A brief introduction to Bayesian Statistics through Astronomical Applications (Lecture 3)

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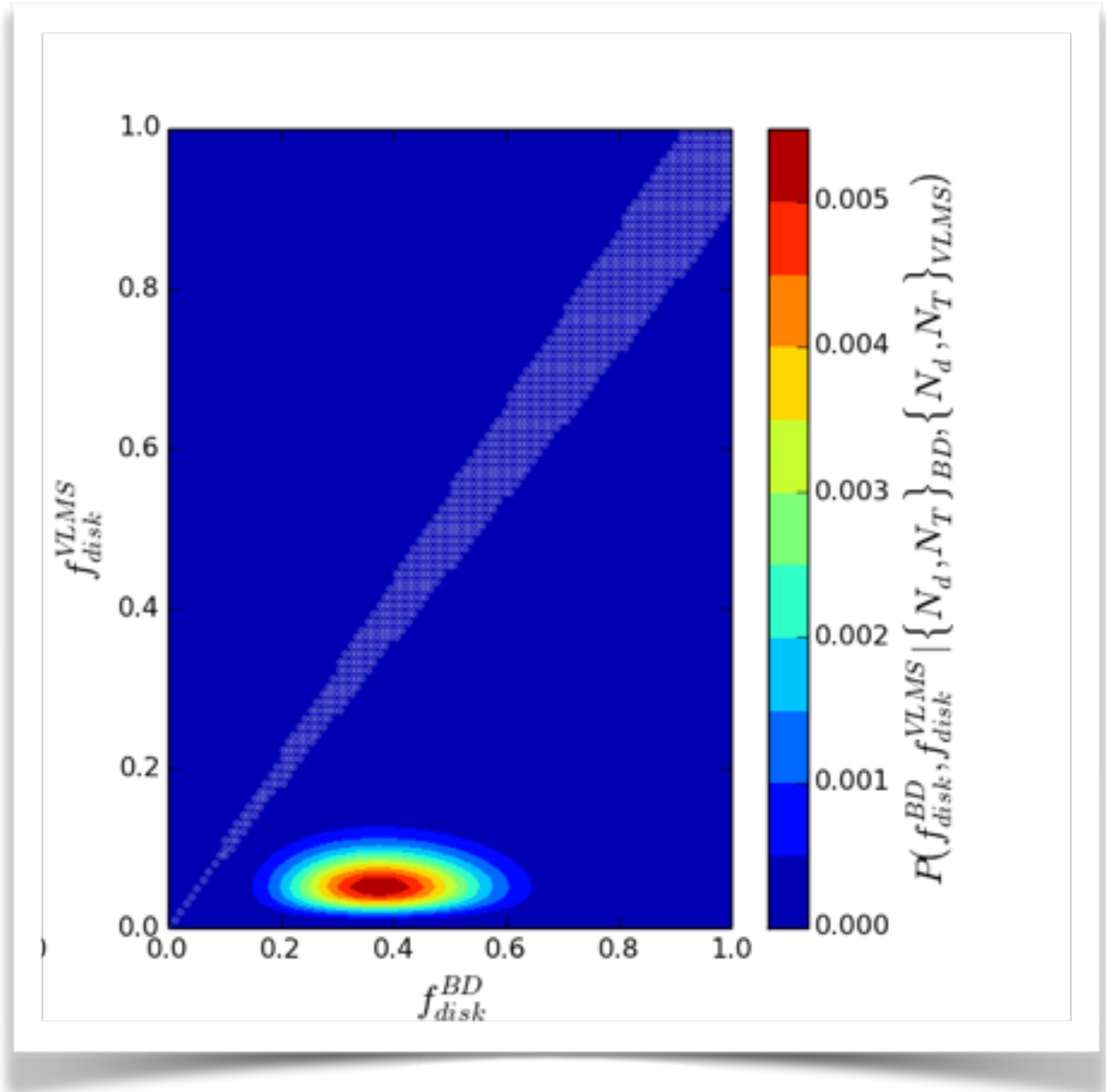
Exploring the parameter space in high dimensionality problems: Markov Chain Monte Carlo

Computing the Posterior in many-parameter problems

- As we have already discussed, the Posterior can only be found by direct evaluation in problems with very few parameters (<~ 6?)

