Differential Geometric Simulation Methods for Uncertainty Quantification in Complex Model Systems

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Never Mind the Big Data here's the Big Models

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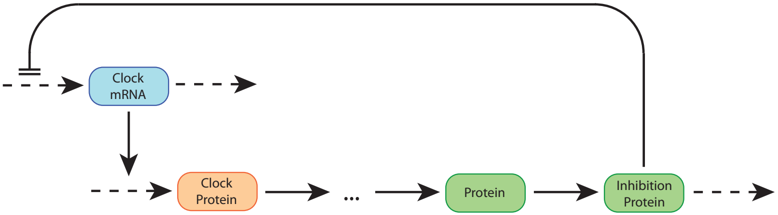
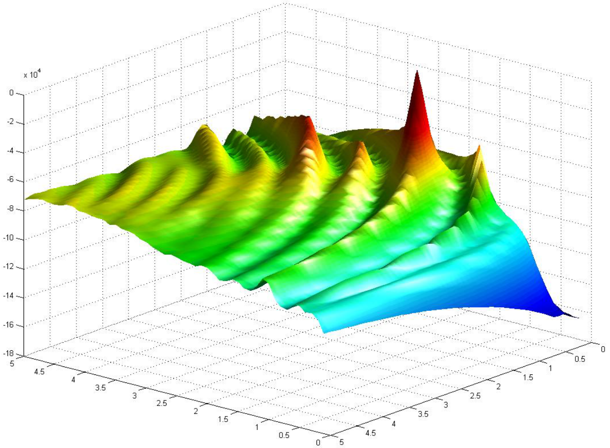
- This talk will concentrate on the issues associated with sampling from the induced measures from such models and associated data

System Identification: Nonlinear ODE Oscillator Model

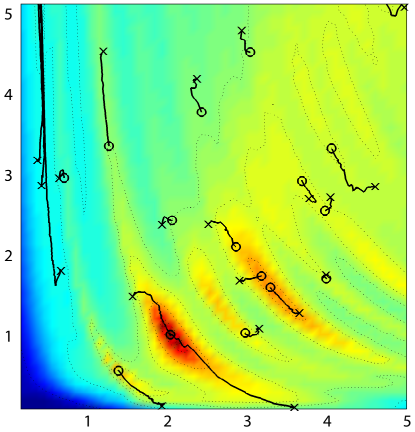


$$
\begin{aligned}
\frac{dx_1}{dt} &= \frac{k_1}{1 + x_n^{\rho}} - m_1 x_1 \\
\frac{dx_2}{dt} &= k_2 x_1 - m_2 x_2 \\
&\vdots \\
\frac{dx_n}{dt} &= k_n x_{n-1} - m_n x_n
\end{aligned}
$$

Systems Identification - Posterior Inference



Mixing of Markov Chains



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- Forward state is w and u the logarithm of distributed thermal conductivity on Ω, n the unit outward normal on Ω, and *Bi* the Biot number.

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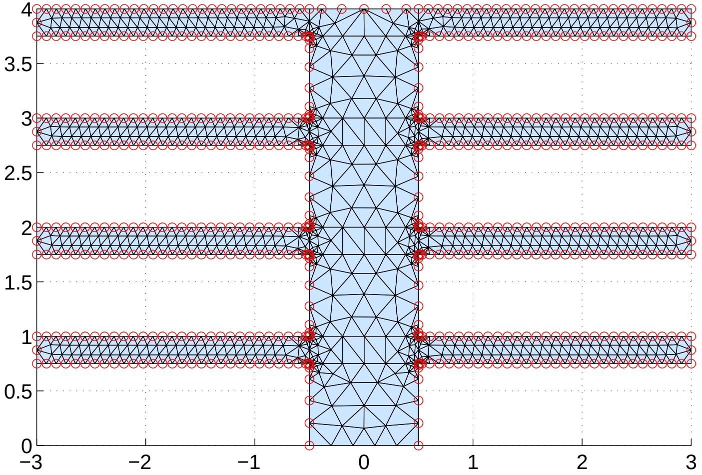

