Lecture Recording

- **Note: These lectures will be recorded and posted onto the IMPRS website**

- Dear participants,

- We will record all lectures on "*Making sense of data: introduction to statistics for gravitational wave astronomy*", including possible Q&A after the presentation, and we will make the recordings publicly available on the IMPRS lecture website at:

    - https://imprs-gw-lectures.aei.mpg.de/2023-making-sense-of-data/

- By participating in this Zoom meeting, you are giving your explicit consent to the recording of the lecture and the publication of the recording on the course website.

Making sense of data: introduction to statistics for gravitational wave astronomy

Part II: Bayesian statistics

Lecture 2: Sampling methods

AEI IMPRS Lecture Course

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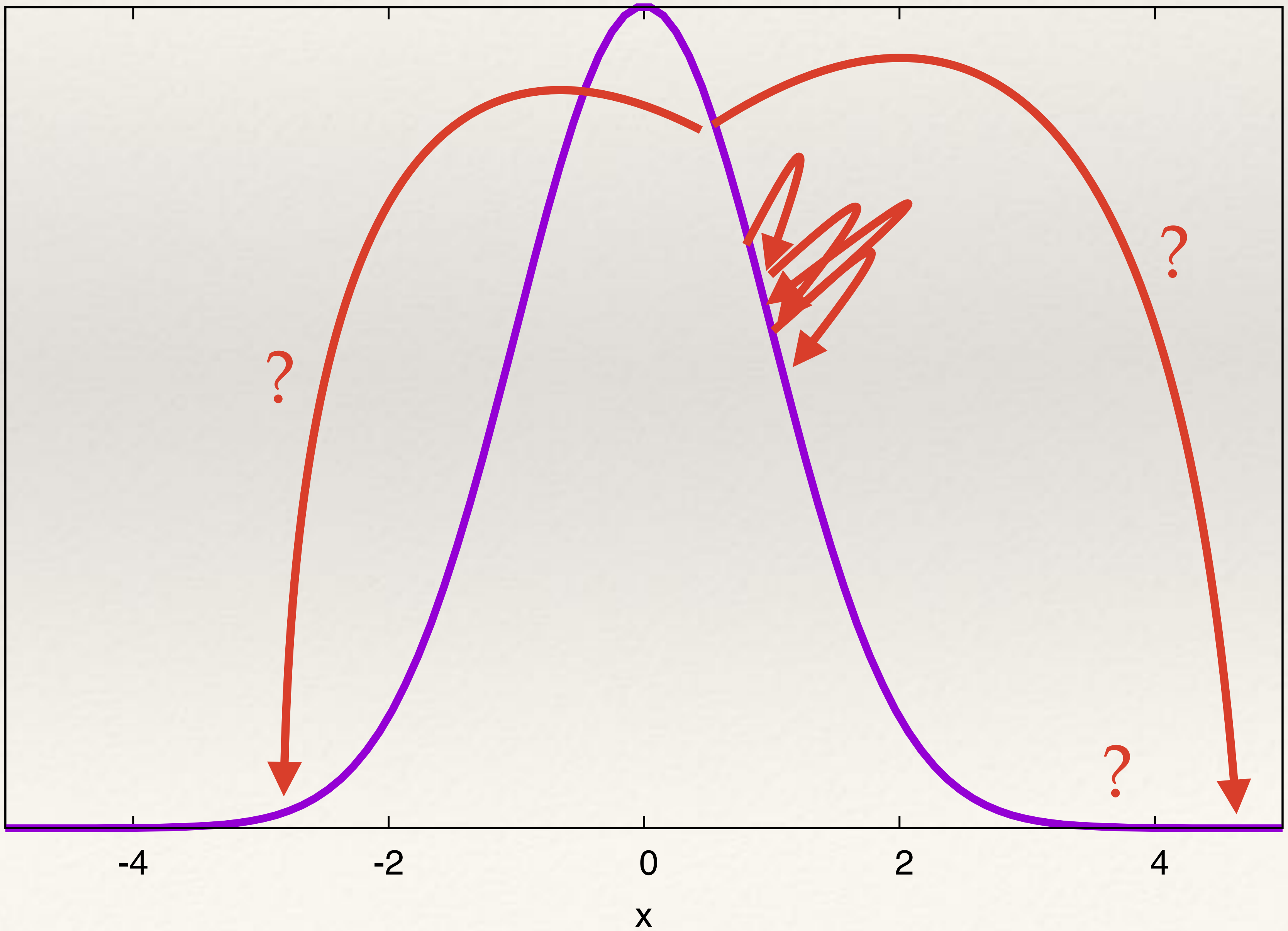


Working with Bayesian Posteriors

- The posterior distribution encodes all information about the parameters of interest after data has been observed. Sometimes these are analytic, but usually not.

- When they are not analytic, they can be approximated by the **Bayesian Central Limit Theorem.** We suppose that $X_1, \ldots, X_n \overset{\text{iid}}{\sim} p(x \mid \boldsymbol{\theta})$ and the prior $p(\boldsymbol{\theta})$ and likelihood $p(x \mid \boldsymbol{\theta})$ are twice differentiable near $\widehat{\boldsymbol{\theta}}_{\text{post}}$, the mode of the posterior distribution. Then, for large *n*,

$$p(\boldsymbol{\theta} \mid \mathbf{x}) \sim \mathrm{N}\left(\widehat{\boldsymbol{\theta}}_{\text{post}}, [I^{\text{post}}(\boldsymbol{\theta}, \mathbf{x})]^{-1}\right)$$

- where

$$I^{\text{post}}(\boldsymbol{\theta}, \mathbf{x}) = -\left[\frac{\partial^2}{\partial\boldsymbol{\theta}\partial\boldsymbol{\theta}^T} \log p(\boldsymbol{\theta} \mid \mathbf{x})\right]_{\boldsymbol{\theta}=\widehat{\boldsymbol{\theta}}_{\text{post}}}$$

Working with Bayesian Posteriors

- As discussed in Lecture 5, the primary application of probability distributions is to compute expectation values of quantities of interest via integration.

- In low numbers of dimensions, such integrals can be computed by **direct evaluation** (numerical integration) on a grid of points.

- In larger numbers of dimensions it is better to use **stochastic (Monte Carlo) sampling**. We draw a set of samples $\{\vec{\theta}_1, \ldots, \vec{\theta}_M\}$ and then approximate

$$\int f(\vec{\theta})p(\vec{\theta}|\mathbf{x})\mathrm{d}\vec{\theta} \approx \frac{1}{M}\sum_{i=1}^{M} f(\vec{\theta}_i)$$

- Monte Carlo integration converges to the true integral asymptotically as *the number of samples M* tends to infinity, which can always be achieved with sufficient computational power, whereas the Central Limit Theorem relies on the number of *observations* to tend to infinity, which is much harder to ensure in practice.

- Samples can be obtained through **direct sampling** or **Markov Chain Monte Carlo**.

Direct sampling: Method of Inversion

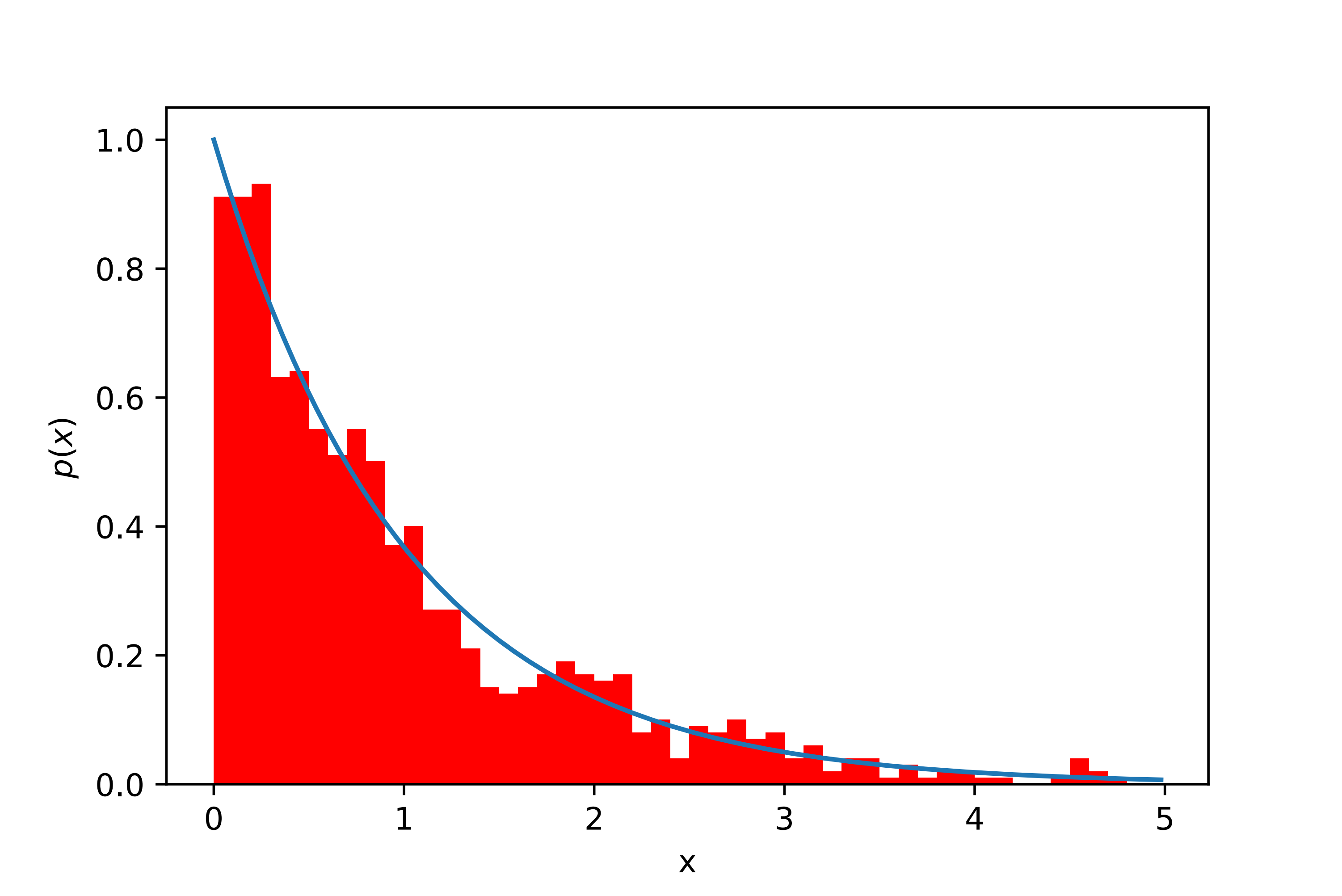
- If the posterior distribution has a cumulative density function (CDF) with a known inverse, samples can be generated by drawing samples from *U[0,1]*.
- If the CDF is denoted by *F*

$$F(\Theta|\mathbf{x}) = \mathbb{P}(\theta \leq \Theta|\mathbf{x})$$

- We simulate

$$u_i \sim U[0,1]$$
$$\theta_i = F^{-1}(u_i|\mathbf{x})$$

- The x_i are samples from *f*.



