of the Levi-Civita connection corresponding to the metric tensor $\mathbf{G}(\mathbf{x}_t)$
- Note $d\mathbf{v}_t + \gamma(\mathbf{x}_t, \mathbf{v}_t)dt$ is the covariant time derivative of velocity and the contravariant form of the potential gradient is simply $\mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)$
- Physically defines acceleration of a particle across manifold under the influence of potential field
- A unit friction or viscous force is included by the term $\mathbf{v}$ and the fluctuating forcing is modelled by the Brownian motion

Second-Order Diffusions

- Define a second-order SDE on a Riemann manifold with the diffusion defined on vector field $\mathbf{v}$ to obtain

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Vector function γ has components $\gamma_k = \sum_{i,j} \Gamma_{ij}^k v^i v^j$
- Each $\Gamma_{i,j}^k$ being the Christofell symbols of the Levi-Civita connection corresponding to the metric tensor $\mathbf{G}(\mathbf{x}_t)$
- Note $d\mathbf{v}_t + \gamma(\mathbf{x}_t, \mathbf{v}_t)dt$ is the covariant time derivative of velocity and the contravariant form of the potential gradient is simply $\mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)$
- Physically defines acceleration of a particle across manifold under the influence of potential field
- A unit friction or viscous force is included by the term $\mathbf{v}$ and the fluctuating forcing is modelled by the Brownian motion
- What has this to do with MCMC?

Second-Order Diffusions

Second-Order Diffusions

- What is invariant measure of this diffusion?

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

$$\frac{dp}{dt} = - v^a \frac{\partial p}{\partial x^a} + \frac{\partial}{\partial v^a}\left[\left(\Gamma^a_{bc} v^b v^c + g^{ab}\frac{\partial \phi}{\partial x^b} + v^a\right) p\right] + g^{ab}\frac{\partial^2 p}{\partial v^a \partial v^b}$$

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

$$\frac{dp}{dt} = \quad - \quad v^a \frac{\partial p}{\partial x^a} + \frac{\partial}{\partial v^a}\left[\left(\Gamma^a_{bc} v^b v^c + g^{ab}\frac{\partial \phi}{\partial x^b} + v^a\right) p\right] + g^{ab}\frac{\partial^2 p}{\partial v^a \partial v^b}$$

- Some schoolboy algebra shows that for $dp/dt = 0$

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

$$\frac{dp}{dt} = - \quad v^a \frac{\partial p}{\partial x^a} + \frac{\partial}{\partial v^a}\left[\left(\Gamma^a_{bc} v^b v^c + g^{ab}\frac{\partial \phi}{\partial x^b} + v^a\right) p\right] + g^{ab}\frac{\partial^2 p}{\partial v^a \partial v^b}$$

- Some schoolboy algebra shows that for $dp/dt = 0$

$$\frac{dp}{p} = \left[-\frac{1}{2}\frac{\partial g_{ab}}{\partial x^c} v^a v^b + \frac{\partial}{\partial x^c}\log\sqrt{|g|} - \frac{\partial \phi}{\partial x^x}\right] dx^c$$

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

$$\frac{dp}{dt} = - \quad v^a \frac{\partial p}{\partial x^a} + \frac{\partial}{\partial v^a}\left[\left(\Gamma^a_{bc} v^b v^c + g^{ab}\frac{\partial \phi}{\partial x^b} + v^a\right) p\right] + g^{ab}\frac{\partial^2 p}{\partial v^a \partial v^b}$$

- Some schoolboy algebra shows that for $dp/dt = 0$

$$\frac{dp}{p} = \left[-\frac{1}{2}\frac{\partial g_{ab}}{\partial x^c} v^a v^b + \frac{\partial}{\partial x^c}\log\sqrt{|g|} - \frac{\partial \phi}{\partial x^x}\right] dx^c$$

- Therefore the above second-order SDE is satisfied by invariant densities $t \to \infty$ of the form

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

$$\frac{dp}{dt} = - \quad v^a \frac{\partial p}{\partial x^a} + \frac{\partial}{\partial v^a}\left[\left(\Gamma^a_{bc} v^b v^c + g^{ab}\frac{\partial \phi}{\partial x^b} + v^a\right) p\right] + g^{ab}\frac{\partial^2 p}{\partial v^a \partial v^b}$$