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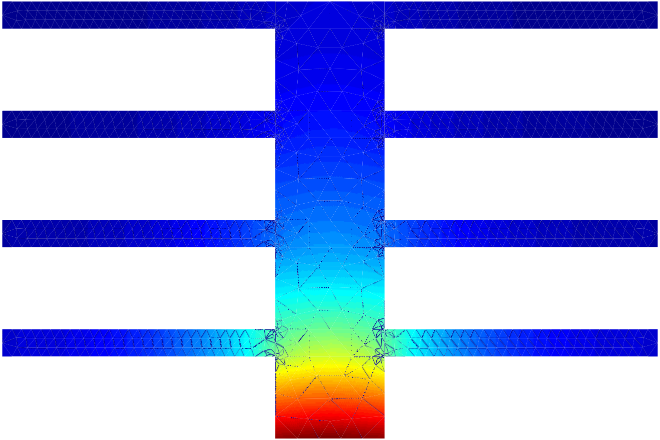

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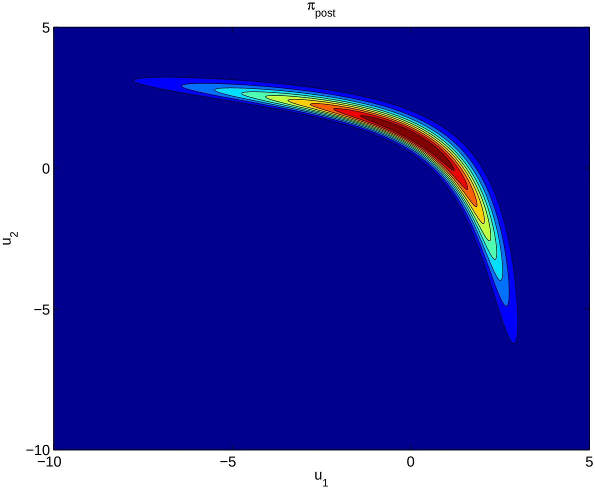
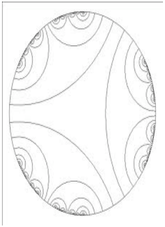
- Consider induced bivariate posterior for varying forms of prior Gaussian measure



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.

`http://www2.warwick.ac.uk/mgirolami`

Talk Outline

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- Further Work and Conclusions

Motivation Simulation Based Inference

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

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- Success of MCMC reliant upon appropriate proposal design

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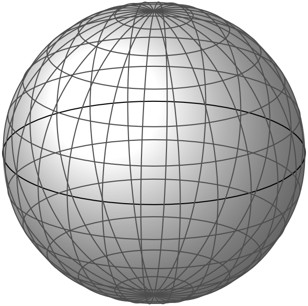
- Can geometric structure be employed in Monte Carlo methodology?

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): $d = 3$, $n = 2$

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



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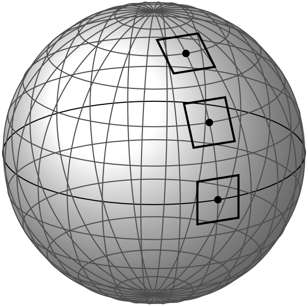
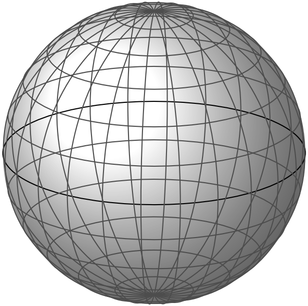
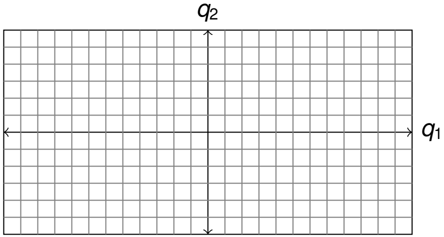


$x \in \mathbb{R}^d$ are the embedded coordinates

Coordinate systems and Riemannian metrics

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





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

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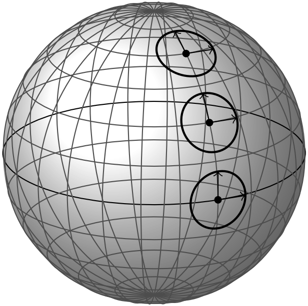