- We would like to have a way of exploring the parameter space efficiently, spending more computation time around high-probability areas than around low probability ones



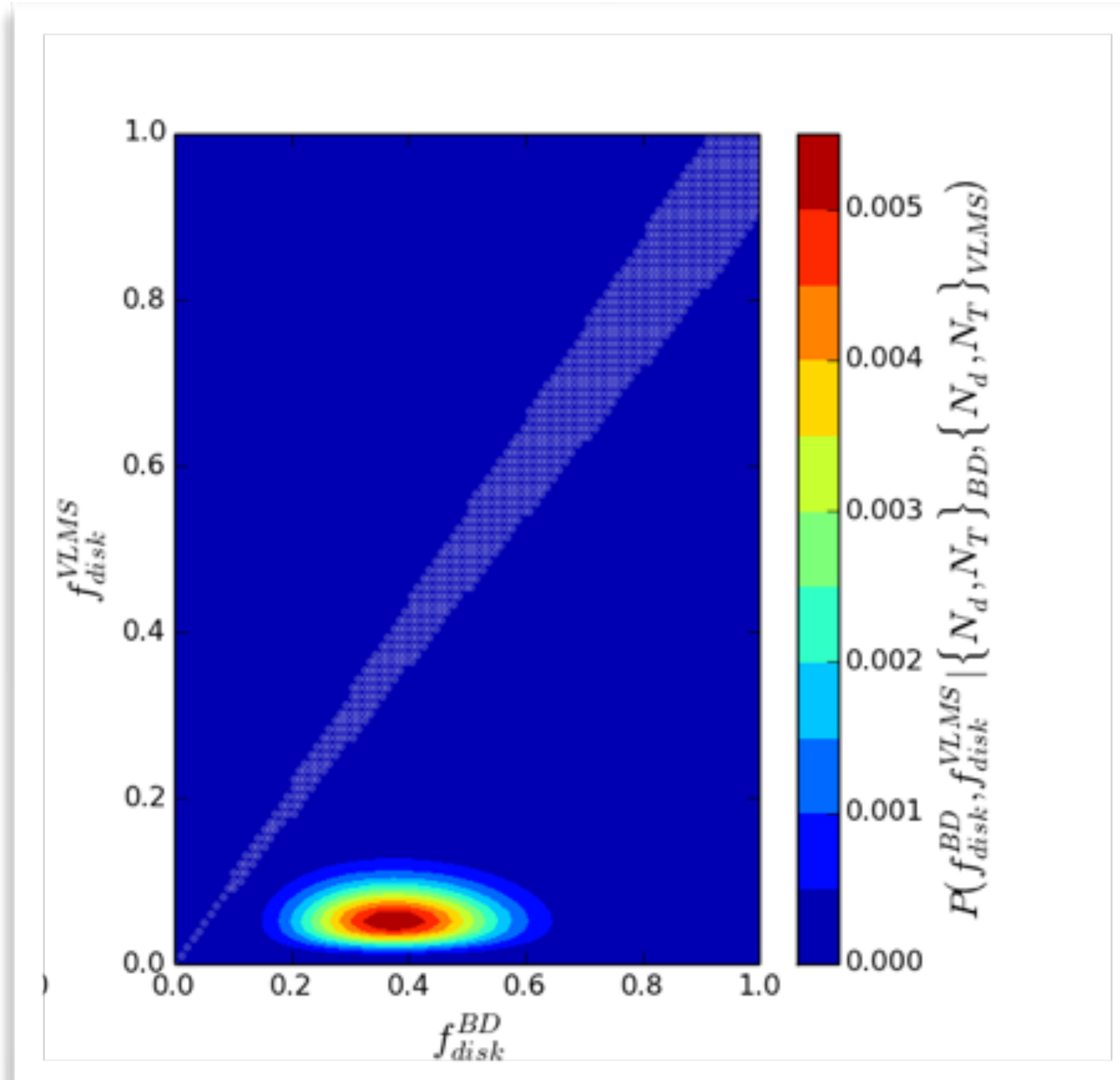
Obtaining samples from the Posterior

- One way is to try to obtain Posterior samples, i.e. a random realisation of the Posterior PDF

- If one has a random realisation of the Posterior with N samples, the Posterior is simply the N-dimensional histogram of this samples