- Some schoolboy algebra shows that for $dp/dt = 0$

$$\frac{dp}{p} = \left[-\frac{1}{2}\frac{\partial g_{ab}}{\partial x^c} v^a v^b + \frac{\partial}{\partial x^c}\log\sqrt{|g|} - \frac{\partial \phi}{\partial x^x}\right] dx^c$$

- Therefore the above second-order SDE is satisfied by invariant densities $t \to \infty$ of the form

$$p(\mathbf{x}, \mathbf{v}) \propto \det(\mathbf{G}(\mathbf{x})) \exp\left(-\frac{1}{2}\mathbf{v}^{\mathsf{T}}\mathbf{G}(\mathbf{x})\mathbf{v} - \phi(\mathbf{x})\right)$$

Second-Order Diffusions

- What is invariant measure of this diffusion?
- The Fokker-Planck equation for the diffusion follows as

$$\frac{dp}{dt} = - \quad v^a \frac{\partial p}{\partial x^a} + \frac{\partial}{\partial v^a}\left[\left(\Gamma^a_{bc} v^b v^c + g^{ab}\frac{\partial \phi}{\partial x^b} + v^a\right) p\right] + g^{ab}\frac{\partial^2 p}{\partial v^a \partial v^b}$$

- Some schoolboy algebra shows that for $dp/dt = 0$

$$\frac{dp}{p} = \left[-\frac{1}{2}\frac{\partial g_{ab}}{\partial x^c} v^a v^b + \frac{\partial}{\partial x^c}\log\sqrt{|g|} - \frac{\partial \phi}{\partial x^x}\right] dx^c$$

- Therefore the above second-order SDE is satisfied by invariant densities $t \to \infty$ of the form

$$p(\mathbf{x}, \mathbf{v}) \propto \det(\mathbf{G}(\mathbf{x})) \exp\left(-\frac{1}{2}\mathbf{v}^{\mathsf{T}}\mathbf{G}(\mathbf{x})\mathbf{v} - \phi(\mathbf{x})\right)$$

- So for $\phi(\mathbf{x}) = -\log \pi(\mathbf{x}) + \frac{1}{2}\log\det(\mathbf{G}(\mathbf{x}))$ then it follows that marginally

$$p(\mathbf{x}) = \exp\left(-\phi(\mathbf{x})\right) = \pi(\mathbf{x})$$

- Numerical integration forms basis of MCMC scheme..... however

Second-Order Diffusions

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- is transformed to

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- is transformed to

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\ d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- is transformed to

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\ d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- where vector function $\boldsymbol{\nu}$ has elements $-\partial_i g^{ab} p_a p_b$

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- is transformed to

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\
d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- where vector function $\boldsymbol{\nu}$ has elements $-\partial_i g^{ab} p_a p_b$
- Invariant measure with density

$$
p(\mathbf{x}, \mathbf{p}) \propto \frac{1}{\det(\mathbf{G}(\mathbf{x}))} \exp\left(-\frac{1}{2}\mathbf{p}^{\mathsf{T}}\mathbf{G}^{-1}(\mathbf{x})\mathbf{p} - \phi(\mathbf{x})\right)
$$

Second-Order Diffusions

- Transform the system of SDE's from the configuration to phase space such that transformed variable $\mathbf{p}_t = \mathbf{G}(\mathbf{x}_t)\mathbf{v}_t$

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- is transformed to

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\ d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- where vector function $\boldsymbol{\nu}$ has elements $-\partial_i g^{ab} p_a p_b$
- Invariant measure with density

$$p(\mathbf{x}, \mathbf{p}) \propto \frac{1}{\det(\mathbf{G}(\mathbf{x}))} \exp\left(-\frac{1}{2}\mathbf{p}^{\mathsf{T}}\mathbf{G}^{-1}(\mathbf{x})\mathbf{p} - \phi(\mathbf{x})\right)$$

- Stochastic Hamiltonian on Manifold - using symplectic integrator samples drawn from invariant density via RMHMC

Geodesic flow as proposal mechanism

Geodesic flow as proposal mechanism

- Intuitive that proposal mechanism follow direct paths - geodesics

Geodesic flow as proposal mechanism

- Intuitive that proposal mechanism follow direct paths - geodesics
- Consider Thermodynamic Integral - basis for Path & Bridge sampling

