Markov Chain Monte Carlo using the Hamiltonian method

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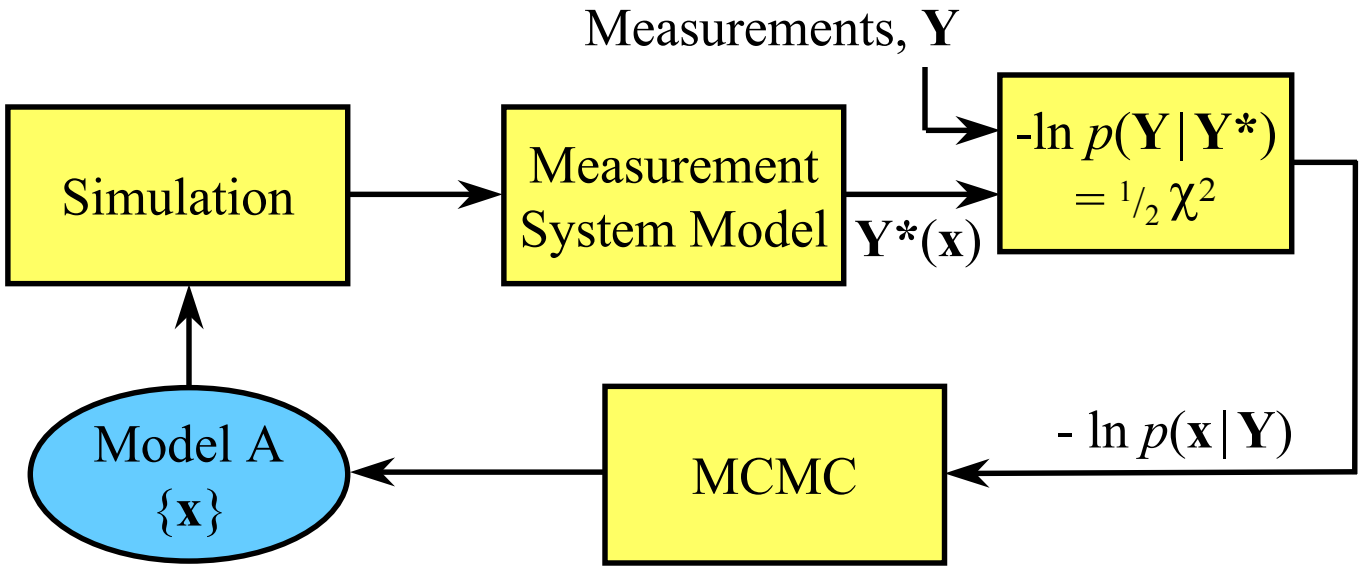
Acknowledgements

- MCMC experts
  - Dave Higdon, Frank Alexander, Julian Besag, Jim Guberantus, John Skilling, Malvin Kalos
- General discussions
  - Greg Cunningham, Richard Silver

MCMC in Bayesian data analysis



- - log(likelihood) distribution is result of calculation; function of model parameters **x**
- Markov Chain Monte Carlo (MCMC) algorithm draws random samples of **x** from posterior probability $p(\mathbf{x}|\mathbf{Y})$
- Produces plausible set of parameters {**x**}; therefore model realization

MCMC - problem statement

- Parameter space of n dimensions represented by vector $\mathbf{x}$
- Given an "arbitrary" **target** probability density function (pdf), $q(\mathbf{x})$, draw a set of samples $\{\mathbf{x}_k\}$ from it
- Only requirement typically is that, given $\mathbf{x}$, one be able to evaluate $Cq(\mathbf{x})$, where C is an unknown constant, that is, $q(\mathbf{x})$ need not be normalized
- Although focus here is on continuous variables, MCMC can be applied to discrete variables as well