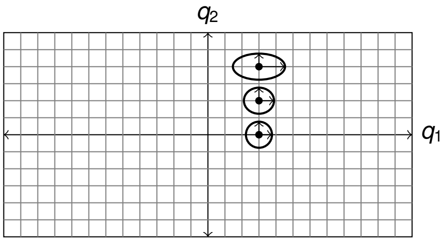

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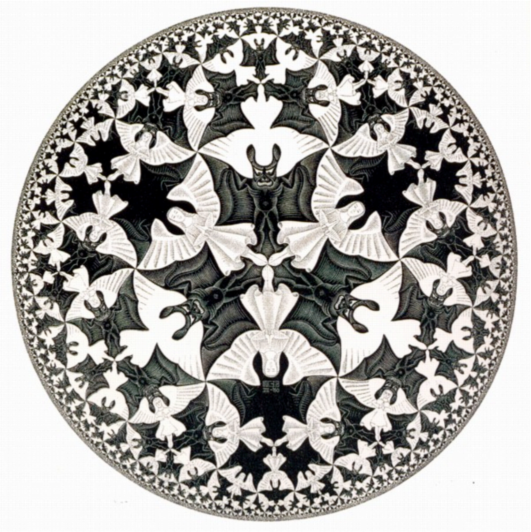
The Euclidean metric $\|\cdot\|$ induces a Riemannian metric G in the coordinate system:

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

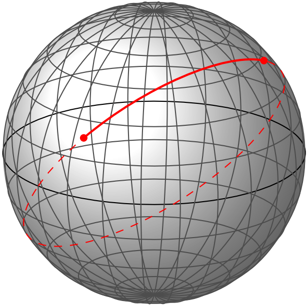
M.C. Escher, Heaven and Hell, 1960

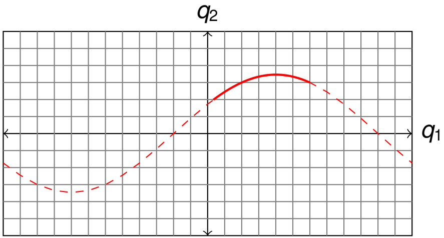


Geodesics

Geodesics are the paths of shortest distance.

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





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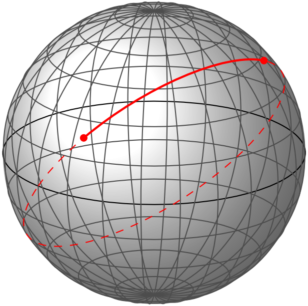
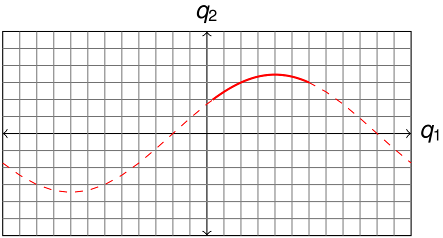


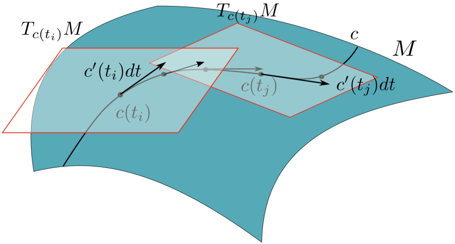


Given an initial velocity $v(0) \perp x(0)$, we have a nice explicit form

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

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

Geometric Concepts in MCMC



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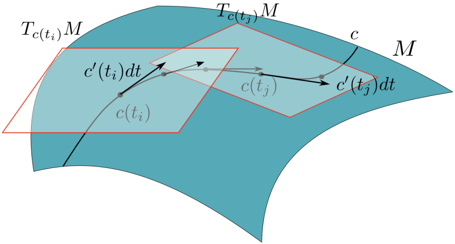

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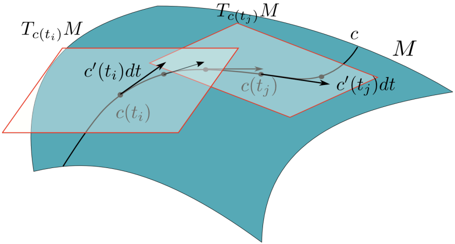

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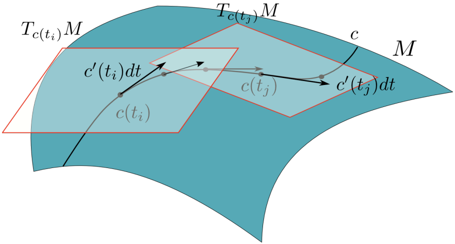
- Christoffel symbols - characterise Levi-Civita connection on manifold

Geometric Concepts in MCMC



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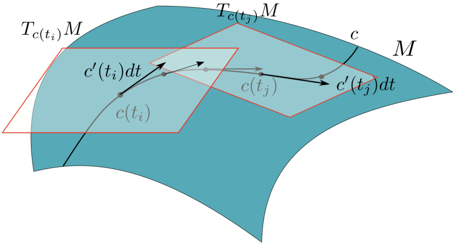