Geodesic flow as proposal mechanism

- Intuitive that proposal mechanism follow direct paths - geodesics
- Consider Thermodynamic Integral - basis for Path & Bridge sampling
- For $\boldsymbol{\theta} \in \mathbb{R}^D$ with $p(y|\boldsymbol{\theta}) = q(y|\boldsymbol{\theta})z(\boldsymbol{\theta})^{-1}$ denote $U(y, \boldsymbol{\theta}) = \partial_{\boldsymbol{\theta}} \log q(y|\boldsymbol{\theta})$ and let $\boldsymbol{\theta}(t)$ be a function of index t

Geodesic flow as proposal mechanism

- Intuitive that proposal mechanism follow direct paths - geodesics
- Consider Thermodynamic Integral - basis for Path & Bridge sampling
- For $\boldsymbol{\theta} \in \mathbb{R}^D$ with $p(y|\boldsymbol{\theta}) = q(y|\boldsymbol{\theta})z(\boldsymbol{\theta})^{-1}$ denote $U(y,\boldsymbol{\theta}) = \partial_{\boldsymbol{\theta}} \log q(y|\boldsymbol{\theta})$ and let $\boldsymbol{\theta}(t)$ be a function of index t

$$\lambda = \log\left(\frac{z(\boldsymbol{\theta}(t_2))}{z(\boldsymbol{\theta}(t_1))}\right) = \int_{t_1}^{t_2} E_{y|\boldsymbol{\theta}(t)}\left\{\sum_d \dot{\boldsymbol{\theta}}_d(t) U_d(y,\boldsymbol{\theta})\right\} dt$$

Geodesic flow as proposal mechanism

- Intuitive that proposal mechanism follow direct paths - geodesics
- Consider Thermodynamic Integral - basis for Path & Bridge sampling
- For $\boldsymbol{\theta} \in \mathbb{R}^D$ with $p(y|\boldsymbol{\theta}) = q(y|\boldsymbol{\theta})z(\boldsymbol{\theta})^{-1}$ denote $U(y, \boldsymbol{\theta}) = \partial_{\boldsymbol{\theta}} \log q(y|\boldsymbol{\theta})$ and let $\boldsymbol{\theta}(t)$ be a function of index t

$$\lambda = \log \left(\frac{z(\boldsymbol{\theta}(t_2))}{z(\boldsymbol{\theta}(t_1))} \right) = \int_{t_1}^{t_2} E_{y|\boldsymbol{\theta}(t)} \left\{ \sum_d \dot{\boldsymbol{\theta}}_d(t) U_d(y, \boldsymbol{\theta}) \right\} dt$$

- Quality of N-sample path estimate $\hat{\lambda}$ is $var(\hat{\lambda})$ i.e. independent sampling

Geodesic flow as proposal mechanism

- Intuitive that proposal mechanism follow direct paths - geodesics
- Consider Thermodynamic Integral - basis for Path & Bridge sampling
- For $\boldsymbol{\theta} \in \mathbb{R}^D$ with $p(y|\boldsymbol{\theta}) = q(y|\boldsymbol{\theta})z(\boldsymbol{\theta})^{-1}$ denote $U(y, \boldsymbol{\theta}) = \partial_{\boldsymbol{\theta}} \log q(y|\boldsymbol{\theta})$ and let $\boldsymbol{\theta}(t)$ be a function of index t

$$\lambda = \log\left(\frac{z(\boldsymbol{\theta}(t_2))}{z(\boldsymbol{\theta}(t_1))}\right) = \int_{t_1}^{t_2} E_{y|\boldsymbol{\theta}(t)}\left\{\sum_d \dot{\boldsymbol{\theta}}_d(t) U_d(y, \boldsymbol{\theta})\right\} dt$$

- Quality of N-sample path estimate $\hat{\lambda}$ is $var(\hat{\lambda})$ i.e. independent sampling

$$\frac{1}{N}\left[\int_{t_1}^{t_2} \sum_{i,j} \left(g_{ij}\dot{\boldsymbol{\theta}}_i(t)\dot{\boldsymbol{\theta}}_j(t)\right) dt - \lambda^2\right] = \frac{1}{N}\left[\int_{t_1}^{t_2} \sum_{i,j} \left(g^{ij} p_i(t) p_j(t)\right) dt - \lambda^2\right]$$

where $g_{ij} = E_{y|\boldsymbol{\theta}(t)}\{U_i(y, \boldsymbol{\theta}) U_j(y, \boldsymbol{\theta})\}$ and $p_i(t) = \sum_j g_{ij}\dot{\boldsymbol{\theta}}_j(t)$