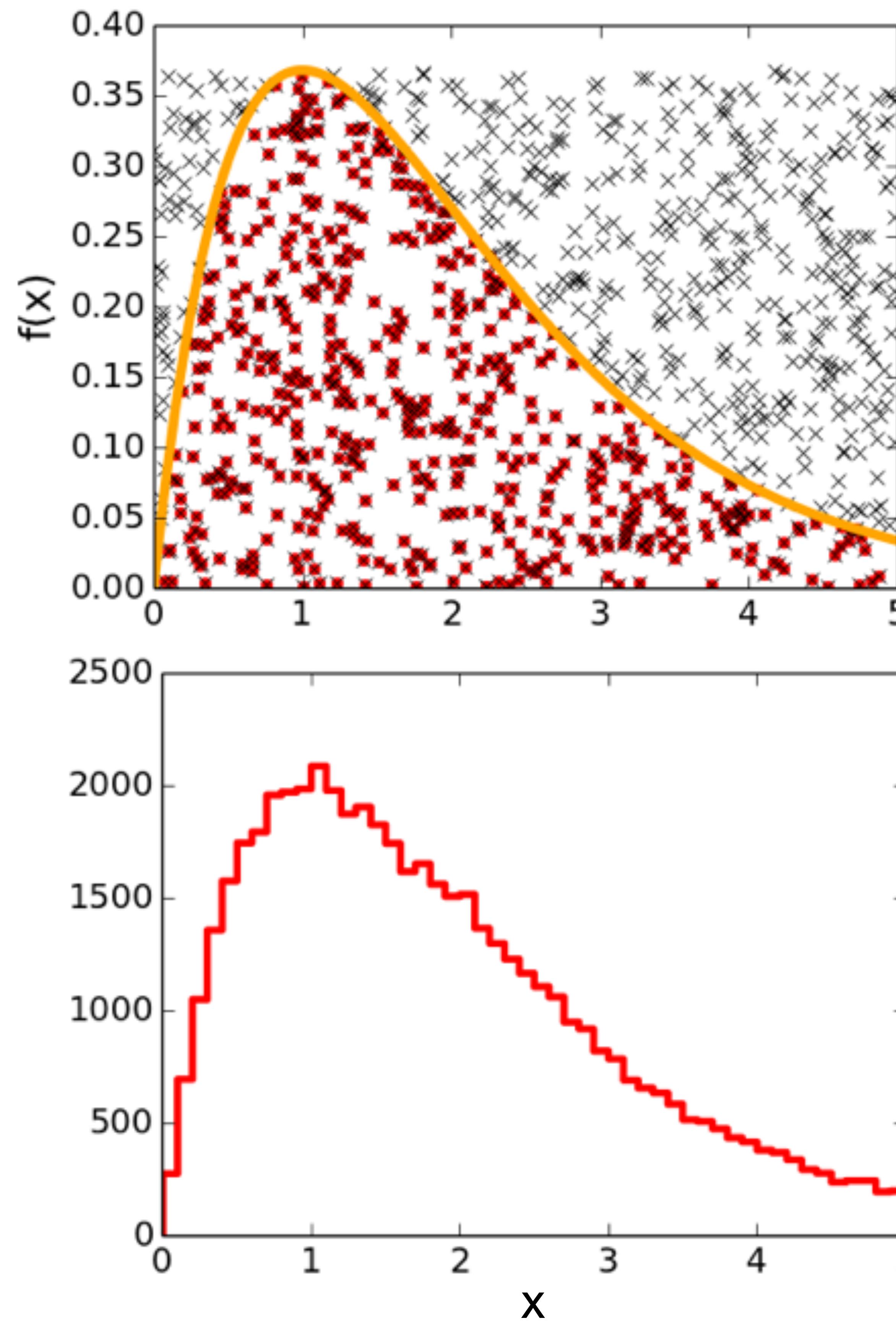
- Having posterior samples, Marginalization is trivial, just the histogram in any lower number of dimensions is the marginal posterior!