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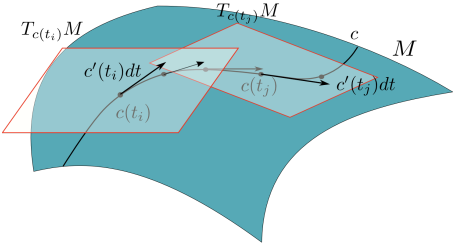

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Fisher–Rao metric

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:

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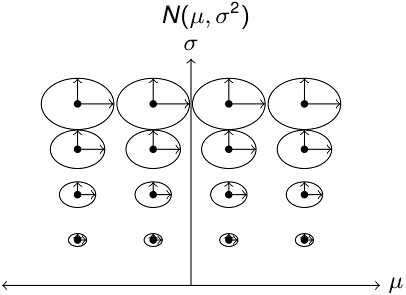

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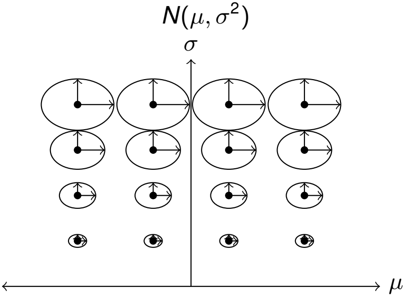

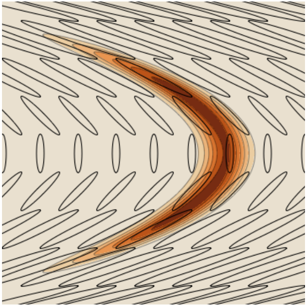

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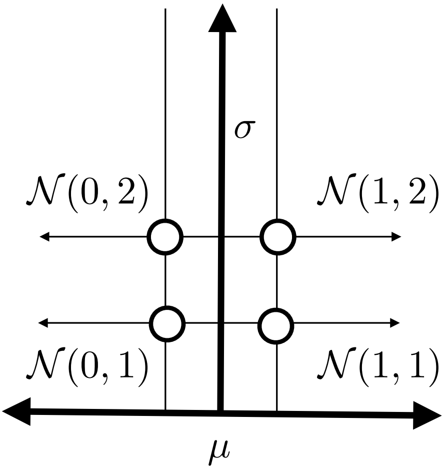
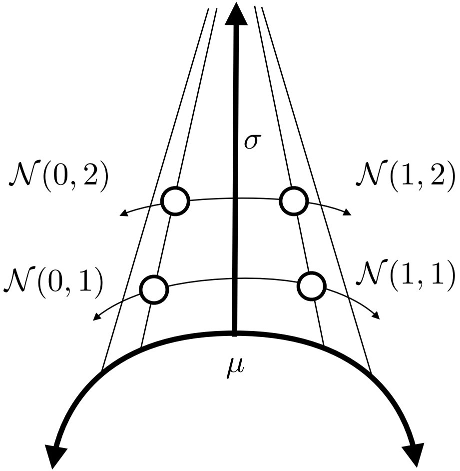
Normal Density - Euclidean Parameter space



Normal Density - Riemannian Functional space



Langevin Diffusion on Riemannian manifold

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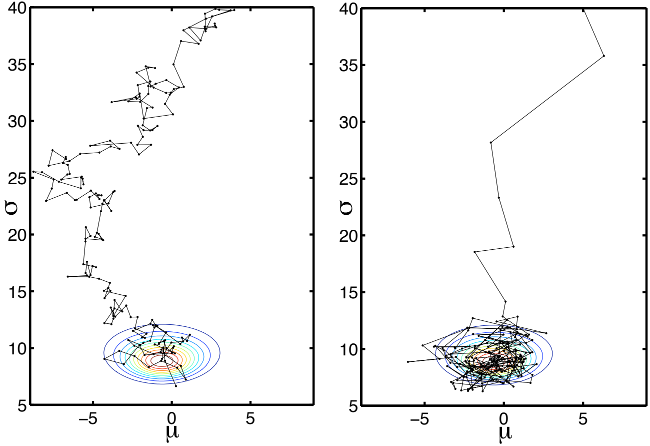