Geodesic flow as proposal mechanism

- Variance of estimate can be minimised by employing path that minimises

$$\int_{t1}^{t2} \dot{\boldsymbol{\theta}}(t)^{\mathsf{T}} \mathbf{G}(\boldsymbol{\theta}(t)) \dot{\boldsymbol{\theta}}(t) dt = \int_{t1}^{t2} \mathbf{p}(t)^{\mathsf{T}} \mathbf{G}^{-1}(\boldsymbol{\theta}(t)) \mathbf{p}(t) dt = \int_{t1}^{t2} H(\boldsymbol{\theta}(t), \mathbf{p}(t)) dt$$

Geodesic flow as proposal mechanism

- Variance of estimate can be minimised by employing path that minimises

$$\int_{t1}^{t2} \dot{\boldsymbol{\theta}}(t)^{\mathsf{T}} \mathbf{G}(\boldsymbol{\theta}(t)) \dot{\boldsymbol{\theta}}(t) dt = \int_{t1}^{t2} \mathbf{p}(t)^{\mathsf{T}} \mathbf{G}^{-1}(\boldsymbol{\theta}(t)) \mathbf{p}(t) dt = \int_{t1}^{t2} H(\boldsymbol{\theta}(t), \mathbf{p}(t)) dt$$

where $H(\boldsymbol{\theta}(t), \mathbf{p}(t))$ is Hamiltonian defined on the manifold with position specific metric tensor $g_{ij}(\boldsymbol{\theta})$

Geodesic flow as proposal mechanism

- Variance of estimate can be minimised by employing path that minimises

$$\int_{t1}^{t2} \dot{\boldsymbol{\theta}}(t)^{\mathsf{T}}\mathbf{G}(\boldsymbol{\theta}(t))\dot{\boldsymbol{\theta}}(t)dt = \int_{t1}^{t2} \mathbf{p}(t)^{\mathsf{T}}\mathbf{G}^{-1}(\boldsymbol{\theta}(t))\mathbf{p}(t)dt = \int_{t1}^{t2} H(\boldsymbol{\theta}(t),\mathbf{p}(t))dt$$

  where $H(\boldsymbol{\theta}(t),\mathbf{p}(t))$ is Hamiltonian defined on the manifold with position specific metric tensor $g_{ij}(\boldsymbol{\theta})$
- This is satisfied by Geodesic equations

$$\frac{d^2\theta^i}{dt^2} + \sum_{k,l}\Gamma^i_{kl}\frac{d\theta^k}{dt}\frac{d\theta^l}{dt} = 0$$

Geodesic flow as proposal mechanism

- Variance of estimate can be minimised by employing path that minimises

$$\int_{t1}^{t2} \dot{\boldsymbol{\theta}}(t)^{\mathsf{T}} \mathbf{G}(\boldsymbol{\theta}(t)) \dot{\boldsymbol{\theta}}(t) dt = \int_{t1}^{t2} \mathbf{p}(t)^{\mathsf{T}} \mathbf{G}^{-1}(\boldsymbol{\theta}(t)) \mathbf{p}(t) dt = \int_{t1}^{t2} H(\boldsymbol{\theta}(t), \mathbf{p}(t)) dt$$

  where $H(\boldsymbol{\theta}(t), \mathbf{p}(t))$ is Hamiltonian defined on the manifold with position specific metric tensor $g_{ij}(\boldsymbol{\theta})$

- This is satisfied by Geodesic equations

$$\frac{d^2\theta^i}{dt^2} + \sum_{k,l} \Gamma^i_{kl} \frac{d\theta^k}{dt} \frac{d\theta^l}{dt} = 0$$

- Replace D 2-order ODEs with $2D$ 1-order ODEs in Hamilton-Jacobi form

$$\frac{d\boldsymbol{\theta}}{dt} = \frac{\partial}{\partial \mathbf{p}} H(\boldsymbol{\theta}, \mathbf{p}) \quad \frac{d\boldsymbol{p}}{dt} = -\frac{\partial}{\partial \boldsymbol{\theta}} H(\boldsymbol{\theta}, \mathbf{p})$$