Uses of MCMC

- Permits evaluation of the expectation values of functions of **x**, e.g.,

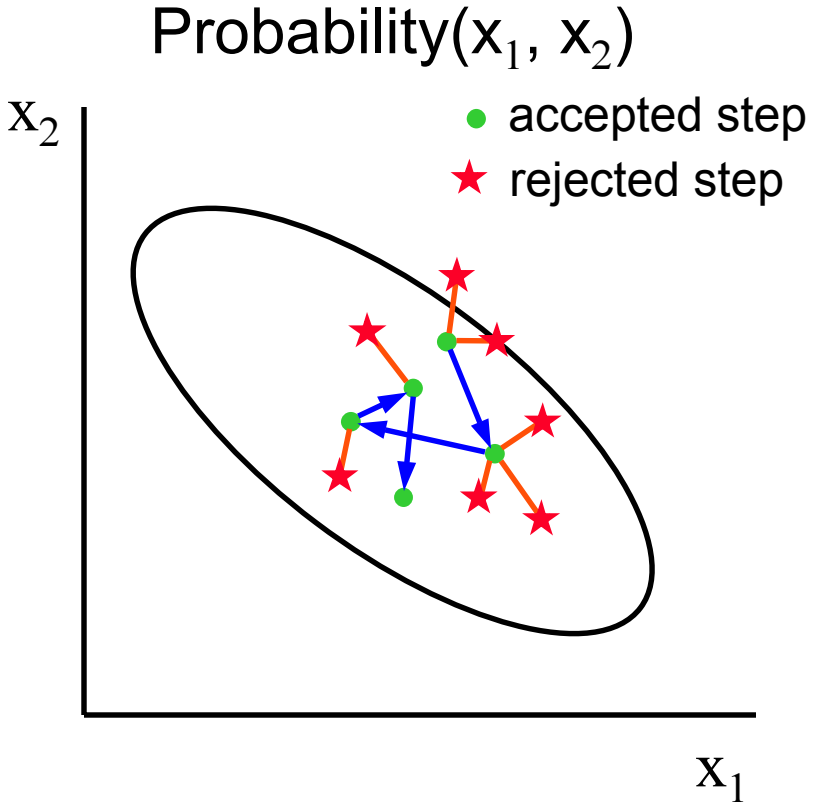
$$\langle f(\mathbf{x})\rangle = \int f(\mathbf{x})\, q(\mathbf{x})\, d\mathbf{x} \cong (1/\mathrm{K})\, \Sigma_k\, f(\mathbf{x}_k)$$

  - typical use is to calculate mean $\langle \mathbf{x} \rangle$ and variance $\langle (\mathbf{x} - \langle \mathbf{x} \rangle)^2 \rangle$
- Useful for evaluating integrals, such as the partition function for properly normalizing the pdf
- Dynamic display of sequences provides visualization of uncertainties in model and range of model variations
- Automatic marginalization; when considering any subset of parameters of an MCMC sequence, the remaining parameters are marginalized over (integrated out)

Metropolis Markov Chain Monte Carlo

Generates sequence of random samples from an arbitrary probability density function

- Metropolis algorithm:
  - draw trial step from symmetric pdf, i.e., $t(\Delta \mathbf{x}) = t(-\Delta \mathbf{x})$
  - accept or reject trial step
  - simple and generally applicable
  - relies only on calculation of target pdf for any **x**



Metropolis algorithm

- Select initial parameter vector $\mathbf{x}_0$
- Iterate as follows: at iteration number k
  (1) create new trial position $\mathbf{x}^* = \mathbf{x}_k + \Delta\mathbf{x}$,
  where $\Delta\mathbf{x}$ is randomly chosen from $t(\Delta\mathbf{x})$
  (2) calculate ratio $r = q(\mathbf{x}^*)/q(\mathbf{x}_k)$
  (3) accept trial position, i.e. set $\mathbf{x}_{k+1} = \mathbf{x}^*$
  if $r \geq 1$ or with probability r, if $r < 1$
  otherwise stay put, $\mathbf{x}_{k+1} = \mathbf{x}_k$