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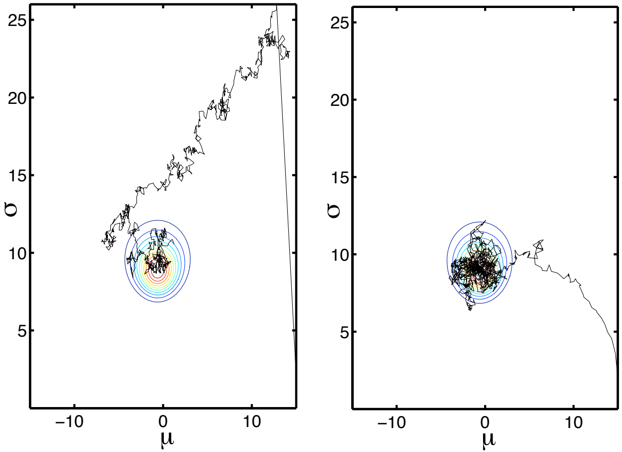

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- What is invariant measure of this diffusion?
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- So for $\phi(\mathbf{x}) = -\log \pi(\mathbf{x}) + \frac{1}{2}\log\det(\mathbf{G}(\mathbf{x}))$ then it follows that marginally

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

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

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Gaussian Mixture Model

- Univariate finite mixture model

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

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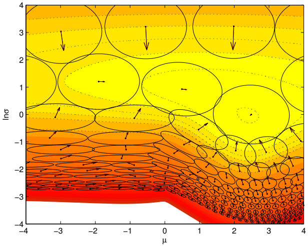
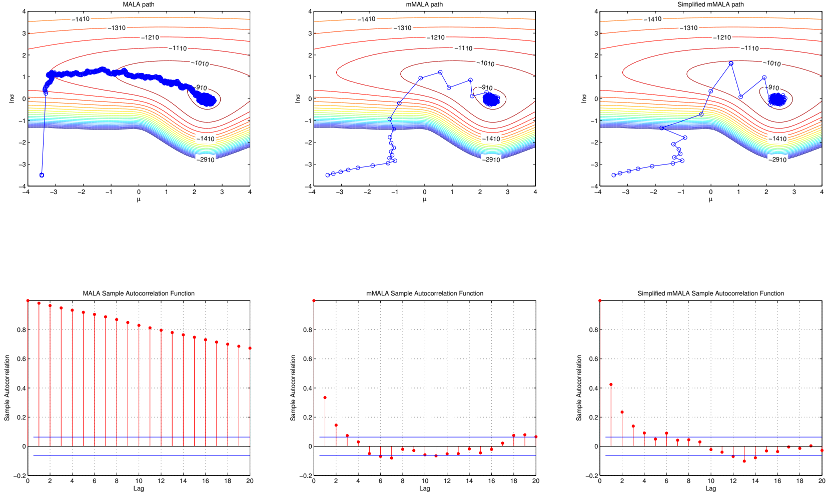


Figure : Arrows correspond to the gradients and ellipses to the inverse metric tensor. Dashed lines are isocontours of the joint log density

Gaussian Mixture Model



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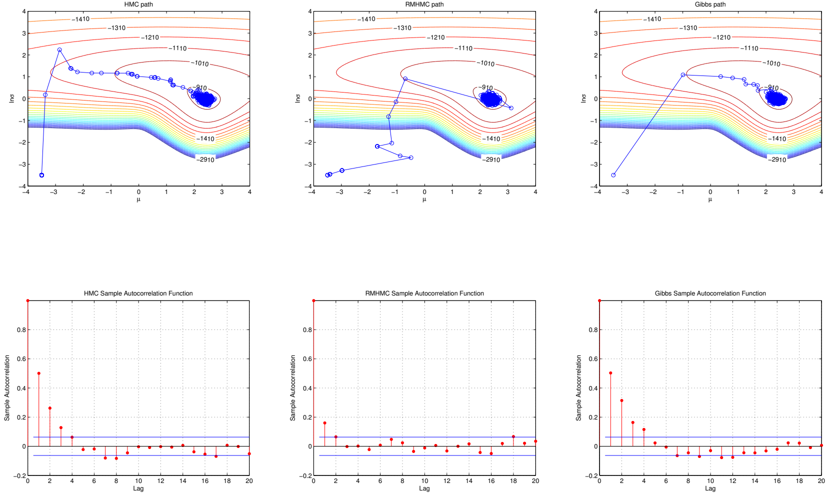

Log-Gaussian Cox Point Process with Latent Field

- The joint density for Poisson counts and latent Gaussian field

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

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- Metric tensors

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

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- 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