Example: exponential with parameter *r*. *p(t | r)* = *r* exp(-*rt*), *F(T)* = *1*-exp(-*rT*), *F*$^{-1}$*(u)* = *ln(1/(1-u))/r.*

Direct sampling: Rejection Sampling

- **Rejection sampling** uses samples drawn from another distribution that "contains" the distribution of interest. The algorithm is

$$\begin{aligned} \theta_i &\sim g(\theta) \\ y_i &\sim U[0, Mg(\theta)] \end{aligned}$$

$$\text{If } y_i \leq p(\theta_i|\mathbf{x}), \text{ accept } \theta_i$$

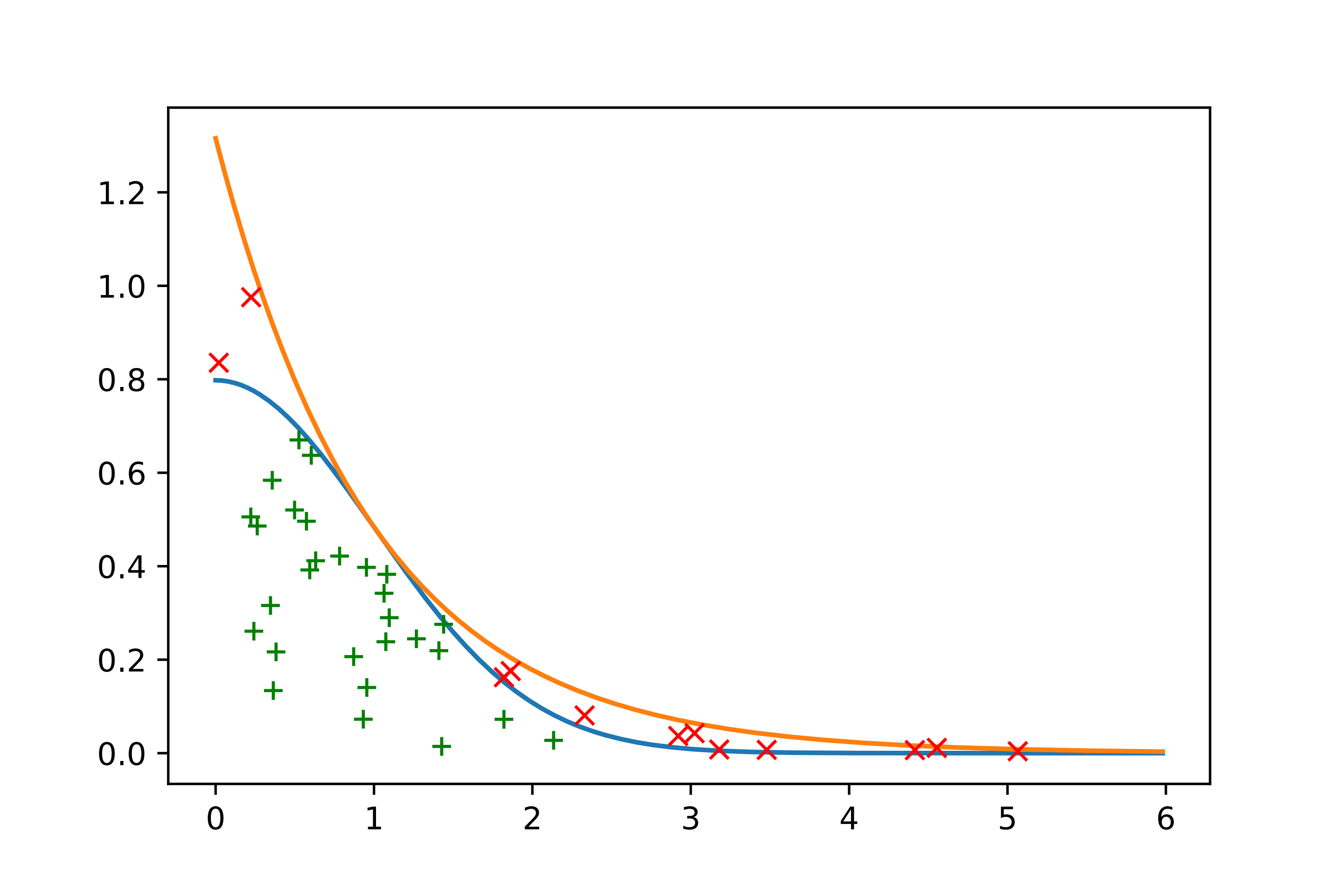
$$\text{as a sample from } p(\theta|\mathbf{x})$$

- We require

$$Mg(\theta) \geq p(\theta|\mathbf{x}) \;\; \forall\, \theta$$

- The "best" rejection method uses

$$M = \sup_{\theta} \left(\frac{p(\theta|\mathbf{x}}{g(\theta)} \right)$$



Example: half-Normal distribution. We want to sample from *N(0,1) I(x > 0)*. We draw samples from *Exp(1)*, for which we need *M = 1.3155*.

Direct sampling: Importance Sampling

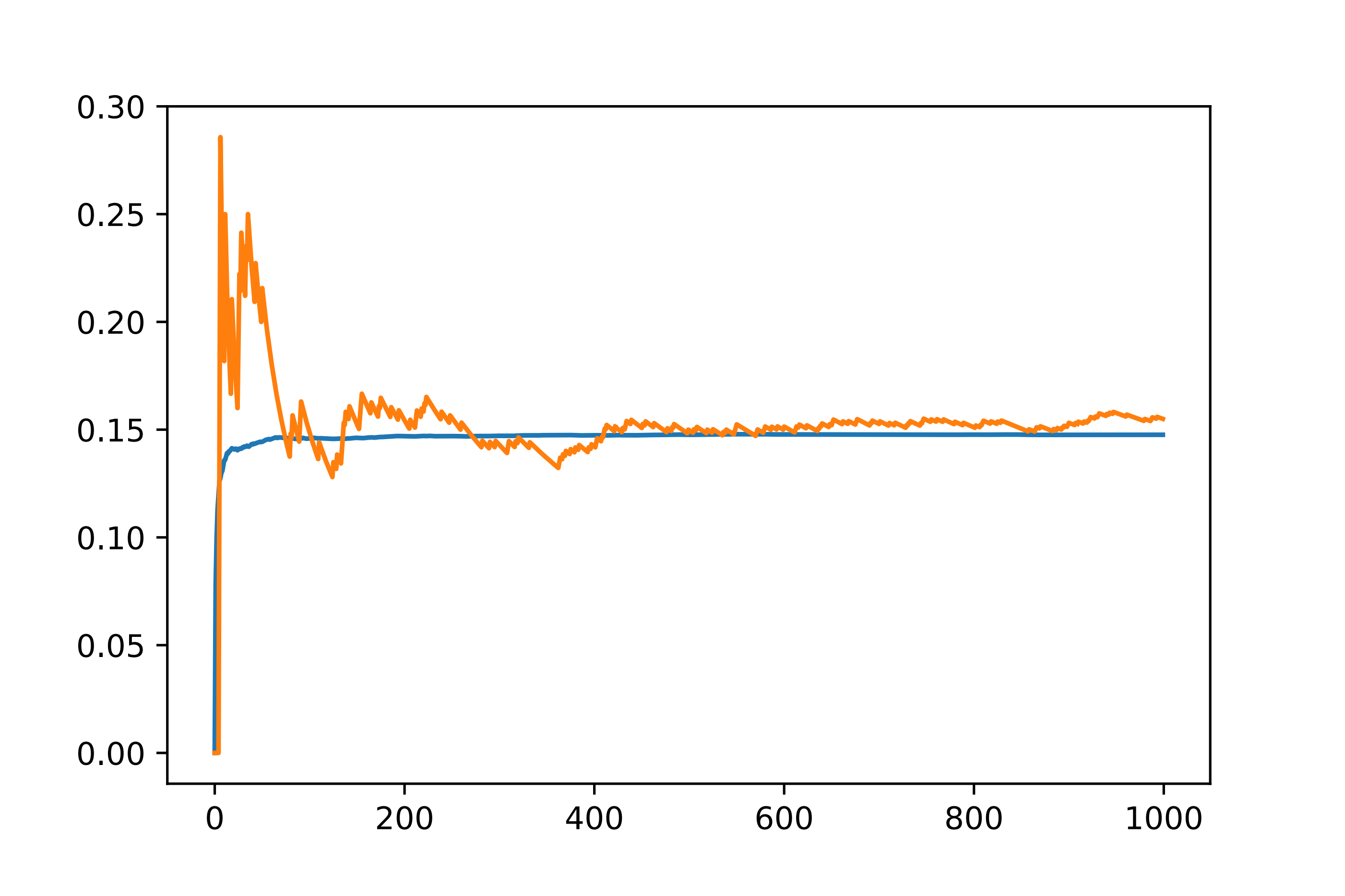
- **Importance sampling** also draws samples from another, easy-to-sample distribution, but now samples are not rejected but given weights

$$w_i = \frac{p(\theta_i|\mathbf{x})}{g(\theta_i)}$$

- Integrals over the posterior are approximated by weighted sums

$$\int f(\theta)p(\theta|\mathbf{x})\,\mathrm{d}\theta \approx \frac{1}{N}\sum_{i=1}^{N} w_i f(\theta_i)$$

- One advantage is that the normalisation of the posterior does not need to be known. But, the algorithm suffers from high sampling variance.