Geodesic flow as proposal mechanism

- Variance of estimate can be minimised by employing path that minimises

$$\int_{t1}^{t2} \dot{\boldsymbol{\theta}}(t)^{\mathsf{T}} \mathbf{G}(\boldsymbol{\theta}(t))\dot{\boldsymbol{\theta}}(t)dt = \int_{t1}^{t2} \mathbf{p}(t)^{\mathsf{T}} \mathbf{G}^{-1}(\boldsymbol{\theta}(t))\mathbf{p}(t)dt = \int_{t1}^{t2} H(\boldsymbol{\theta}(t), \mathbf{p}(t))dt$$

  where $H(\boldsymbol{\theta}(t), \mathbf{p}(t))$ is Hamiltonian defined on the manifold with position specific metric tensor $g_{ij}(\boldsymbol{\theta})$
- This is satisfied by Geodesic equations

$$\frac{d^2\theta^i}{dt^2} + \sum_{k,l} \Gamma^i_{kl} \frac{d\theta^k}{dt}\frac{d\theta^l}{dt} = 0$$

- Replace D 2-order ODEs with $2D$ 1-order ODEs in Hamilton-Jacobi form

$$\frac{d\boldsymbol{\theta}}{dt} = \frac{\partial}{\partial \mathbf{p}} H(\boldsymbol{\theta}, \mathbf{p}) \quad \frac{d\mathbf{p}}{dt} = -\frac{\partial}{\partial \boldsymbol{\theta}} H(\boldsymbol{\theta}, \mathbf{p})$$

- Solving Hamilton equations defines lowest variance / shortest path between two densities on manifold

Second-Order Diffusions

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\
d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\ d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Employ symplectic integrator e.g. RMHMC for drift term

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\
d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Employ symplectic integrator e.g. RMHMC for drift term
- Note that OU diffusion process corresponds to ad-hoc partial momentum updating

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\ d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Employ symplectic integrator e.g. RMHMC for drift term
- Note that OU diffusion process corresponds to ad-hoc partial momentum updating
- Solid theoretical basis amenable to analysis of algorithm performance

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\
d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Employ symplectic integrator e.g. RMHMC for drift term
- Note that OU diffusion process corresponds to ad-hoc partial momentum updating
- Solid theoretical basis amenable to analysis of algorithm performance
- Phase space defined on co-tangent bundle with symplectic forms in place

Second-Order Diffusions

- Stochastic Hamiltonian on Manifold driven by conditional Ornstein-Uhlenbeck process

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{G}^{-1}(\mathbf{x}_t)\mathbf{p}_t dt \\
d\mathbf{p}_t &= -\boldsymbol{\nu}(\mathbf{x}_t, \mathbf{p}_t)dt - \nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{p}_t dt + \sqrt{2\mathbf{G}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Employ symplectic integrator e.g. RMHMC for drift term
- Note that OU diffusion process corresponds to ad-hoc partial momentum updating
- Solid theoretical basis amenable to analysis of algorithm performance
- Phase space defined on co-tangent bundle with symplectic forms in place
- What of the configuration space?

Second-Order Diffusions

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$\begin{aligned} d\mathbf{x}_t &= \mathbf{v}_t dt \\ d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t \end{aligned}$$

- Drift function can be seen to describe Lagrangian dynamics

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Drift function can be seen to describe Lagrangian dynamics
- OU diffusion driving overall process

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Drift function can be seen to describe Lagrangian dynamics
- OU diffusion driving overall process
- Construct explicit integrator for dynamics - with volume correction

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Drift function can be seen to describe Lagrangian dynamics
- OU diffusion driving overall process
- Construct explicit integrator for dynamics - with volume correction
- Preserves original Hamiltonian dynamics - high proposal acceptance rates

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Drift function can be seen to describe Lagrangian dynamics
- OU diffusion driving overall process
- Construct explicit integrator for dynamics - with volume correction
- Preserves original Hamiltonian dynamics - high proposal acceptance rates
- Speed improvement over implicit symplectic integrator between 2x to 10x