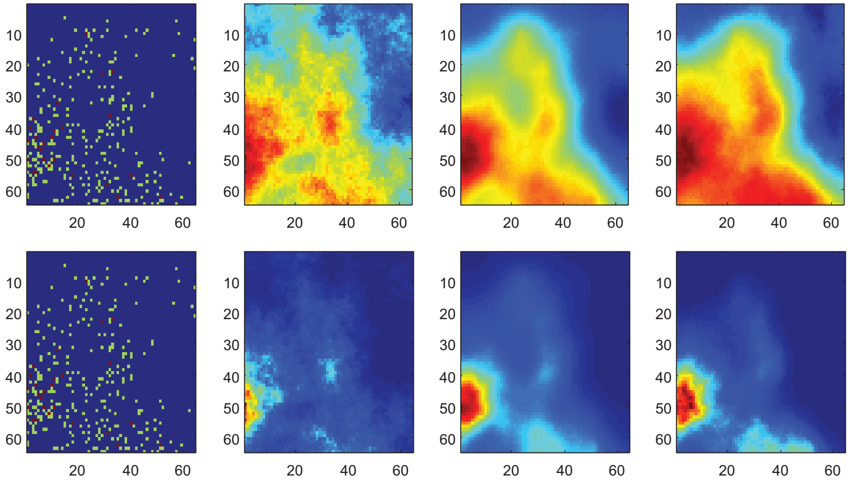

Figure : Data, Latent Field, Poisson Mean Field

RMHMC 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	$\times 7070$

Illustrative Heat Conduction Problem

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-e^{u} \nabla w \cdot \mathrm{n} &= u \;\, \mathrm{Bi} \quad on \quad \partial\Omega / \, \Gamma_R \\
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Illustrative Heat Conduction Problem

- Heat conduction problem governed by an elliptic partial differential equation in the open and bounded domain Ω:

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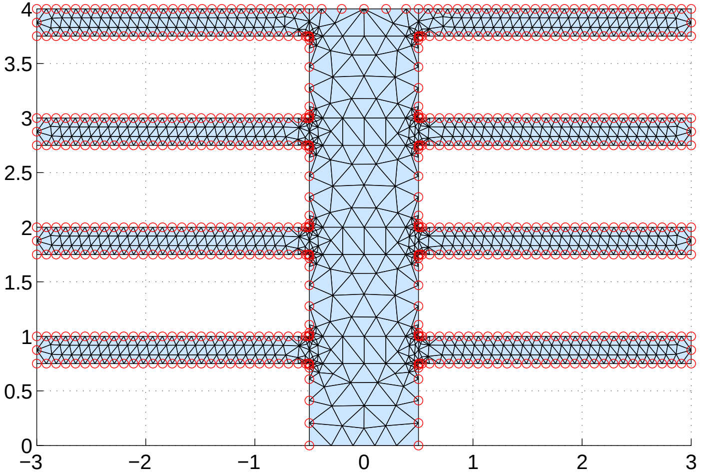

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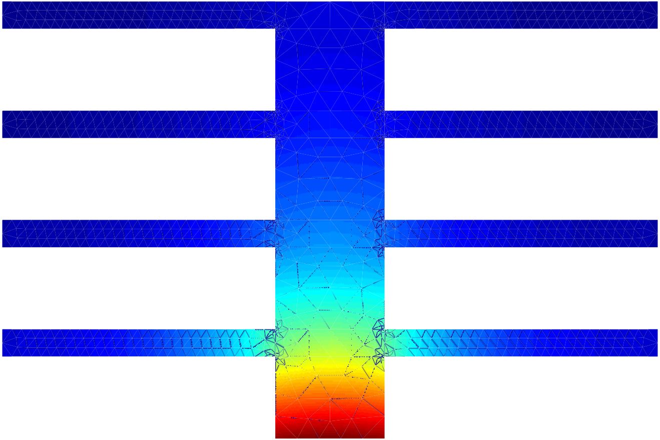
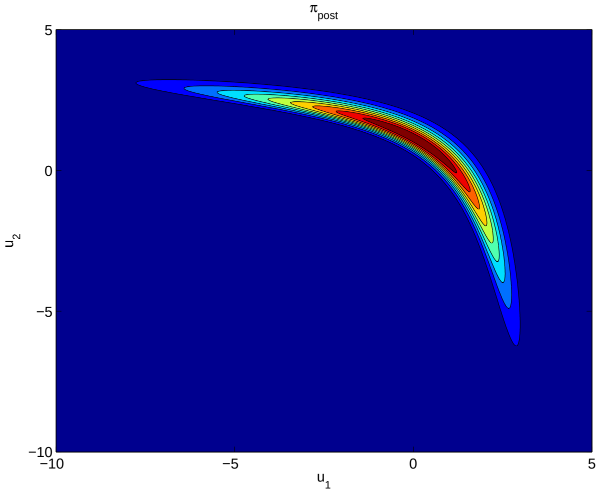