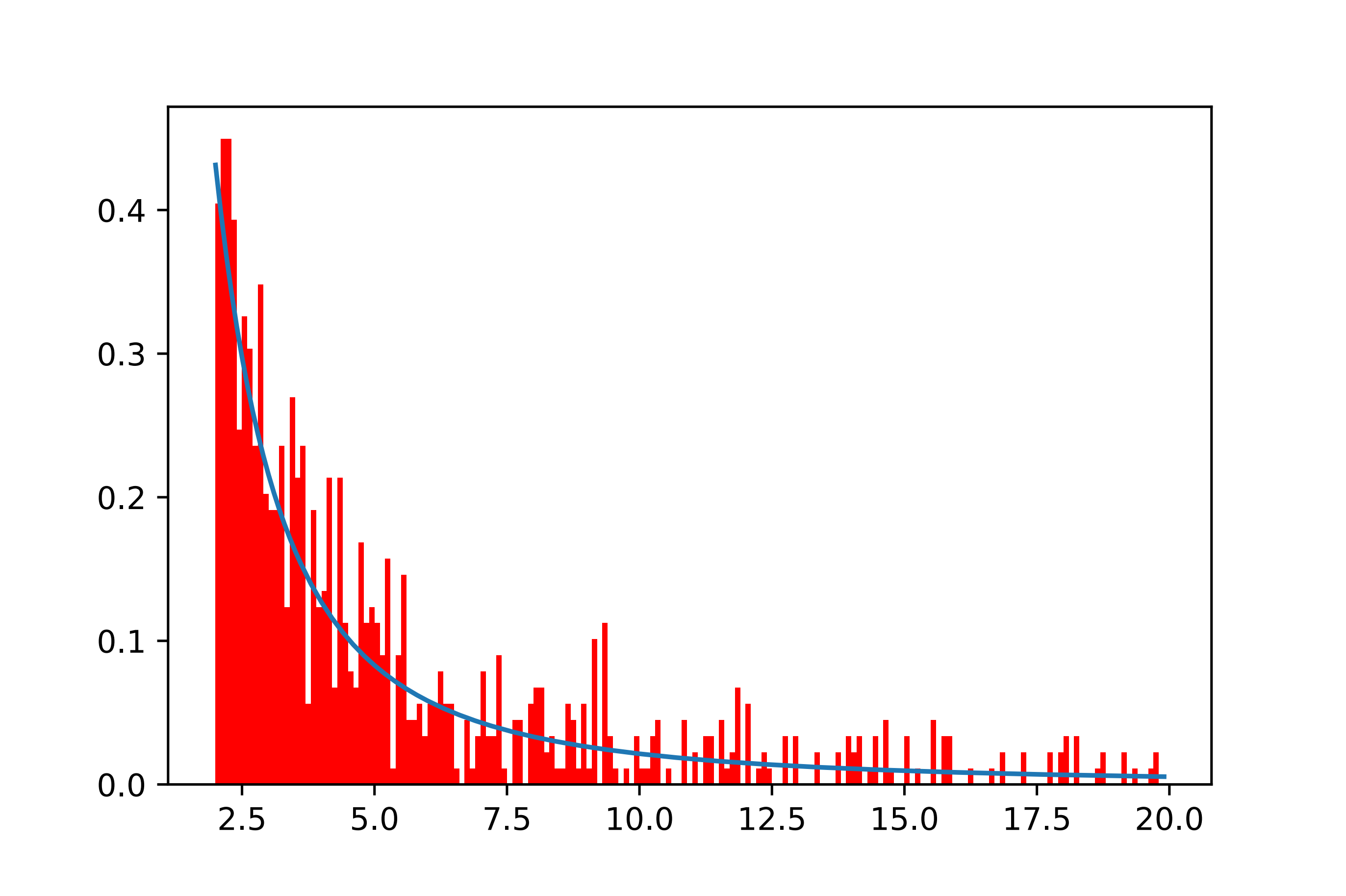
Example: Cauchy distribution. We want samples from $p(\theta) = 1/(\pi(1+\theta^2))$. We draw samples from $g(\theta) = 2/\theta^2$ and use importance sampling to estimate $\mathbb{P}(\theta > 2)$.

Direct sampling: Sampling importance Resampling

- **Sampling importance resampling** is a variant of importance sampling.
- Importance samples are first drawn using the algorithm on the previous slide and the weights renormalised

$$w_i = \frac{w_i}{\sum_{j=1}^{n} w_j}$$

- New samples are then drawn at random, with replacement, from the first set, with relative probabilities given by w_i.
- This is a form of **particle filtering**. It can suffer from **particle depletion**, when a small number of samples carry the majority of the weight.



Example: histogram of resampled points from first 1000 importance samples from previous slide.

Markov Chain Monte Carlo

- Often direct sampling methods cannot be devised, because the target distribution is too complicated. In those cases, stochastic methods can be used based on Markov Chain Monte Carlo methods.

- The idea is to generate a reversible Markov chain (i.e., a sequence such that each element depends only on the previous one and not longer past history), with a stationary distribution that equals the target distribution.

- Such a Markov chain must satisfy *detailed balance*

$$p(\vec{\theta})\, p(\vec{\theta}, \vec{\theta}') = p(\vec{\theta}')\, p(\vec{\theta}', \vec{\theta})$$

- In which

$$p(\vec{\theta}, \vec{\theta}') = p(\vec{\theta}_i = \vec{\theta}' | \vec{\theta}_{i-1} = \vec{\theta})$$

- and $p(\vec{\theta})$ denotes the target distribution, in our case $p(\vec{\theta}|d, M)$.

Gibbs Sampling

- **Gibbs sampling** draws consecutive samples from the full conditional distributions. It relies on the conditionals taking known forms. The algorithm is as follows
    - Initialise the parameters at some starting values

      $$\boldsymbol{\theta}^{(0)} = (\theta_1^{(0)}, \ldots, \theta_p^{(0)})$$

    - For *s* = *1, …, S:*
        - Draw $\theta_1^{(s)} \sim p(\theta_1 \mid \theta_2^{(s-1)}, \theta_3^{(s-1)}, \ldots, \theta_p^{(s-1)}, \mathbf{x})$
        - Draw $\theta_2^{(s)} \sim p(\theta_2 \mid \theta_1^{(s)}, \theta_3^{(s-1)}, \ldots, \theta_p^{(s-1)}, \mathbf{x})$
        - ….
        - Draw $\theta_p^{(s)} \sim p(\theta_p \mid \theta_1^{(s)}, \theta_2^{(s)}, \ldots, \theta_{p-1}^{(s)}, \mathbf{x})$
- For sufficiently large *s* $(\theta_1^{(s)}, \ldots, \theta_p^{(s)}) \overset{\text{approx.}}{\sim} p(\theta_1, \ldots, \theta_p \mid \mathbf{x})$

Metropolis Hastings Algorithm

- Gibbs sampling relies on being able to define the full conditional distributions. When this is not possible, the Metropolis-Hastings algorithm provides another way to compute a suitable Markov chain.

- We initialise by choosing a (random) starting point. Then, at step i:

  - propose a new point, $\vec{\theta}'$, by drawing from a *proposal distribution,* $q(\vec{\theta}', \vec{\theta}_i)$.

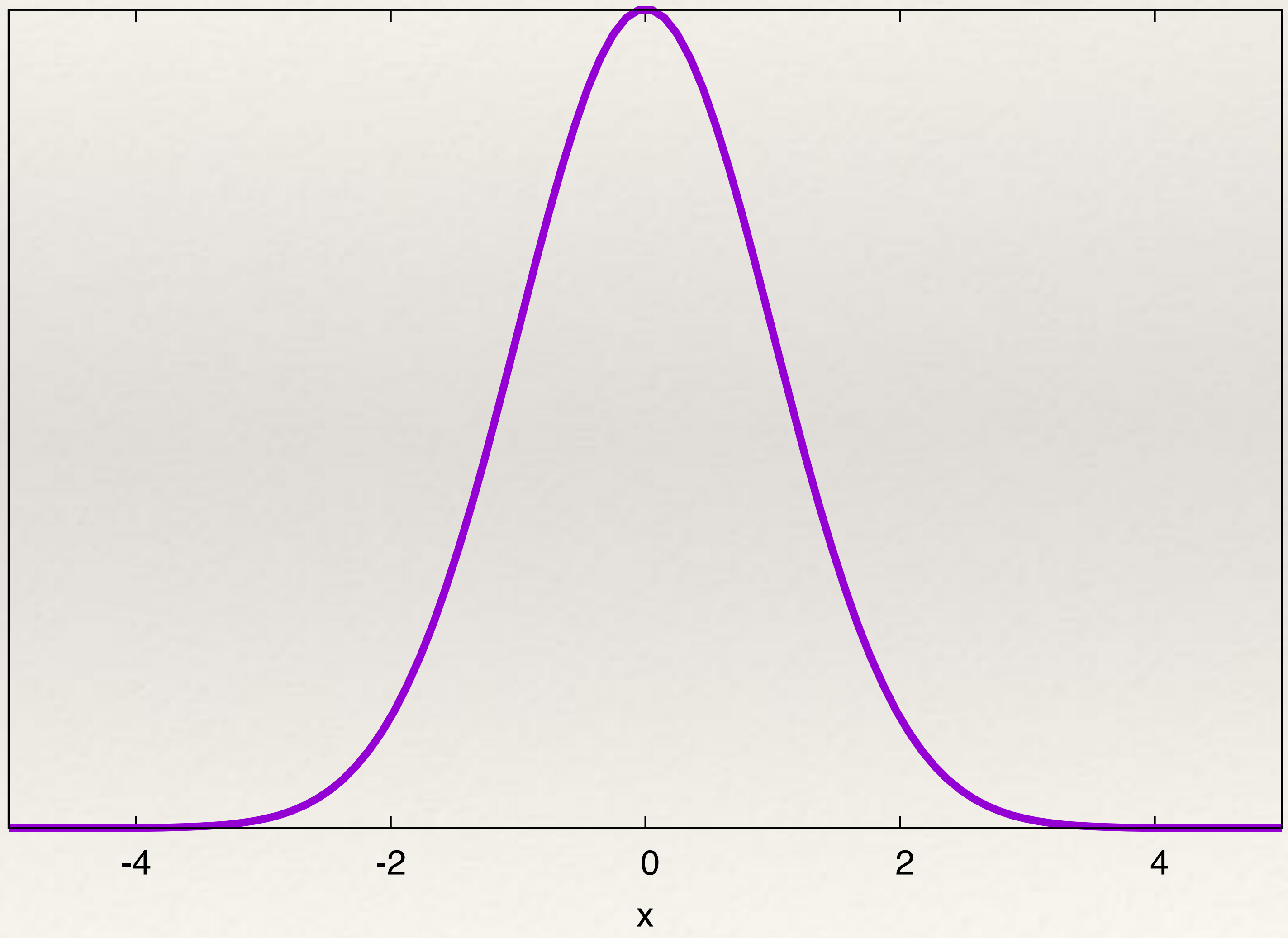
  - evaluate the target distribution at the new point. Compute the *Metropolis-Hastings ratio*

$$\mathcal{H} = \frac{p(\vec{\theta}')q(\vec{\theta}_i, \vec{\theta}')}{p(\vec{\theta}_i)q(\vec{\theta}', \vec{\theta}_i)}$$

  - and draw a random sample, α, from a U[0,1] distribution. If $\alpha < \mathcal{H}$ then set $\vec{\theta}_{i+1} = \vec{\theta}'$, otherwise set $\vec{\theta}_{i+1} = \vec{\theta}_i$. NB if $\mathcal{H} > 1$the proposed move is definitely accepted.