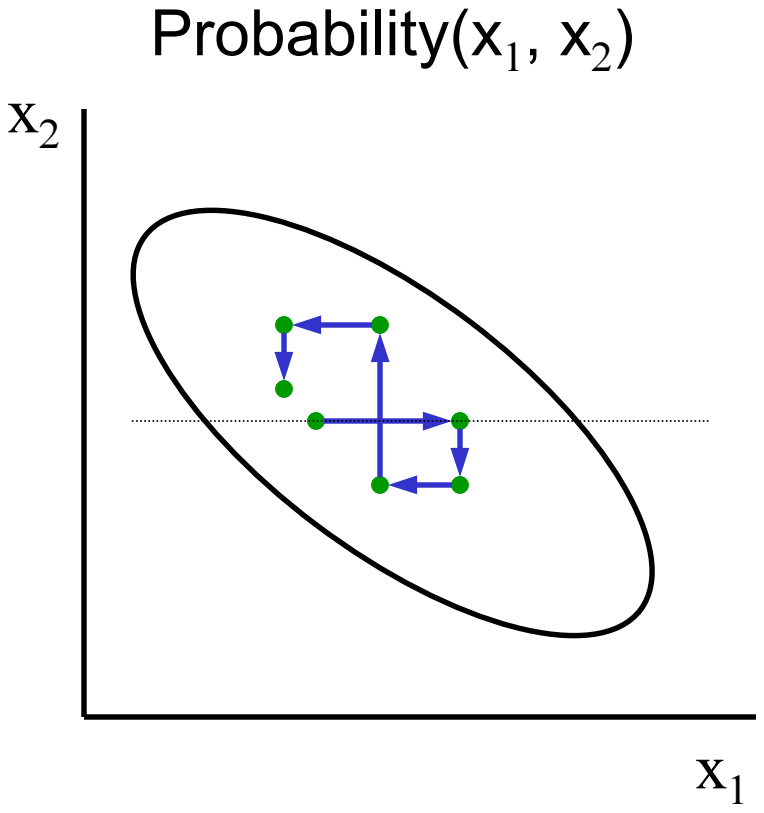
- Requires only computation of $q(\mathbf{x})$
- Creates Markov chain since $\mathbf{x}_{k+1}$ depends only on $\mathbf{x}_k$

Gibbs algorithm

- Vary only one component of **x** at a time
- Draw new value of x_j from conditional pdf

$$q(x_j | x_1 x_2 \ldots x_{j-1} x_{j+1} \ldots)$$

- Cycle through all components



Hamiltonian method

- Often called **hybrid method** because it alternates Gibbs & Metropolis steps
- Associate with each parameter x_i a momentum p_i
- Define a Hamiltonian (sum of potential and kinetic energy):

$$H = \varphi(\mathbf{x}) + \Sigma\, p_i^2/(2\, m_i) \ ,$$

where $\varphi = -\log\,(q(\mathbf{x}))$

- Objective is to draw samples from new pdf:

$$q'(\mathbf{x}, \mathbf{p}) \propto \exp(-\,H(\mathbf{x}, \mathbf{p})) = q(\mathbf{x})\, \exp(-\Sigma\, p_i^2/(2\, m_i))$$

- Then set of samples $\{\mathbf{x}_k\}$ represent draws from $q(\mathbf{x})$; **p** dependence marginalized out

Hamiltonian algorithm

- Gibbs step: randomly sample momentum distribution
- Follow trajectory of constant *H* using leapfrog algorithm:

$$p_i(t+\frac{\tau}{2}) = p_i(t) - \frac{\tau}{2}\frac{\partial\varphi}{\partial x_i}\bigg|_{\mathbf{x}(t)}$$