- Uncertainties can be easily computed as the standard deviation or percentiles in the resulting histograms



Posterior Samples: Von Neumann Rejection

- A simple way of doing this is with the Von Neumann Rejection Technique, also known as Accept-Reject:
    - Generate random uniformly-distributed samples (x,y) with $x_o<x<x_f$ and $0<y<max(Posterior)$
    - Accept only the samples for which $y<Posterior(x)$
    - … that's it, the accepted points are distributed as the posterior
- This is quite simple and works in any number of dimensions!
- **However…**



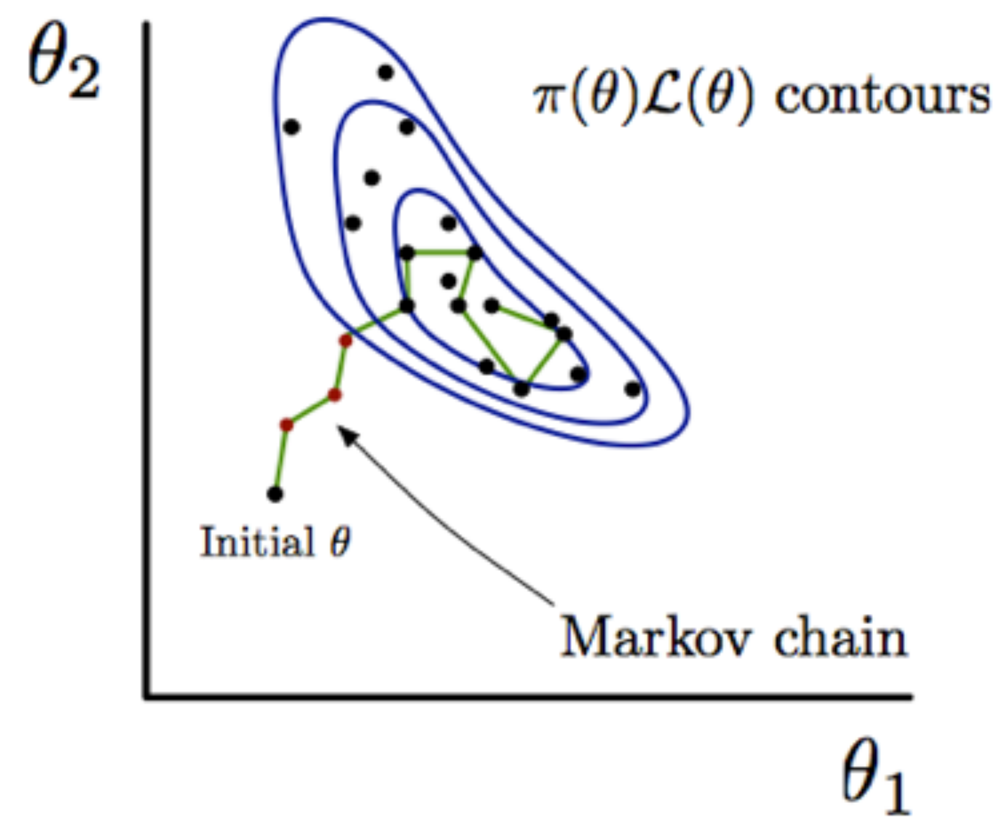
Posterior samples: Markov Chain Monte Carlo

- Von Neumann rejection can still be very inefficient for most problems, so Markov Chain Monte Carlo (MCMC) is preferred

- The idea of MCMC is to start from a point and explore the parameter space by taking steps that may be accepted or rejected, such that the Markov chain:

    - Tends to walk towards higher probability areas

    - Tends to avoid low probability areas



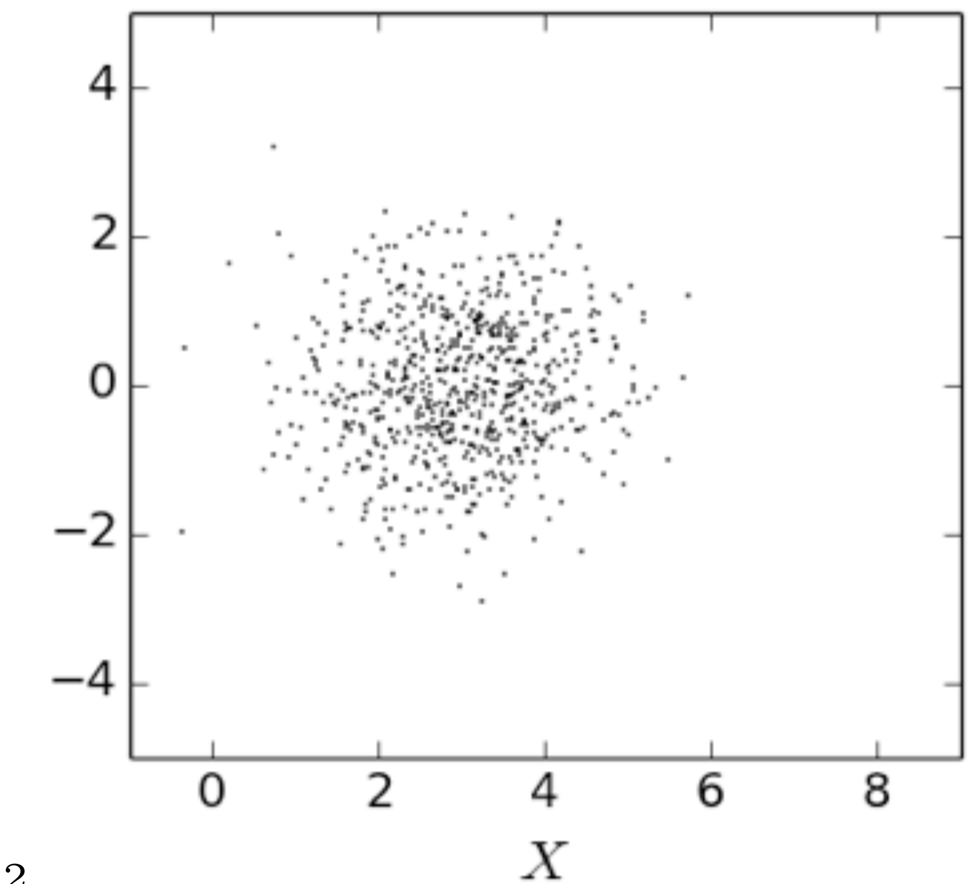
(from Tom Loredo's Lecture Notes)

- Note that the samples are not completely independent, there is some correlation

- After a while, the chain 'forgets' the initial conditions and the accepted (independent) samples have a PDF that is proportional to the Posterior

A two-parameter problem

- We observe the following distribution of N pairs (xi,yi)



- It seems reasonable to assume they were drawn from a random distribution, so lets use a gaussian model with known σx=σy=1 and μX,μY the unknown means in the X and Y directions

- The likelihood is expressed as

$$P(\{x_i, y_i\}|\mu_X, \mu_Y) = \prod_{i=1}^{N} e^{\frac{1}{2}[(x_i - \mu_X)^2 + (y_i - \mu_Y)^2]}$$

- Assuming a uniform prior probability for μX,μY, the posterior is therefore given by

$$P(\mu_X, \mu_Y|\{x_i, y_i\}) = \prod_{i=1}^{N} e^{\frac{1}{2}[(x_i - \mu_X)^2 + (y_i - \mu_Y)^2]}$$

MCMC: The Metropolis-Hastings Recipe

from Hogg et al. 2010

- 1-Choose an initial position for the model params $\{\mu_i\}$
- 2-Advance a step (in one parameter) randomly -> μ_{i+1}
- 3-Evaluate the posterior at current position $P(\mu_{i+1})$
- 4-Draw a random number R with uniform probability in the range $0<R<1$
  - If $R<P(\mu_{i+1})/P(\mu_i)$, keep the point and add it to the chain
  - if not, go back to the previous step and re-add it to the chain
  - repeat …
  - **the set of $\{\mu_i\}$ obtained is a random realization of the Posterior !**