Proposal Distributions

- Sampling efficiency is strongly influenced by the choice of proposal distribution.
- Uniform proposal (random sampling) very inefficient - better to use a grid.
- Ideally want a proposal tuned to the distribution you are sampling.
- A Gaussian is often a good choice, but need to tune width.



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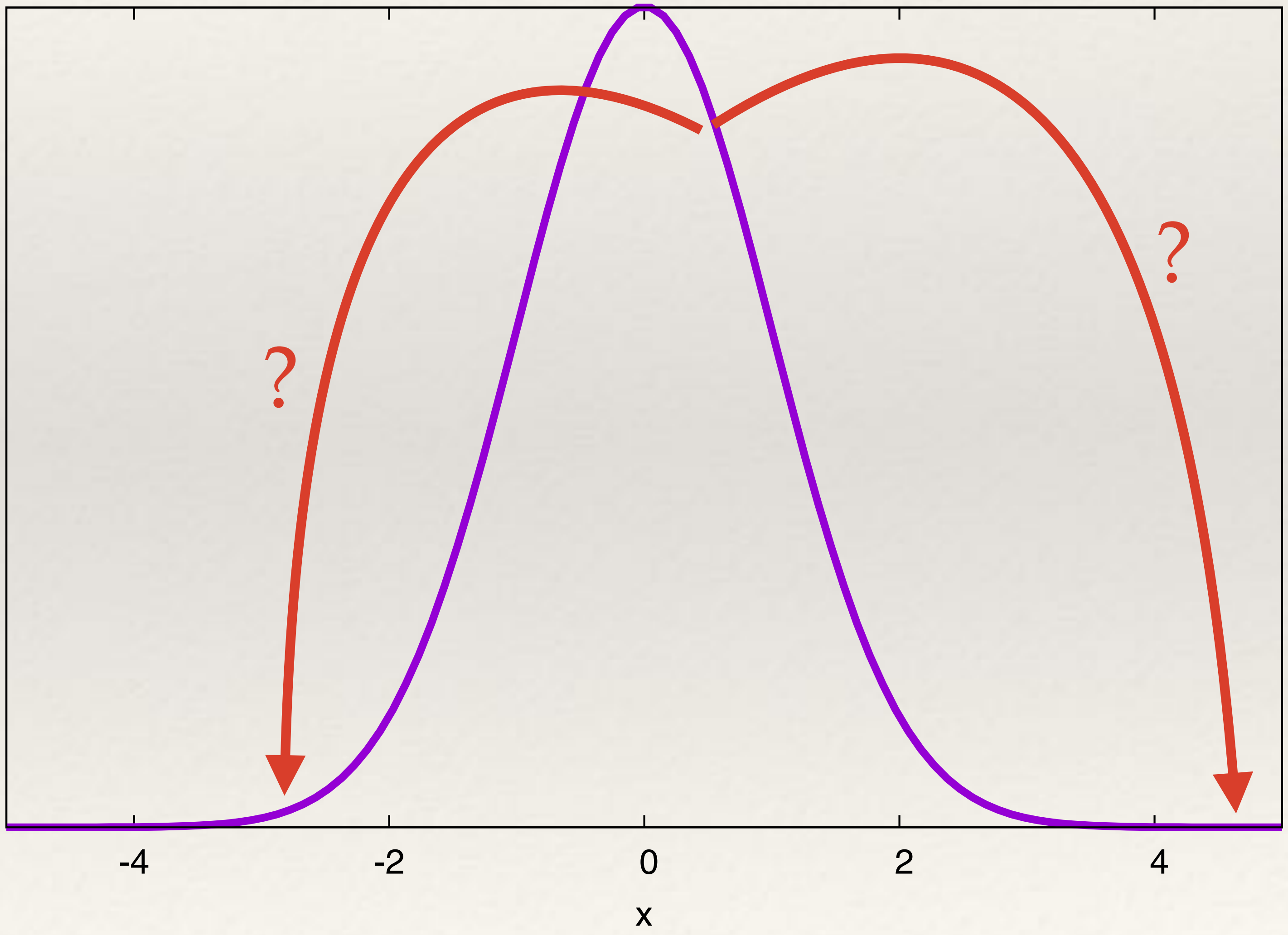

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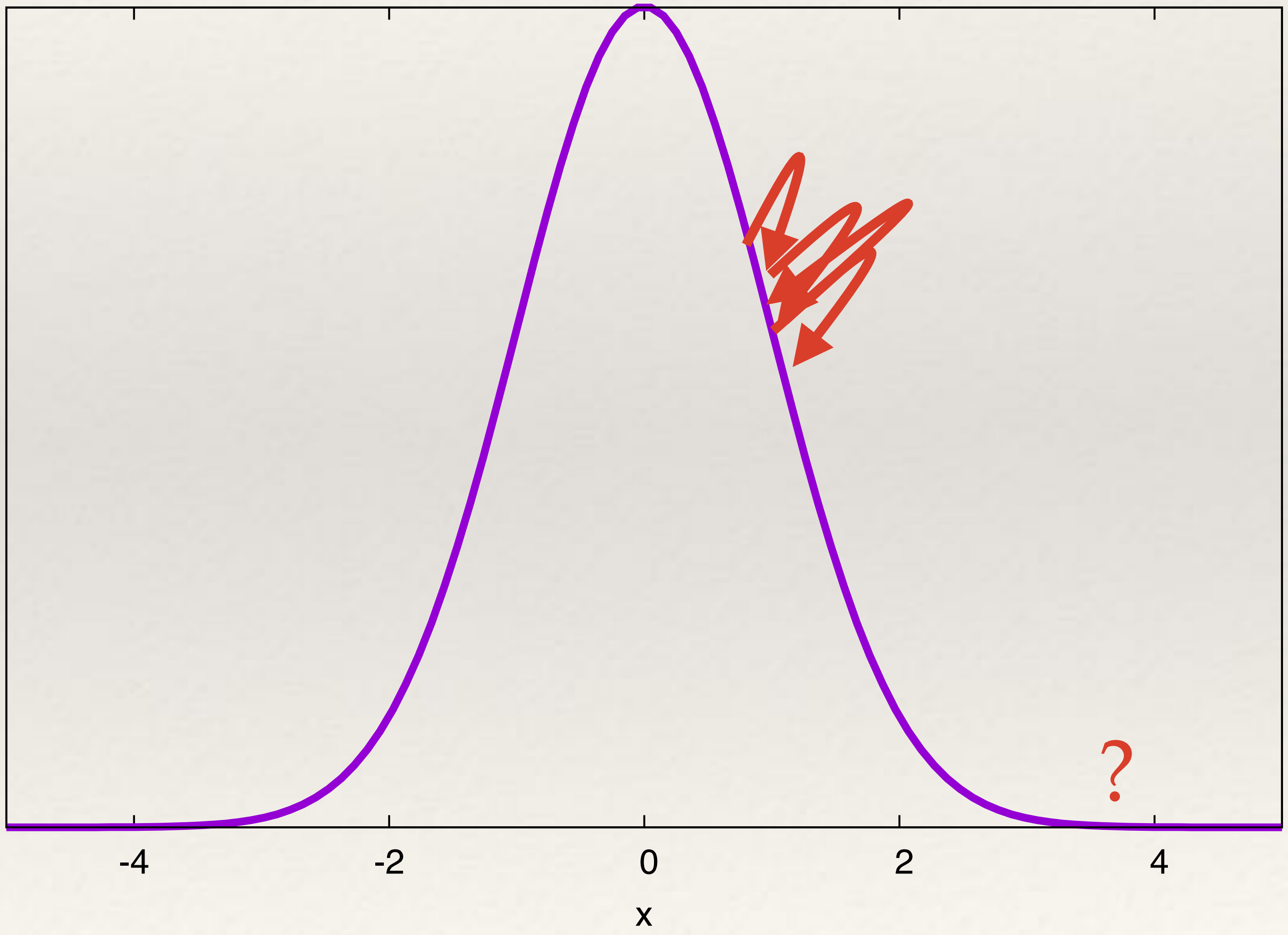
- A Gaussian is often a good choice, but need to tune width.
  - **too wide:** low acceptance rate;
  - **too narrow:** high acceptance rate; low effective samples.



Annealing

- One way to accelerate convergence is to use *simulated annealing*.