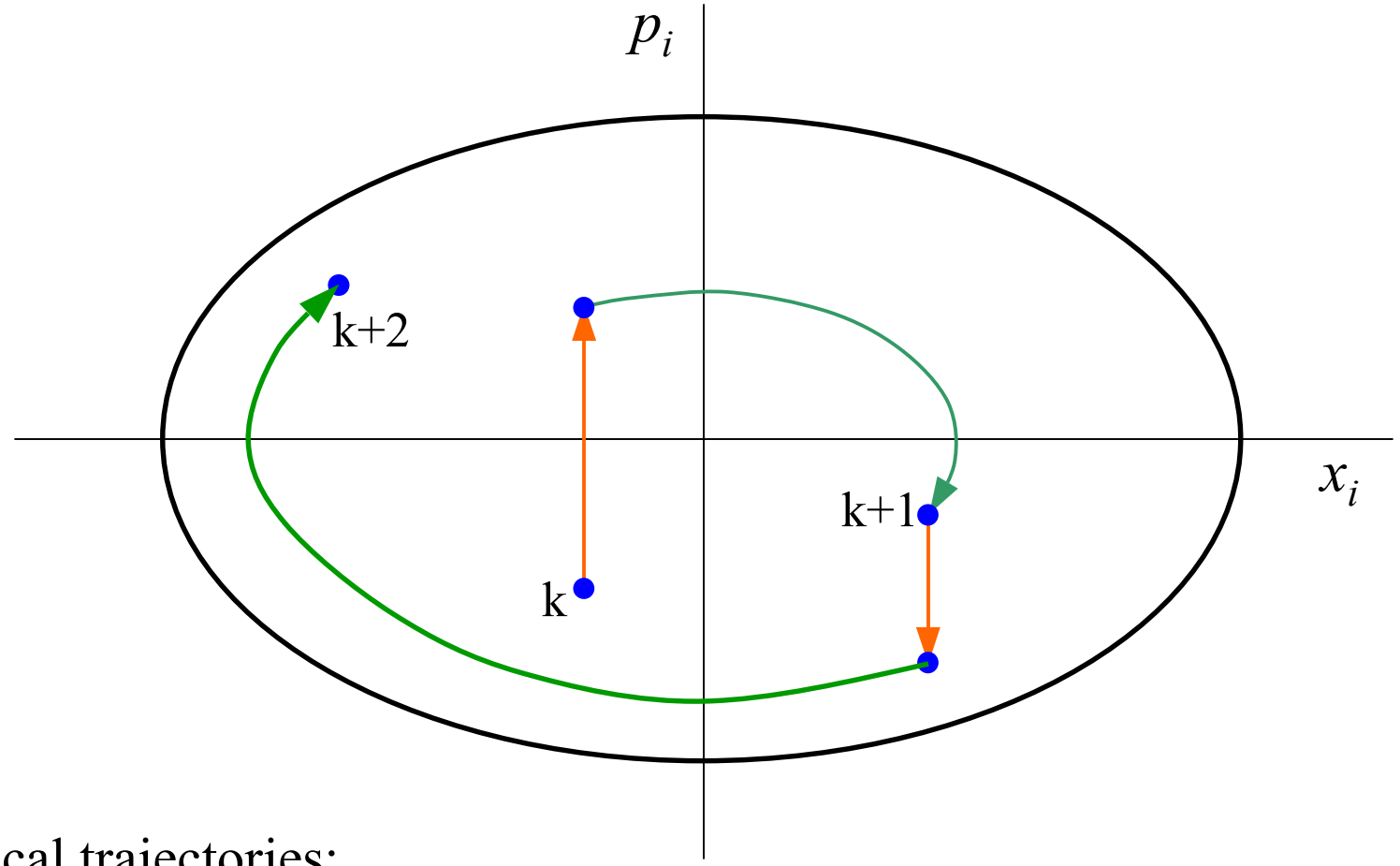
$$x_i(t+\tau) = x_i(t+\tau) + \frac{\tau}{m_i}p_i(t+\frac{\tau}{2})$$

$$p_i(t+\tau) = p_i(t+\frac{\tau}{2}) - \frac{\tau}{2}\frac{\partial\varphi}{\partial x_i}\bigg|_{\mathbf{x}(t+\tau)}$$

  where τ is leapfrog time step

- Metropolis step: accept or reject on basis of *H* at beginning and end of H trajectory

Hamiltonian hybrid algorithm



Typical trajectories:

red path - Gibbs sample from momentum distribution

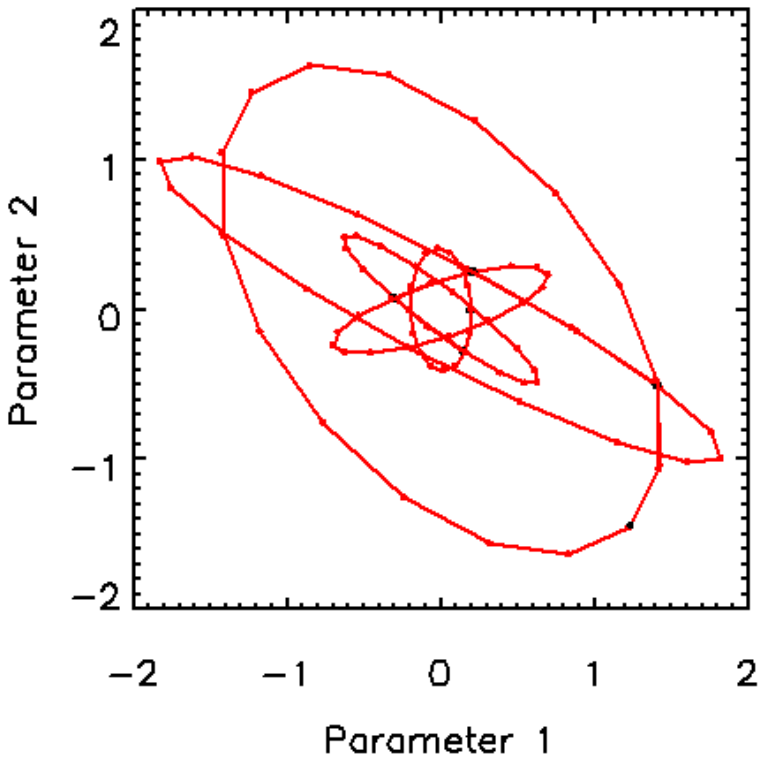
green path - trajectory with constant H, follow by Metropolis

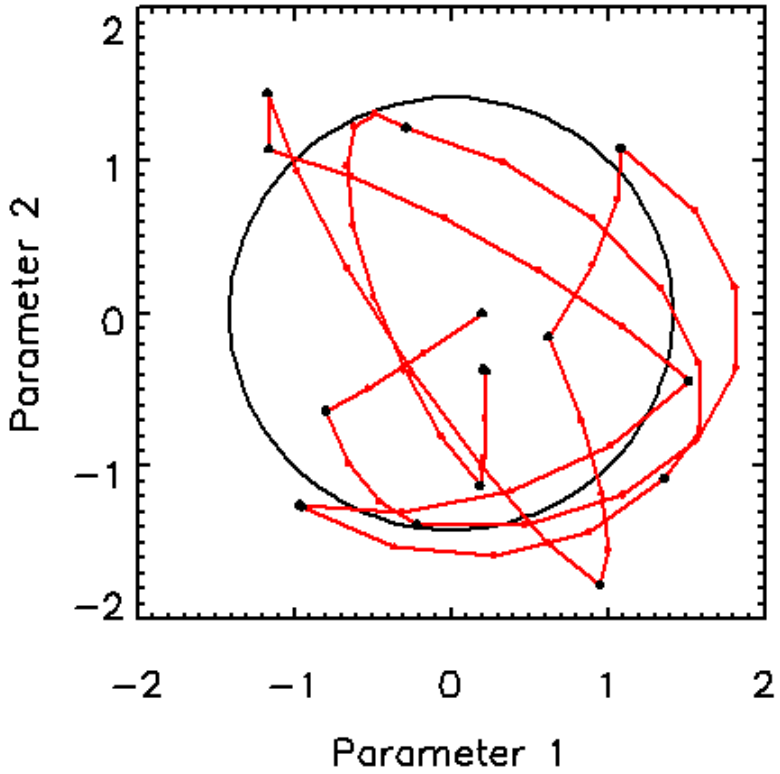
Hamiltonian algorithm

- Gibbs step - easy because draws are from uncorrelated Gaussian
- H trajectories followed by several leapfrog steps permit long jumps in (**x**, **p**) space, with little change in H
  - specify total time = T ; number of leapfrog steps = T/τ
- Metropolis step - no rejections if H is unchanged

- Adjoint differentiation efficiently provides gradient

2D isotropic Gaussian distribution





Long H trajectories - shows ellipses when $\sigma_1 = \sigma_2 = 1$, $m_1 = m_2 = 1$