Illustrative Heat Conduction Problem

- Take one finite element discretisation of domain and one observation at leftmost boundary

Illustrative Heat Conduction Problem

- Take one finite element discretisation of domain and one observation at leftmost boundary
- Consider induced bivariate posterior for varying forms of prior Gaussian measure



Hamiltonian on Riemann Manifold

The dynamics for k-th component of $\mathbf{u}$ is given by Hamiltons equations

$$\frac{d\mathbf{u}_k}{dt} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} = \left(\mathbf{G}(\mathbf{u})^{-1}\mathbf{p}\right)_k$$

$$\frac{d\mathbf{p}_k}{dt} = -\frac{\partial \mathcal{H}}{\partial \mathbf{u}_k} = -\nabla_k J(\mathbf{u}) - \frac{1}{2} Tr\left[\mathbf{G}(\mathbf{u})^{-1}\frac{\partial\, \mathbf{G}(\mathbf{u})}{\partial \mathbf{u}_k}\right] + \frac{1}{2}\mathbf{p}^T \mathbf{G}(\mathbf{u})^{-1}\frac{\partial\, \mathbf{G}(\mathbf{u})}{\partial \mathbf{u}_k}\mathbf{G}(\mathbf{u})^{-1}\mathbf{p}$$

Gradient

Gradient

$$\langle \nabla \mathcal{J}(u), \tilde{u} \rangle = \int_\Omega \tilde{u} e^u \nabla w \cdot \nabla \lambda \, d\Omega,$$

First Order Forward

$$\int_\Omega e^u \nabla w \cdot \nabla \hat{\lambda} \, d\Omega + \int_{\partial\Omega \setminus \Gamma_R} Bi \, w \hat{\lambda} \, ds = \int_{\Gamma_R} \hat{\lambda} \, ds,$$

First Order Adjoint

$$\int_\Omega e^u \nabla \lambda \cdot \nabla \hat{w} \, d\Omega + \int_{\partial\Omega \setminus \Gamma_R} Bi \, \lambda \hat{w} \, ds = -\frac{1}{\sigma^2} \sum_{j=1}^{K} \left(w(\mathbf{x}_j) - d_j \right) \hat{w}(\mathbf{x}_j),$$

Hamiltonian on Riemann Manifold

The dynamics for k-th component of u is given by Hamiltons equations

$$\frac{du_k}{dt} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} = \left(\mathbf{G}(u)^{-1}\mathbf{p}\right)_k$$

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Hessian/Fisher Information Matrix

Fisher Matrix-Vector Product

$$\left\langle \langle G(u), \tilde{u} \rangle , u^2 \right\rangle = \int_\Omega \tilde{u} e^u \nabla w \cdot \nabla \tilde{\lambda}^2 \, d\Omega,$$

Second Order Forward

$$\int_\Omega e^u \nabla w^2 \cdot \nabla \hat{\lambda} \, d\Omega + \int_{\partial\Omega \backslash \Gamma_R} Bi \, w^2 \hat{\lambda} \, ds = - \int_\Omega u^2 e^u \nabla w \cdot \nabla \hat{\lambda} \, d\Omega,$$

Second Order Adjoint

$$\int_\Omega e^u \nabla \tilde{\lambda}^2 \cdot \nabla \hat{w} \, d\Omega + \int_{\partial\Omega \backslash \Gamma_R} Bi \, \tilde{\lambda}^2 \hat{w} \, ds = -\frac{1}{\sigma^2} \sum_{j=1}^{K} w^2 (\mathbf{x}_j) \, \hat{w} (\mathbf{x}_j) \, .$$

Hamiltonian on Riemann Manifold

The dynamics for k-th component of u is given by Hamiltons equations

$$\frac{du_k}{dt} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} = \left(\mathbf{G}(u)^{-1}\mathbf{p}\right)_k$$

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Derivative of Fisher Information Matrix

Derivative of Fisher Matrix-Matrix product

$$\left\langle\left\langle\left\langle T\left(u\right),\tilde{u}\right\rangle,u^2\right\rangle,u^3\right\rangle := \left\langle\nabla\left\langle\left\langle G\left(u\right),\tilde{u}\right\rangle,u^2\right\rangle,u^3\right\rangle$$
$$= \int_\Omega \tilde{u}u^3 e^u \nabla w \cdot \nabla\tilde{\lambda^2}\,d\Omega + \int_\Omega \tilde{u}e^u \nabla w^3 \cdot \nabla\tilde{\lambda^2}\,d\Omega + \int_\Omega \tilde{u}e^u \nabla w \cdot \nabla\lambda^{2,3}\,d\Omega$$