- "Heat up" posterior by making the replacement

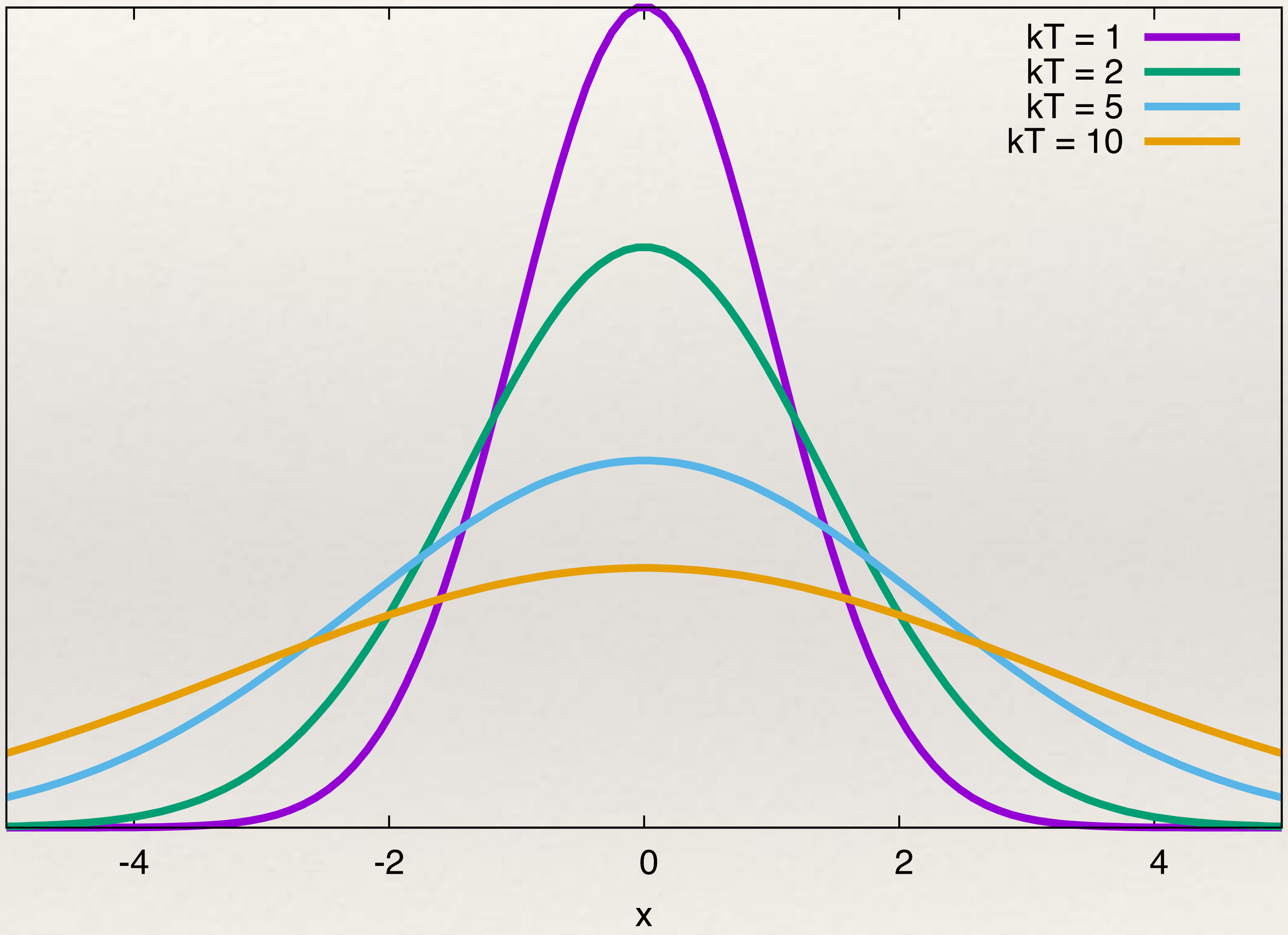
$$p(\vec{\theta}|d, M) \rightarrow \left[p(\vec{\theta}|d, M)\right]^{\beta}$$

- where

$$\beta = \frac{1}{kT}$$

- Choosing a high temperature smoothes out the posterior which can then be more easily sampled.

- Allows identification of interesting parts of parameter space.



Annealing

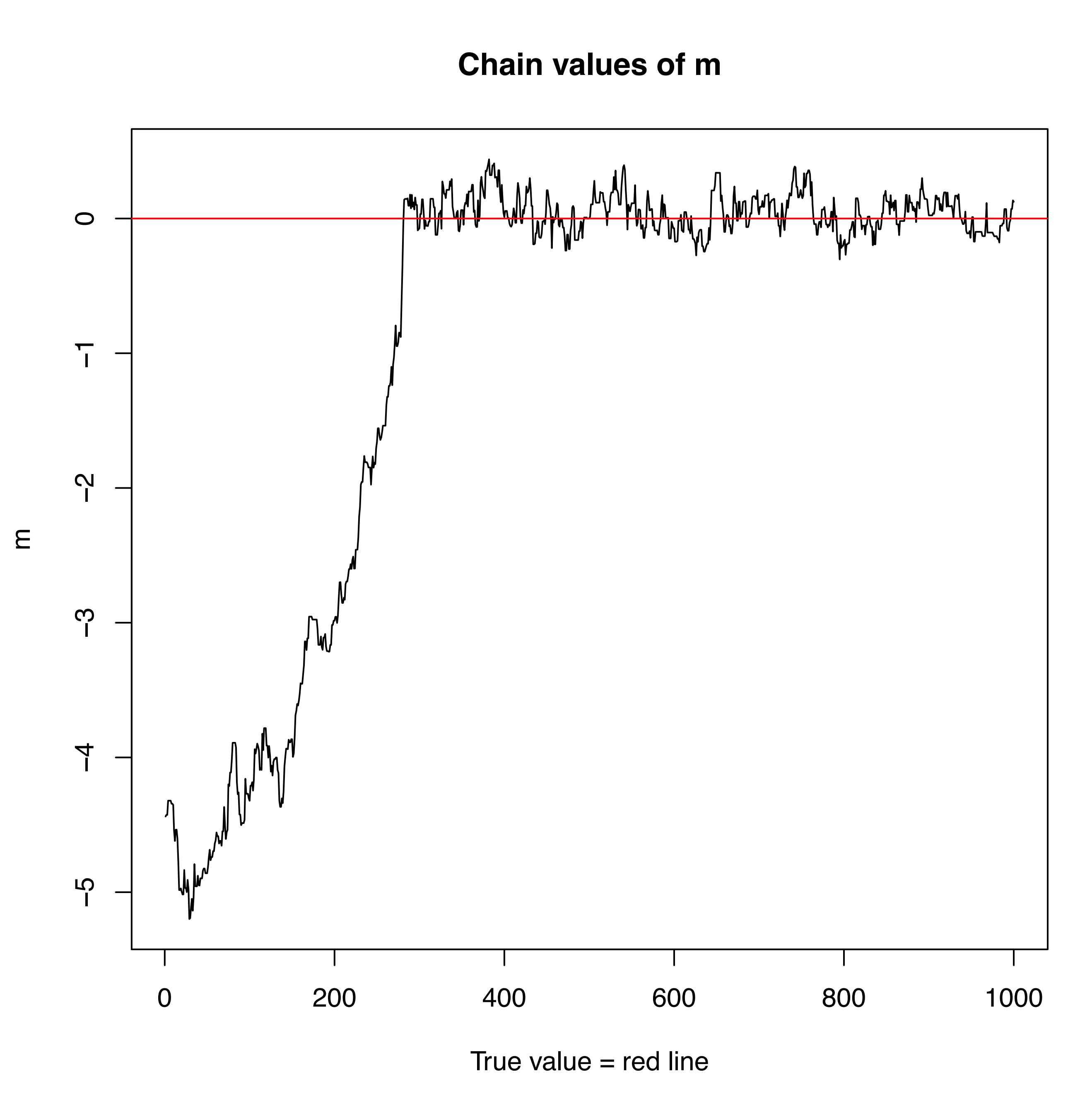
- It is common to use *parallel tempering*. A sequence of M MCMC chains are run simultaneously at different temperatures, $\{T_1, \ldots, T_M\}$.
- The chains can exchange information, which is achieved by proposing a swap of the states of two chains with different temperatures. The swap is accepted with probability

$$\min\left(1, \frac{p_i(\vec{\theta}_j)\, p_j(\vec{\theta}_i)}{p_i(\vec{\theta}_i)\, p_j(\vec{\theta}_j)}\right)$$

- where i, j label the two temperature chains, $\vec{\theta}_k$ denotes the current state of the k'th chain and $p_k(\vec{\theta})$ denotes the target (annealed) distribution for the k'th chain.

Burn-in

- The MCMC chain does not sample from the target distribution immediately.
- There is a residual "memory" of the initial state. Need to discard the first few samples.
- This is called the **burn-in**.
- Can identify number of samples to discard by looking at *trace plots*.
- Usually a few hundred to a thousand samples is sufficient for burn-in.



Autocorrelation and Effective sample size

- Consecutive samples in the MCMC chain are not independent samples from the target distribution.

- Can use all samples for posterior inference *but* do need to know how many *independent* samples the chain contains in order to assess the precision of inferences.

- Compute the (lag-k) autocorrelation

$$\rho_k = \frac{\sum_{i=1}^{N-k}(x_i - \bar{x})(x_{i+k} - \bar{x})}{\sum_{i=1}^{N}(x_i - \bar{x})^2}$$

- where x now denotes one of the components of $\vec{\theta}$. Choose *k*=*K* large enough that the autocorrelation $\rho_k << 1$. The **effective sample size** is $\sim N/K$ and formally defined

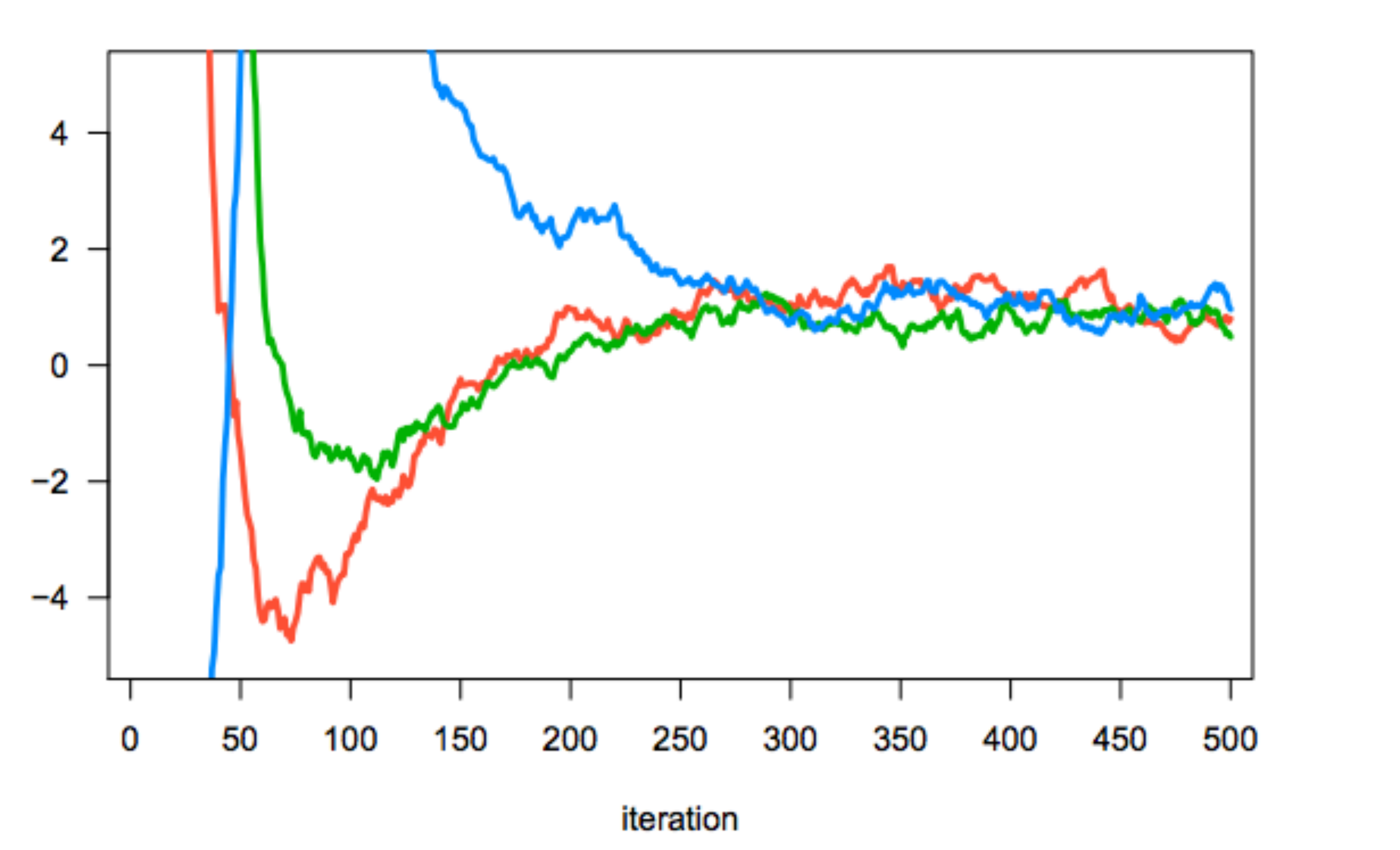
$$\mathrm{ESS} = \frac{N}{1 + 2\sum_{i=1}^{\infty}\rho_k}$$

- Can "thin" chain by keeping only every *K*'th sample without affecting accuracy of posterior inference.