Randomize length of H trajectories to obtain good sampling of pdf

MCMC Efficiency

– Estimate of a quantity from its samples from a pdf $q(v)$

$$\tilde{v} = \frac{1}{N_k} \Sigma\, v_k$$

– For N independent samples drawn from a pdf, variance in estimate:

$$\mathrm{var}(\tilde{v}) = \frac{\mathrm{var}(v)}{N}$$

– For N samples from an MCMC sequence with target pdf $q(v)$

$$\mathrm{var}(\tilde{v}) = \frac{\mathrm{var}(v)}{\eta N}$$

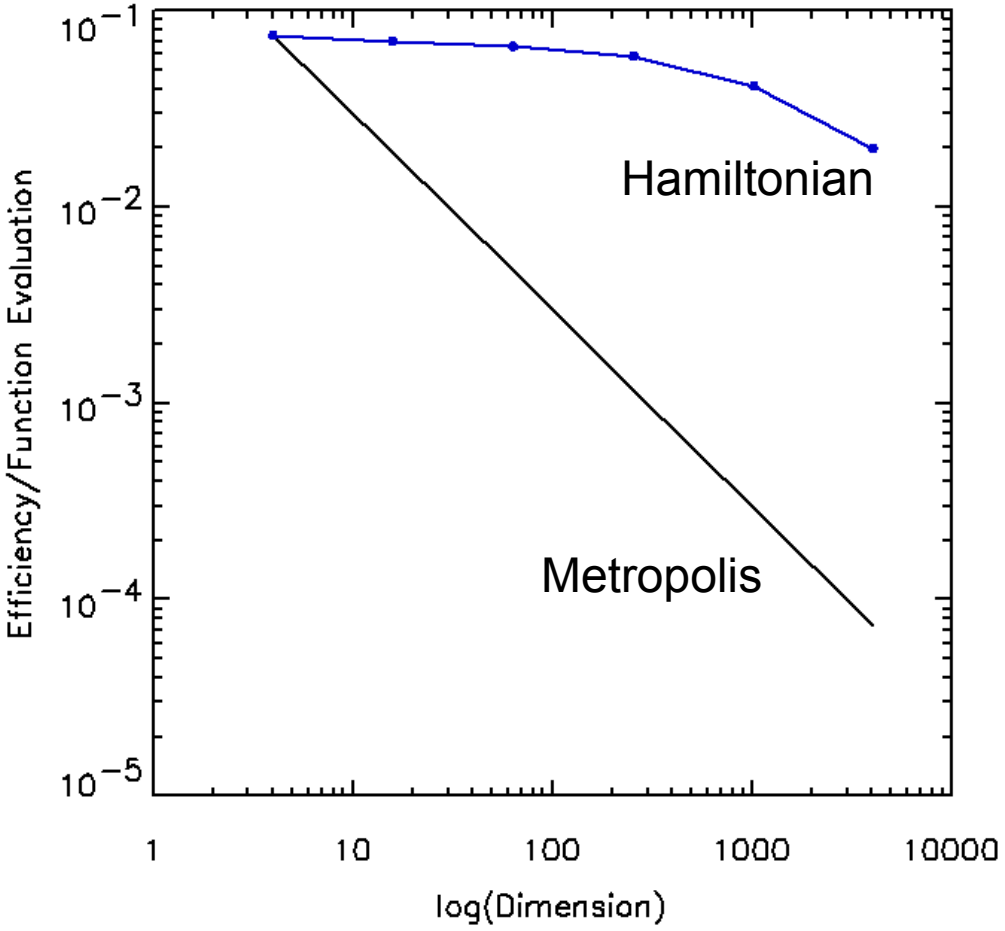
where η is the sampling efficiency

– Thus, η^{-1} iterations needed for one statistically independent sample

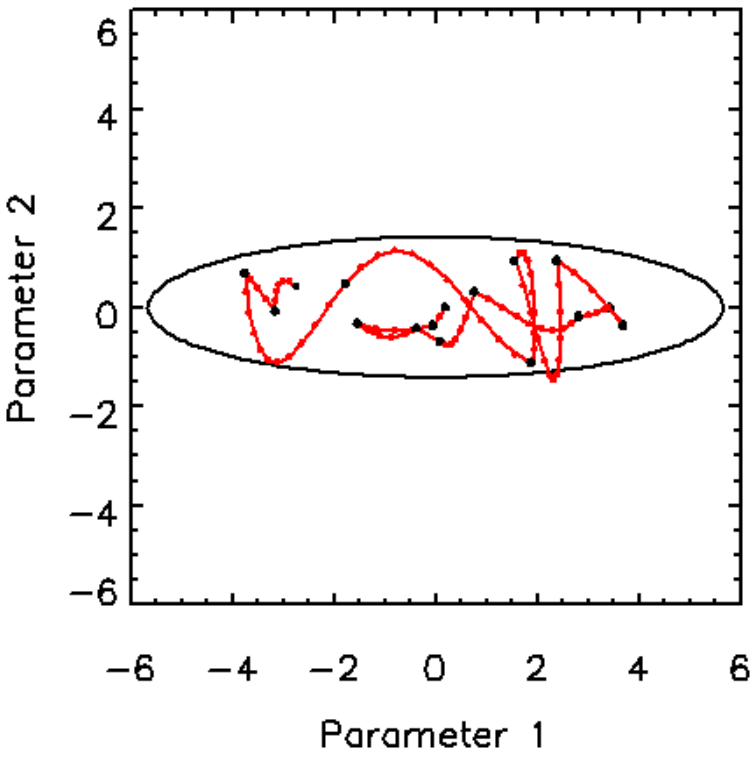
– Let v = variance because aim is to estimate variance of target pdf

n-D isotropic Gaussian distributions

- MCMC efficiency versus number dimensions
  - Hamiltonian method: drops little