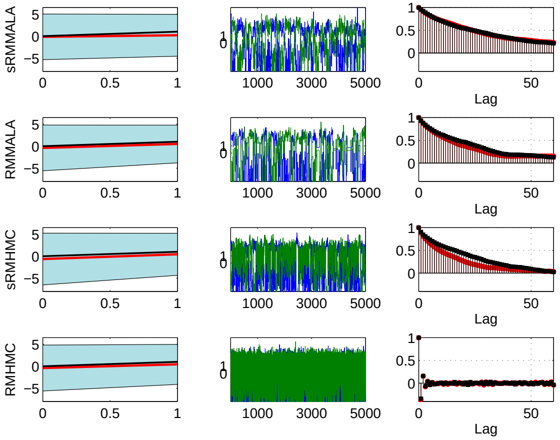
Third Order Forward

$$\int_\Omega e^u \nabla w^3 \cdot \nabla\hat{\lambda}\,d\Omega + \int_{\partial\Omega\setminus\Gamma_R} Bi\,w^3\hat{\lambda}\,ds = -\int_\Omega u^3 e^u \nabla w \cdot \nabla\hat{\lambda}\,d\Omega.$$

Third Order Adjoint

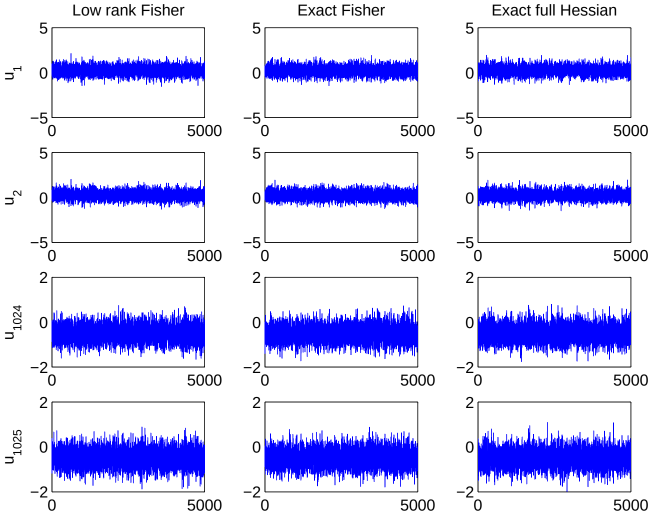
$$\int_\Omega e^u \nabla\lambda^{2,3} \cdot \nabla\hat{w}\,d\Omega + \int_{\partial\Omega\setminus\Gamma_R} Bi\,\lambda^{2,3}\hat{w}\,ds = -\frac{1}{\sigma^2}\sum_{j=1}^{K} w^{2,3}\left(\mathbf{x}_j\right)\hat{w}\left(\mathbf{x}_j\right)$$
$$-\int_\Omega u^3 e^u \nabla\tilde{\lambda^2} \cdot \nabla\hat{w}\,d\Omega,$$

Two-parameter Case



- $\varepsilon = 0.7$ for simRMMALA and RMMALA
- $\varepsilon = 0.02$, $L = 100$ for simRMHMC and RMHMC

1025-parameter Case



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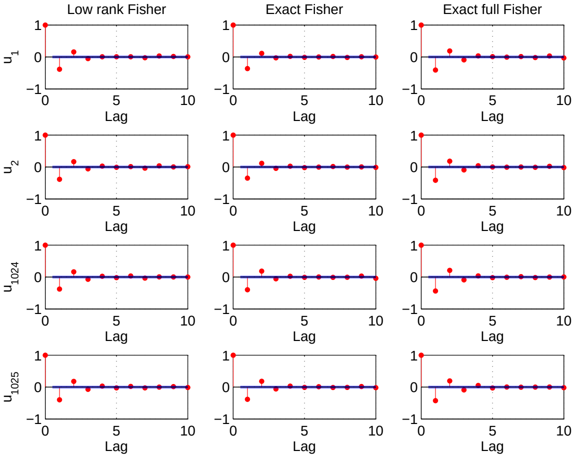

Bui-Thanh, T., and Girolami, M., *Solving Large-scale PDE using Riemann Manifold Hamiltonian MCMC*, **Inverse Problems, 30, 92014) 114014, IoP Publishing**.

Conclusion and Discussion

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