Second-Order Diffusions

- This SDE defined on co-tangent bundle - non-symplectic forms

$$
\begin{aligned}
d\mathbf{x}_t &= \mathbf{v}_t dt \\
d\mathbf{v}_t &= -\gamma(\mathbf{x}_t, \mathbf{v}_t)dt - \mathbf{G}^{-1}(\mathbf{x}_t)\nabla_{\mathbf{x}_t}\phi(\mathbf{x}_t)dt - \mathbf{v}_t dt + \sqrt{2\mathbf{G}^{-1}(\mathbf{x}_t)}d\mathbf{W}_t
\end{aligned}
$$

- Drift function can be seen to describe Lagrangian dynamics
- OU diffusion driving overall process
- Construct explicit integrator for dynamics - with volume correction
- Preserves original Hamiltonian dynamics - high proposal acceptance rates
- Speed improvement over implicit symplectic integrator between 2x to 10x
- Lagrangian Dynamical Monte Carlo
  `http://arxiv.org/abs/1211.3759`

Gaussian Mixture Model

- Univariate finite mixture model

$$p(x|\mu,\sigma^2) = 0.7 \times \mathcal{N}(x|0,\sigma^2) + 0.3 \times \mathcal{N}(x|\mu,\sigma^2)$$

Gaussian Mixture Model

- Univariate finite mixture model

$$p(x|\mu, \sigma^2) = 0.7 \times \mathcal{N}(x|0, \sigma^2) + 0.3 \times \mathcal{N}(x|\mu, \sigma^2)$$

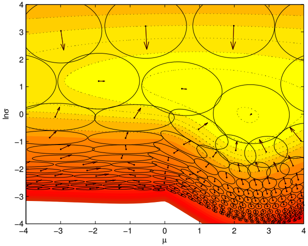
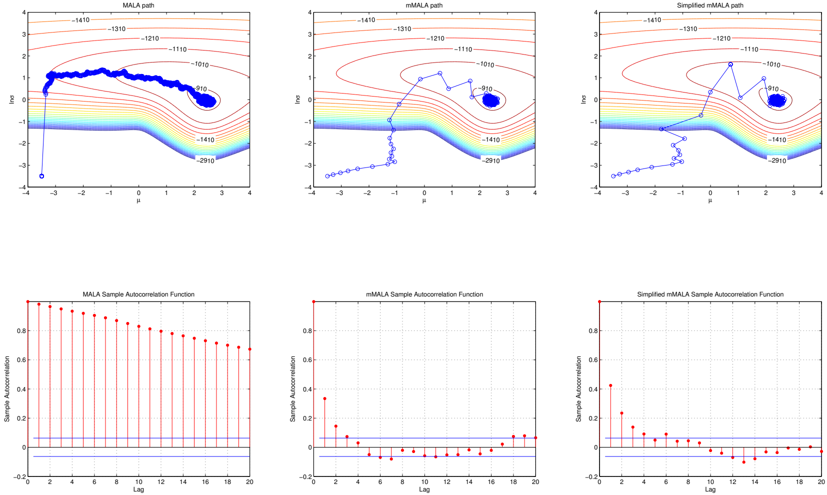
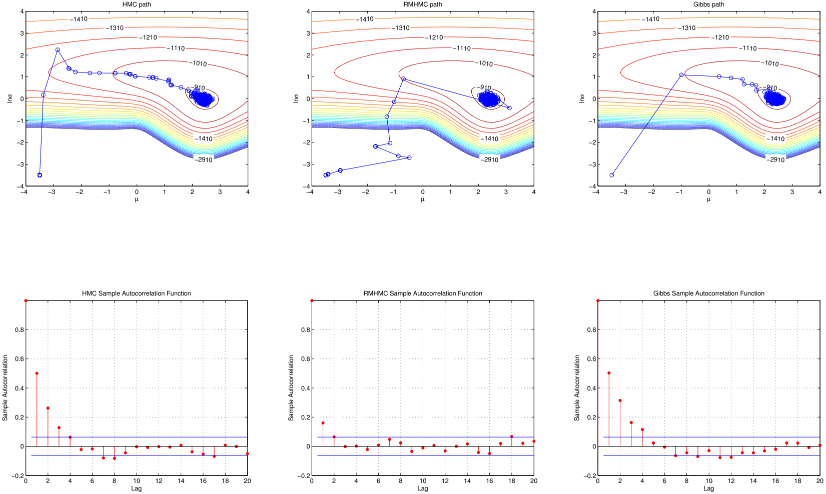