  - Metropolis method: goes as $0.3/n$
- Hamiltonian method much more efficient at high dimensions



2D nonisotropic Gaussian distribution



- Nonisotropic Gaussian target pdf: $\sigma_1 = 4$, $\sigma_2 = 1$, $m_1 = m_2 = 1$
- Randomize length of H trajectories to get random sampling
- Convergence: determine whether sequence samples target pdf

Convergence test statistic

- Variance integral

$$\mathrm{var}(x_i) = \int (x_i - \bar{x}_i)^2 \, p(\mathbf{x}) d\mathbf{x}$$

$$= \int \frac{1}{3} (x_i - \bar{x}_i)^3 \nabla \varphi(\mathbf{x}) \, p(\mathbf{x}) \, d\mathbf{x} + \frac{1}{3} (x_i - \bar{x}_i)^3 \, p(\mathbf{x}) \Big|$$

  by integration by parts and $\varphi(\mathbf{x}) = -\log(p(\mathbf{x}))$

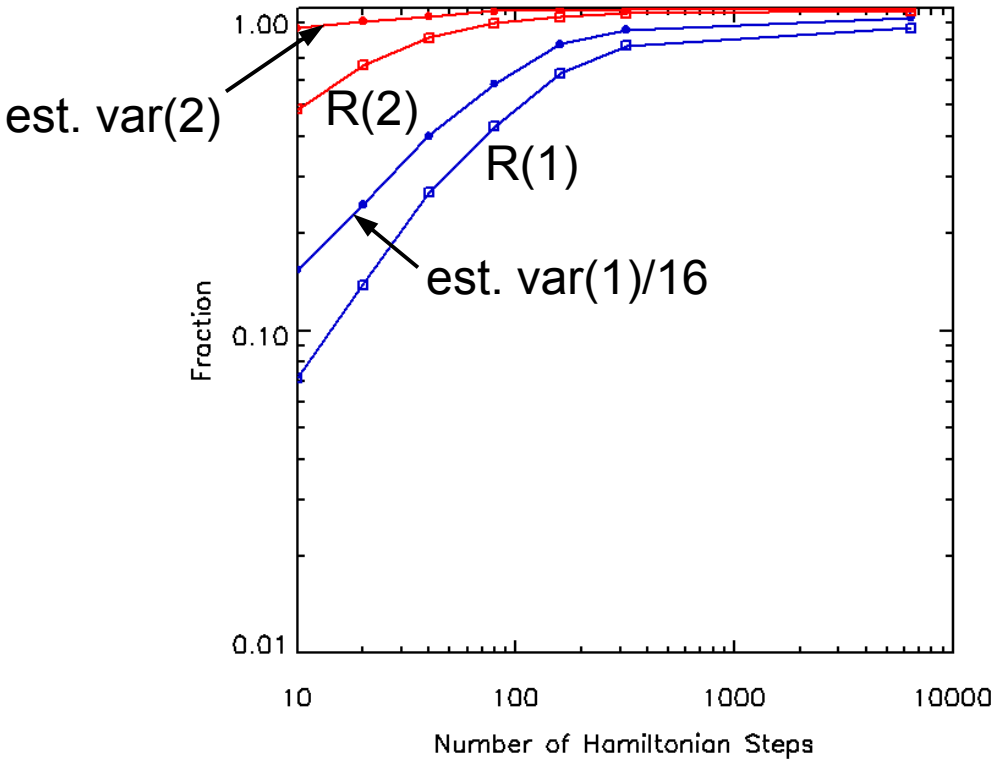
  - limits are typically $\pm\infty$ and last term is usually 0
  - thus, integrals are equal