Diagnostics

- There are various techniques to diagnose the quality of results from a given MCMC run.
    - compute acceptance rate, i.e., fraction of proposed points that are accepted. Acceptance rate ~25% is optimal.
    - look at one and two dimensional posterior distributions — do they look smooth and well sampled?
    - look at trace plots — is the chain moving back and forth or unidirectionally?
    - run multiple MCMC chains starting at different points. Do they give consistent results?

Diagnostics



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    - look at trace plots — is the chain moving back and forth or unidirectionally?
    - run multiple MCMC chains starting at different points. Do they give consistent results?
    - use Gelman-Rubin convergence diagnostic.

Gelman-Rubin convergence diagnostic

- Run m (at least 2) chains and discard first half of samples from each.
- Calculate the within-chain variance

$$W = \frac{1}{m}\sum_{j=1}^{m}\frac{1}{N-1}\sum_{i=1}^{N}(x_{ij}-\bar{x}_j)^2$$

- Calculate the between-chain variance

$$B = \frac{N}{m-1}\sum_{j=1}^{m}(\bar{x}_j-\bar{\bar{x}})^2, \qquad \bar{\bar{x}} = \frac{1}{m}\sum_{j=1}^{m}\bar{x}_j$$

- Calculate the estimated variance of a given parameter

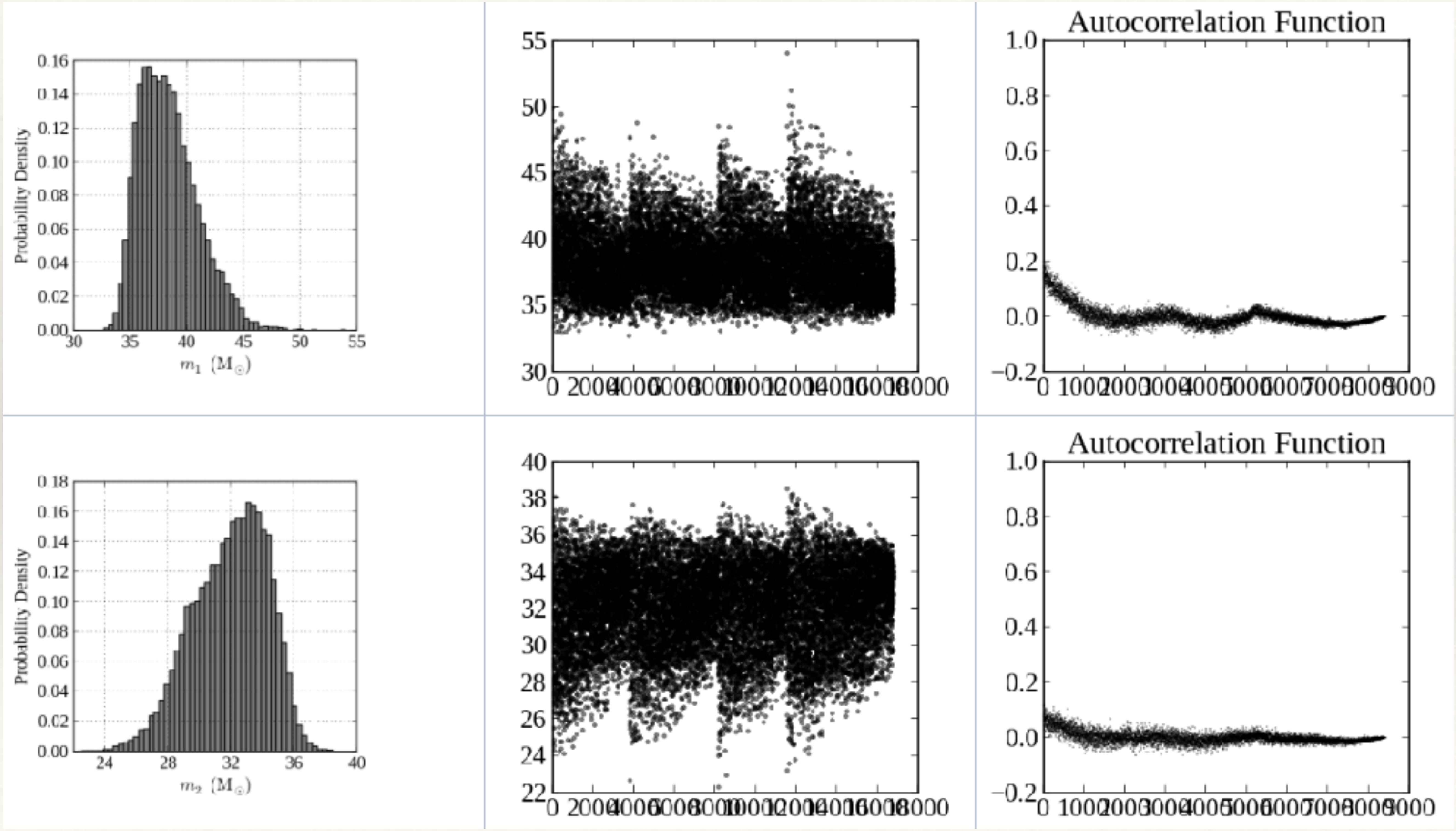
$$\mathrm{Var}(x) = \left(1-\frac{1}{N}\right)W + \frac{1}{N}B$$

- Calculate the potential scale-reduction factor

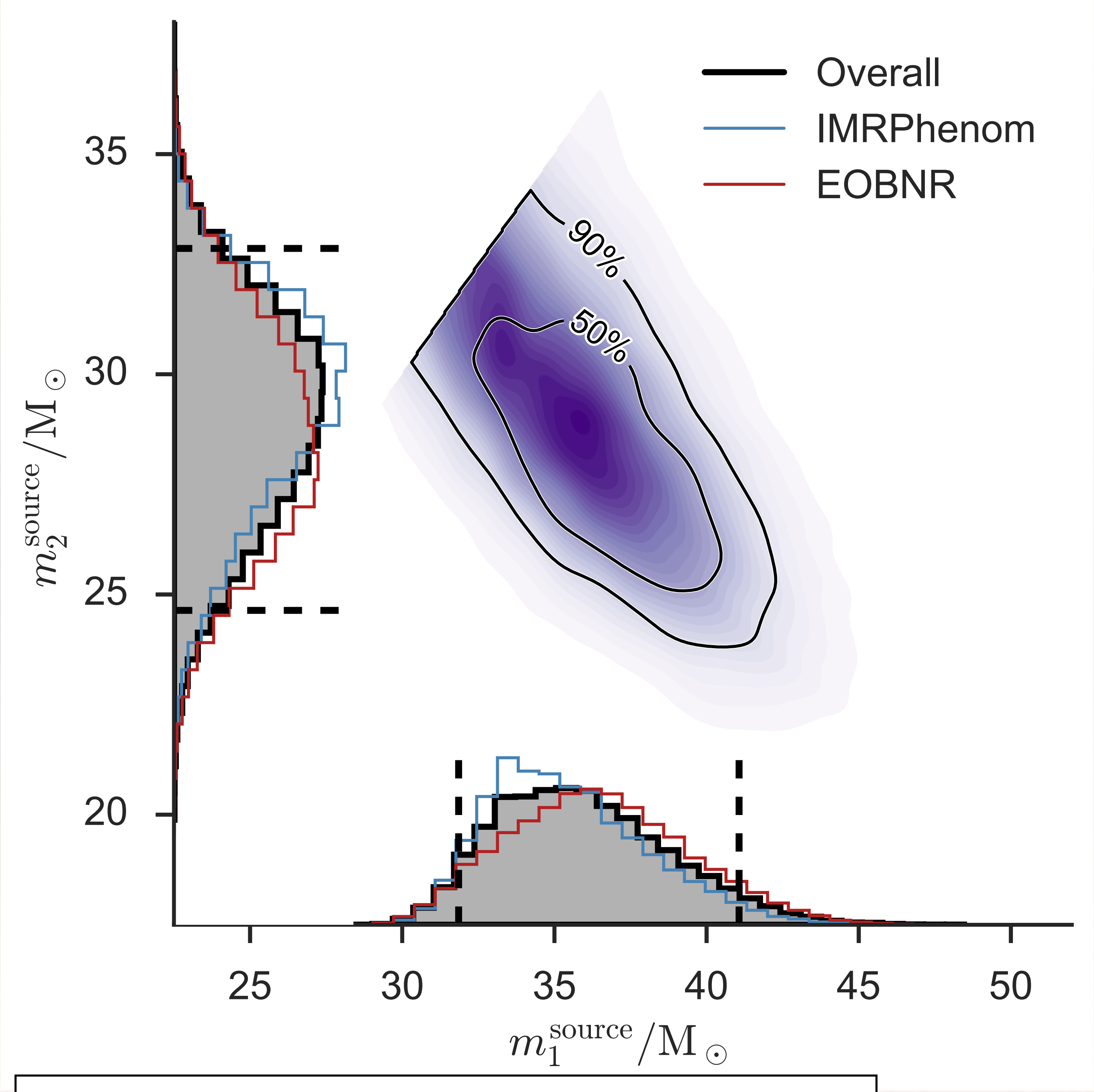
$$\hat{R} = \sqrt{\frac{\hat{\mathrm{Var}}(x)}{W}}$$