Figure: Arrows correspond to the gradients and ellipses to the inverse metric tensor. Dashed lines are isocontours of the joint log density

Gaussian Mixture Model



Gaussian Mixture Model



Log-Gaussian Cox Point Process with Latent Field

- The joint density for Poisson counts and latent Gaussian field

$$p(\mathbf{y}, \mathbf{x}|\mu, \sigma, \beta) \propto \prod_{i,j}^{64} \exp\{y_{i,j}x_{i,j} - m\exp(x_{i,j})\} \exp(-(\mathbf{x} - \mu\mathbf{1})^{\mathsf{T}} \Sigma_\theta^{-1}(\mathbf{x} - \mu\mathbf{1})/2)$$

Log-Gaussian Cox Point Process with Latent Field

- The joint density for Poisson counts and latent Gaussian field

$$p(\mathbf{y}, \mathbf{x}|\mu, \sigma, \beta) \propto \prod_{i,j}^{64} \exp\{y_{i,j}x_{i,j} - m\exp(x_{i,j})\}\exp(-(\mathbf{x}-\mu\mathbf{1})^{\mathsf{T}}\Sigma_{\theta}^{-1}(\mathbf{x}-\mu\mathbf{1})/2)$$

- Metric tensors

$$\begin{aligned} \mathbf{G}(\boldsymbol{\theta})_{i,j} &= \frac{1}{2} trace\left(\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\theta}}}{\partial \theta_i}\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\theta}}}{\partial \theta_j}\right) \\ \mathbf{G}(\mathbf{x}) &= \Lambda + \Sigma_{\boldsymbol{\theta}}^{-1} \end{aligned}$$

where Λ is diagonal with elements $m\exp(\mu + (\Sigma_{\boldsymbol{\theta}})_{i,i})$

Log-Gaussian Cox Point Process with Latent Field

- The joint density for Poisson counts and latent Gaussian field

$$p(\mathbf{y}, \mathbf{x}|\mu, \sigma, \beta) \propto \prod_{i,j}^{64} \exp\{y_{i,j}x_{i,j} - m\exp(x_{i,j})\} \exp(-(\mathbf{x}-\mu\mathbf{1})^{\mathsf{T}}\Sigma_\theta^{-1}(\mathbf{x}-\mu\mathbf{1})/2)$$

- Metric tensors

$$\begin{aligned} \mathbf{G}(\boldsymbol{\theta})_{i,j} &= \frac{1}{2} trace\left(\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\theta}}}{\partial \theta_i}\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\theta}}}{\partial \theta_j}\right) \\ \mathbf{G}(\mathbf{x}) &= \Lambda + \Sigma_{\boldsymbol{\theta}}^{-1} \end{aligned}$$

  where Λ is diagonal with elements $m\exp(\mu + (\Sigma_{\boldsymbol{\theta}})_{i,i})$

- Latent field metric tensor defining flat manifold is 4096×4096, $\mathcal{O}(N^3)$ obtained from parameter conditional

Log-Gaussian Cox Point Process with Latent Field

- The joint density for Poisson counts and latent Gaussian field

$$p(\mathbf{y}, \mathbf{x}|\mu, \sigma, \beta) \propto \prod_{i,j}^{64} \exp\{y_{i,j}x_{i,j} - m\exp(x_{i,j})\} \exp(-(\mathbf{x}-\mu\mathbf{1})^{\mathsf{T}}\Sigma_\theta^{-1}(\mathbf{x}-\mu\mathbf{1})/2)$$

- Metric tensors

$$\begin{aligned} \mathbf{G}(\boldsymbol{\theta})_{i,j} &= \frac{1}{2} trace\left(\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\theta}}}{\partial \theta_i}\boldsymbol{\Sigma}_{\boldsymbol{\theta}}^{-1}\frac{\partial \boldsymbol{\Sigma}_{\boldsymbol{\theta}}}{\partial \theta_j}\right) \\ \mathbf{G}(\mathbf{x}) &= \Lambda + \Sigma_{\boldsymbol{\theta}}^{-1} \end{aligned}$$

  where Λ is diagonal with elements $m\exp(\mu + (\Sigma_{\boldsymbol{\theta}})_{i,i})$