- Form ratio of integrals, computed from samples $\mathbf{x}^k$ from $p(\mathbf{x})$

$$R = \frac{\Sigma \, (x_i^k - \bar{x}_i^k)^3 \, \dfrac{\partial \varphi}{\partial x_i^k}}{3 \Sigma \, (x_i^k - \bar{x}_i^k)^2}$$

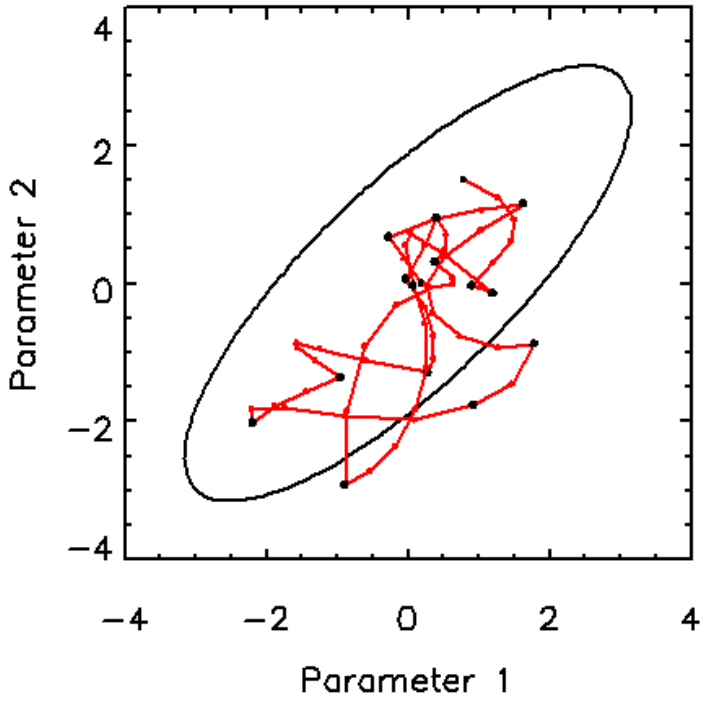
- R tends to be less than 1 when $p(\mathbf{x})$ not adequately sampled

Convergence - 2D nonisotropic Gaussians



- Nonisotropic Gaussian target pdf: $\sigma_1 = 4$, $\sigma_2 = 1$, $m_1 = m_2 = 1$
  - control degree of pdf sampling by using short leapfrog steps ($\tau = 0.2$) and $T_{max} = 2$
- Test statistic R < 1 when estimated variance is deficient

16D correlated Gaussian distribution



- 16D Gaussian pdf related to smoothness prior based on integral of L2 norm of second derivative
- Efficiency/(function evaluation) =
  2.2% (Hamiltonian algorithm)
  0.11% or 1.6% (Metropolis; w/o & with covar. adapt.)

MCMC - Issues

- Identification of convergence to target pdf
  - is sequence in thermodynamic equilibrium with target pdf?
  - validity of estimated properties of parameters (covariance)
- Burn in
  - at beginning of sequence, may need to run MCMC for awhile to achieve convergence to target pdf
- Use of multiple sequences
  - different starting values can help confirm convergence
  - natural choice when using computers with multiple CPUs
- Accuracy of estimated properties of parameters
  - related to efficiency, described above

Conclusions

- MCMC provides good tool for exploring the Bayesian posterior and hence for drawing inferences about models and parameters
- Hamiltonian method
  - based on Hamiltonian dynamics
  - efficiency for isotropic Gaussians is about 7% per function evaluation, independent of number of dimensions
  - much better efficiency than Metropolis for large dimensions
  - more robust to correlations among parameters than Metropolis
- Convergence test based on gradient of -log(probability)

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