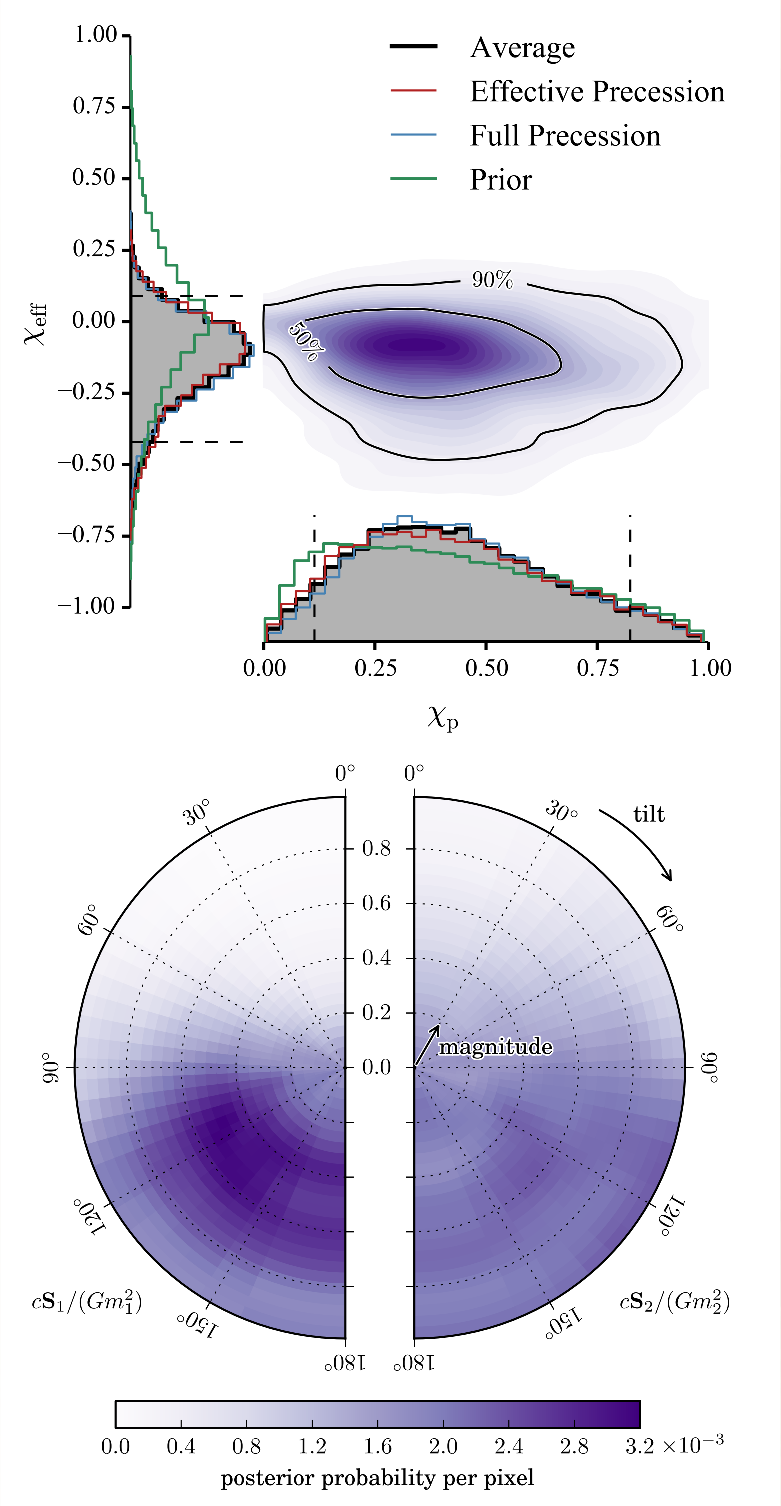
- If R is greater than ~1.1 or 1.2, need to run chains for longer.

Convergence diagnostics: GW150914



Examples of Parameter Posteriors





LVC, *Phys. Rev. Lett.* **116**, 061102 (2016)

Reversible Jump MCMC

- Often the number of sources in the data set is also unknown.
- **Reversible Jump Markov Chain Monte Carlo** is a technique applied in such situations, by periodically proposing jumps **between models**. In GW applications these normally correspond to different numbers of events.
- Represent a proposed move by tuples *(x, u)* and *(x′, u′)*. Here **x** and **x′** denote the parameters of the current and proposed state (which may have different numbers of dimensions) and **u**, **u′** are sets of random numbers that lead to a proposed move from **x** to **x′** and back.
- Generalisation of acceptance ratio is $\alpha = \min\left(1, \frac{p(\mathbf{x}')q(\mathbf{u}')}{p(\mathbf{x})q(\mathbf{u})}\left|\frac{\partial(\mathbf{x}',\mathbf{u}')}{\partial(\mathbf{x},\mathbf{u})}\right|\right)$
- Commonly used when **number** of sources in data unknown. Then it is usual to draw proposed sources for the prior, simplifying the acceptance ratio to

$$\alpha = \min\left(1, \frac{p(\mathbf{x}|\boldsymbol{\theta}')\pi_{N+1}}{p(\mathbf{x}|\boldsymbol{\theta})\pi_N}\right)$$

Integrated detailed balance

- Almost all MCMC algorithms can be expressed in the form of RJMCMC. This follows from imposing the ***integrated detailed balance condition***

$$\int_A \int_{A'} \pi(\boldsymbol{\theta})\mathcal{K}(\boldsymbol{\theta}'|\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}'\mathrm{d}\boldsymbol{\theta} = \int_A \int_{A'} \pi(\boldsymbol{\theta}')\mathcal{K}(\boldsymbol{\theta}|\boldsymbol{\theta}')\mathrm{d}\boldsymbol{\theta}'\mathrm{d}\boldsymbol{\theta}$$

- Representing a proposed move in terms of a draw of random variables **w** and a reversible mapping

$$(\boldsymbol{\theta}', \mathbf{w}') = (h_\theta(\boldsymbol{\theta}, \mathbf{w}), h_w(\boldsymbol{\theta}, \mathbf{w})) \equiv h(\boldsymbol{\theta}, \mathbf{w})$$
$$(\boldsymbol{\theta}, \mathbf{w}) = (h'_\theta(\boldsymbol{\theta}', \mathbf{w}'), h'_w(\boldsymbol{\theta}', \mathbf{w}')) \equiv h'(\boldsymbol{\theta}', \mathbf{w}')$$

- the integrated detailed balance condition is satisfied when

$$\int_A \int_{B'(\boldsymbol{\theta})} \pi(\boldsymbol{\theta})g(\mathbf{w})\alpha(\boldsymbol{\theta}'|\boldsymbol{\theta})\mathrm{d}\mathbf{w}\mathrm{d}\boldsymbol{\theta} = \int_{A'} \int_{B(\boldsymbol{\theta}')} \pi(\boldsymbol{\theta}')g'(\mathbf{w}')\alpha(\boldsymbol{\theta}|\boldsymbol{\theta}')\mathrm{d}\mathbf{w}'\mathrm{d}\boldsymbol{\theta}'$$

- After a change of variable in the integrand we see this will be satisfied when

$$\alpha(\boldsymbol{\theta}'|\boldsymbol{\theta}) = \min\left(1, \frac{\pi(\boldsymbol{\theta}')g'(\mathbf{w}')}{\pi(\boldsymbol{\theta})g(\mathbf{w})}\left|\frac{\partial(\boldsymbol{\theta}', \mathbf{w}')}{\partial(\boldsymbol{\theta}, \mathbf{w})}\right|\right)$$

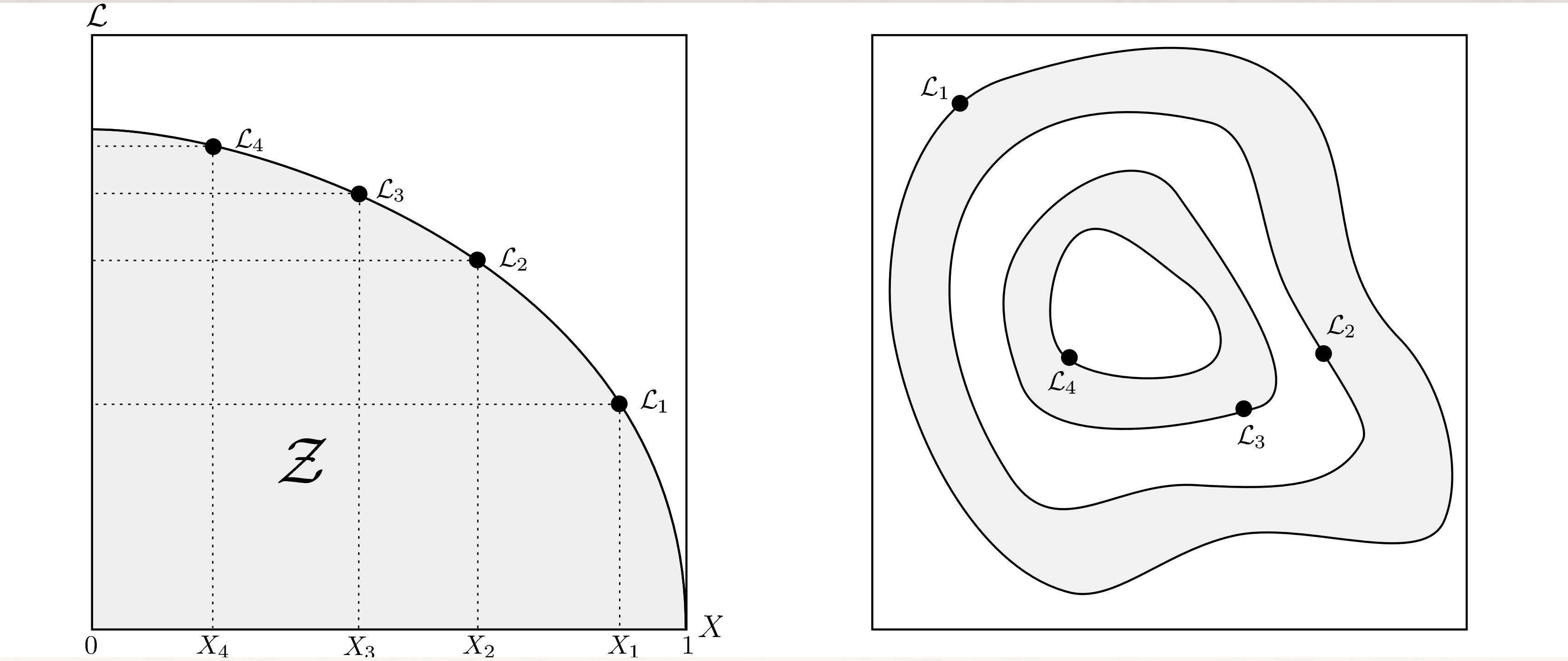
- See lecture notes for various examples.