- Latent field metric tensor defining flat manifold is 4096×4096, $\mathcal{O}(N^3)$ obtained from parameter conditional

- MALA requires transformation of latent field to sample - with separate tuning in transient and stationary phases of Markov chain

RMHMC for Log-Gaussian Cox Point Processes

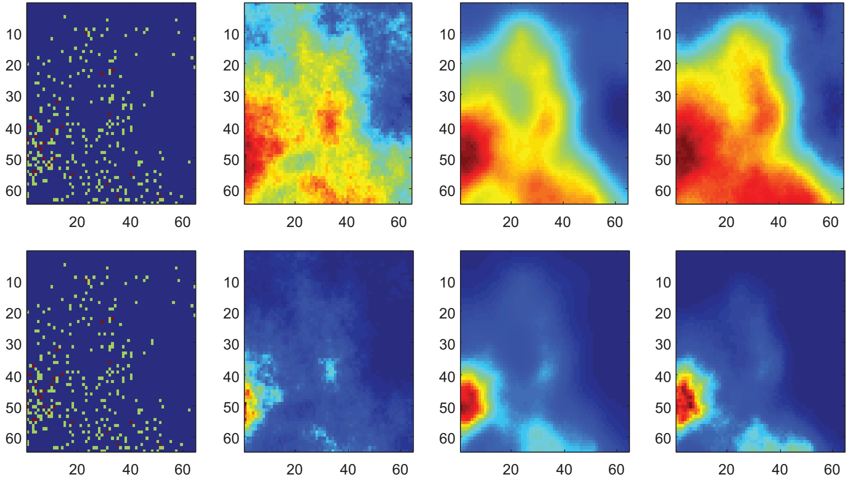


Figure: Data, Latent Field, Poisson Mean Field

RMHC for Log-Gaussian Cox Point Processes

Table: Sampling the latent variables of a Log-Gaussian Cox Process - Comparison of sampling methods

Method	Time	ESS (Min, Med, Max)	s/Min ESS	Rel. Speed
MALA (Transient)	31,577	(3, 8, 50)	10,605	$\times 1$
MALA (Stationary)	31,118	(4, 16, 80)	7836	$\times 1.35$
mMALA	634	(26, 84, 174)	24.1	$\times 440$
RMHMC	2936	(1951, 4545, 5000)	1.5	$\times 7070$

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence
  - Geodesic Monte Carlo on Embedded Manifolds
    `http://arxiv.org/pdf/1301.6064.pdf`

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence
  - Geodesic Monte Carlo on Embedded Manifolds
    `http://arxiv.org/pdf/1301.6064.pdf`
  - Investigate alternative manifold structures

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence
  - Geodesic Monte Carlo on Embedded Manifolds
    `http://arxiv.org/pdf/1301.6064.pdf`
  - Investigate alternative manifold structures
  - Design and effect of metric and connection

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence
  - Geodesic Monte Carlo on Embedded Manifolds
    `http://arxiv.org/pdf/1301.6064.pdf`
  - Investigate alternative manifold structures
  - Design and effect of metric and connection
  - Optimality of Hamiltonian flows as local geodesics

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence
  - Geodesic Monte Carlo on Embedded Manifolds
    `http://arxiv.org/pdf/1301.6064.pdf`
  - Investigate alternative manifold structures
  - Design and effect of metric and connection
  - Optimality of Hamiltonian flows as local geodesics
  - Alternative transition kernels

Conclusion and Discussion

- Geometry of statistical models harnessed in Monte Carlo methods
  - Diffusions that respect structure and curvature of space - Manifold MALA
  - Geodesic flows on model manifold - RMHMC - generalisation of HMC
  - Assessed on correlated & high-dimensional latent variable models
  - Promising capability of methodology
- Ongoing development
  - Theoretical analysis of convergence
  - Geodesic Monte Carlo on Embedded Manifolds
    `http://arxiv.org/pdf/1301.6064.pdf`
  - Investigate alternative manifold structures
  - Design and effect of metric and connection
  - Optimality of Hamiltonian flows as local geodesics
  - Alternative transition kernels
- No silver bullet or cure all - new powerful methodology for MC toolkit

Funding Acknowledgment

- EPSRC Established Career Fellowship
- Royal Society Wolfson Research Merit Award