Nested Sampling

- Nested Sampling (Skilling 04) provides an efficient way to compute evidences, using a 1D integral over the prior

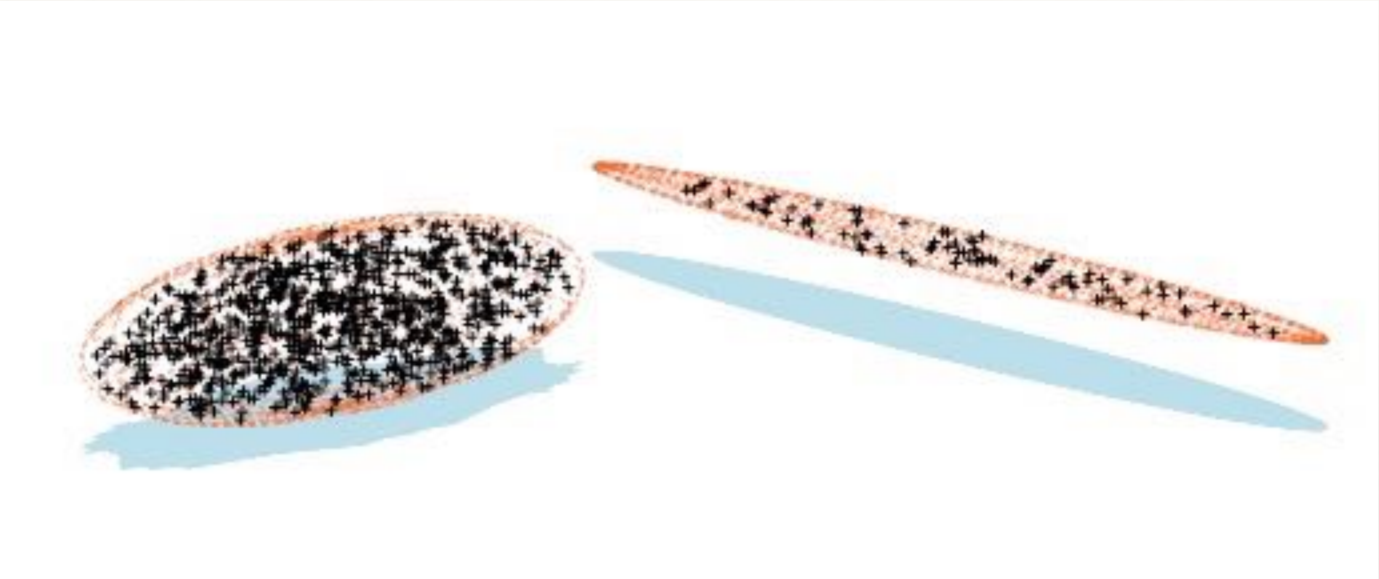
$$\mathcal{Z} = \int \mathcal{L}(\mathbf{\Theta})\pi(\mathbf{\Theta})\mathrm{d}^N\mathbf{\Theta} = \int_0^1 \mathcal{L}(X)\mathrm{d}X, \text{ where } X(\lambda) = \int_{\mathcal{L}(\mathbf{\Theta})>\lambda} \pi(\mathbf{\Theta})\mathrm{d}^N\mathbf{\Theta}$$

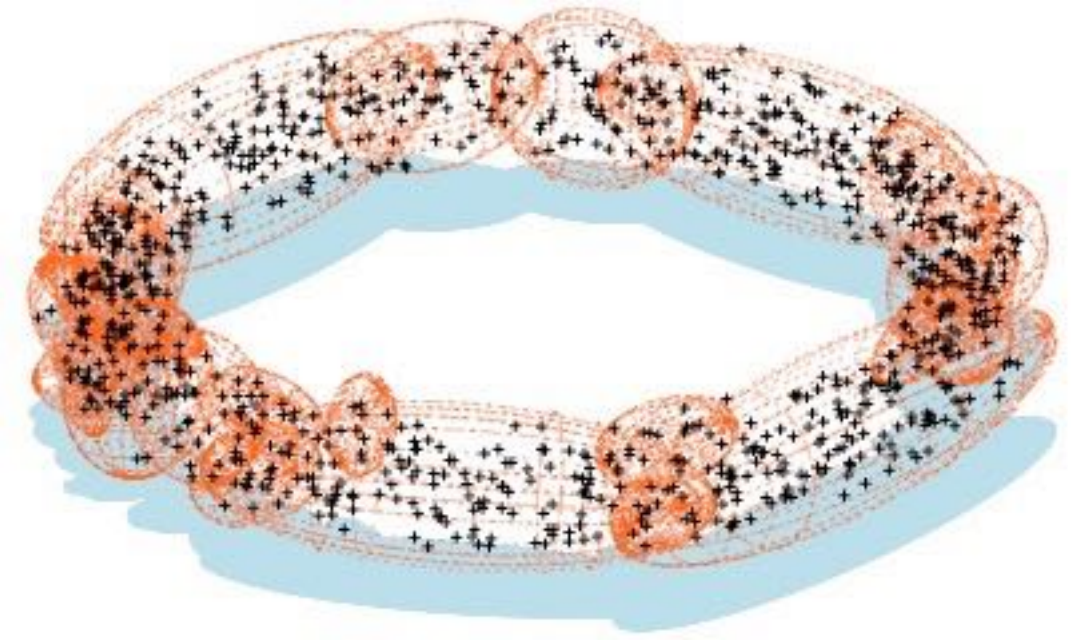
- Use N ‘live points’, initially chosen at random from the prior. At step i, the point of lowest likelihood, $\mathcal{L}_i$, is replaced by a new point with likelihood $\mathcal{L} > \mathcal{L}_i$. The prior volume is reduced by a factor *t*, drawn from $p(t) = Nt^{N-1}$, at each step. We climb through nested contours of increasing likelihood as the algorithm proceeds.



MultiNest

- The trick is to sample efficiently from the prior within the hard constraint that $\mathcal{L} > \mathcal{L}_i$. MultiNest achieves this using an ellipsoidal rejection sampling scheme. The live point set is partitioned into a number of (possibly overlapping) ellipsoids.

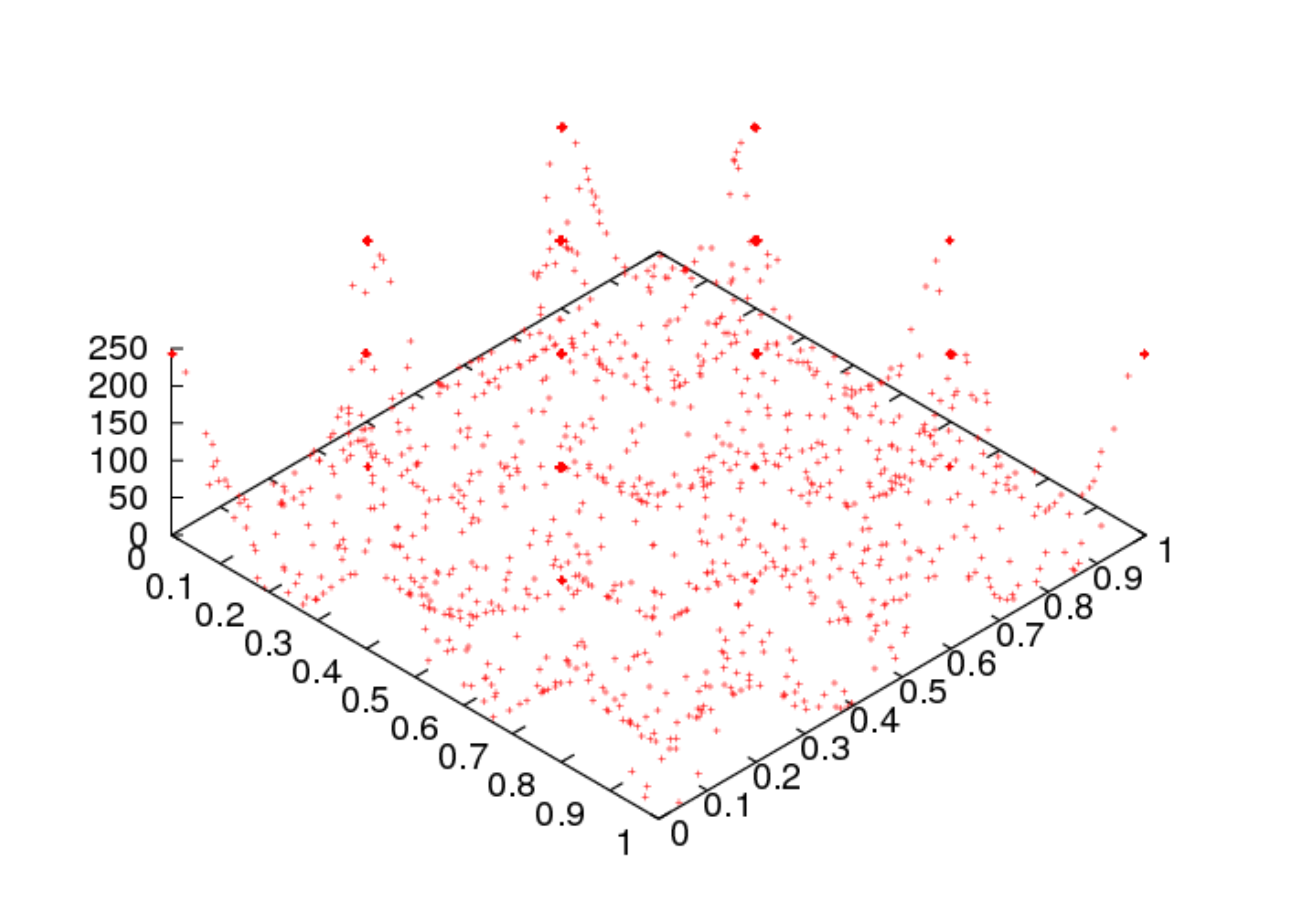




- The algorithm is well suited to exploring likelihoods with multiple modes. Other algorithms (e.g., *cpnest*) update live points using short MCMC explorations.

- Although designed to compute evidences, nested sampling algorithms also return the posterior probability distribution.

MultiNest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