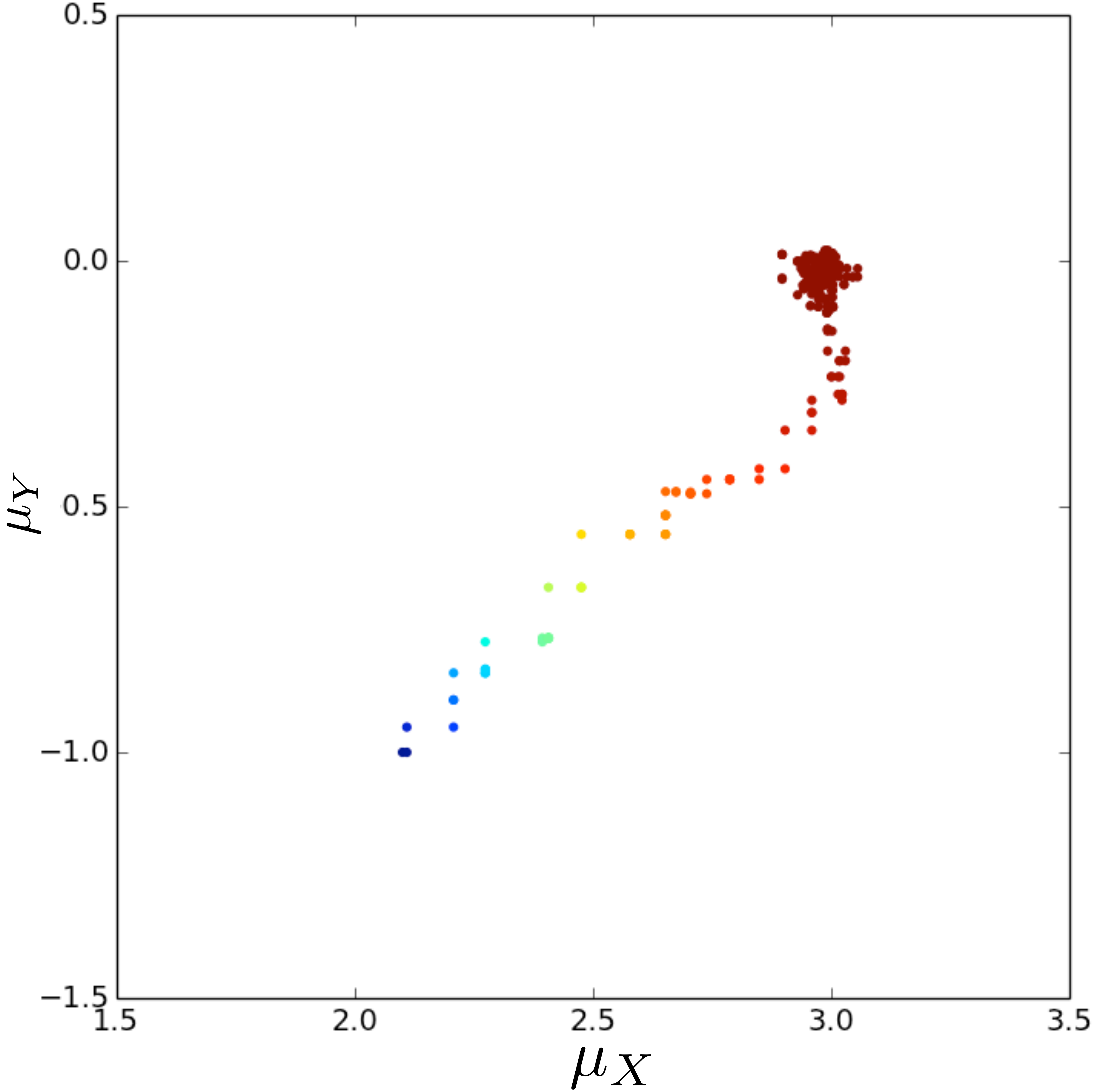
MCMC: The Metropolis-Hastings Recipe

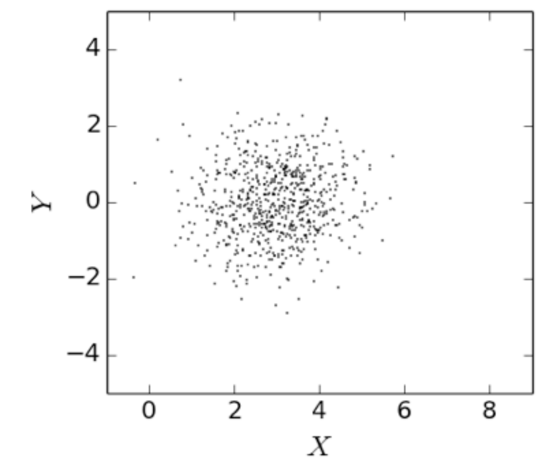
- The step size must be chosen so that the acceptance fraction (fraction of points accepted in the chain) lies between ~0.2 and ~0.5 (see Hogg et. al. 2010 and Foreman-Mackey et al. 2013)

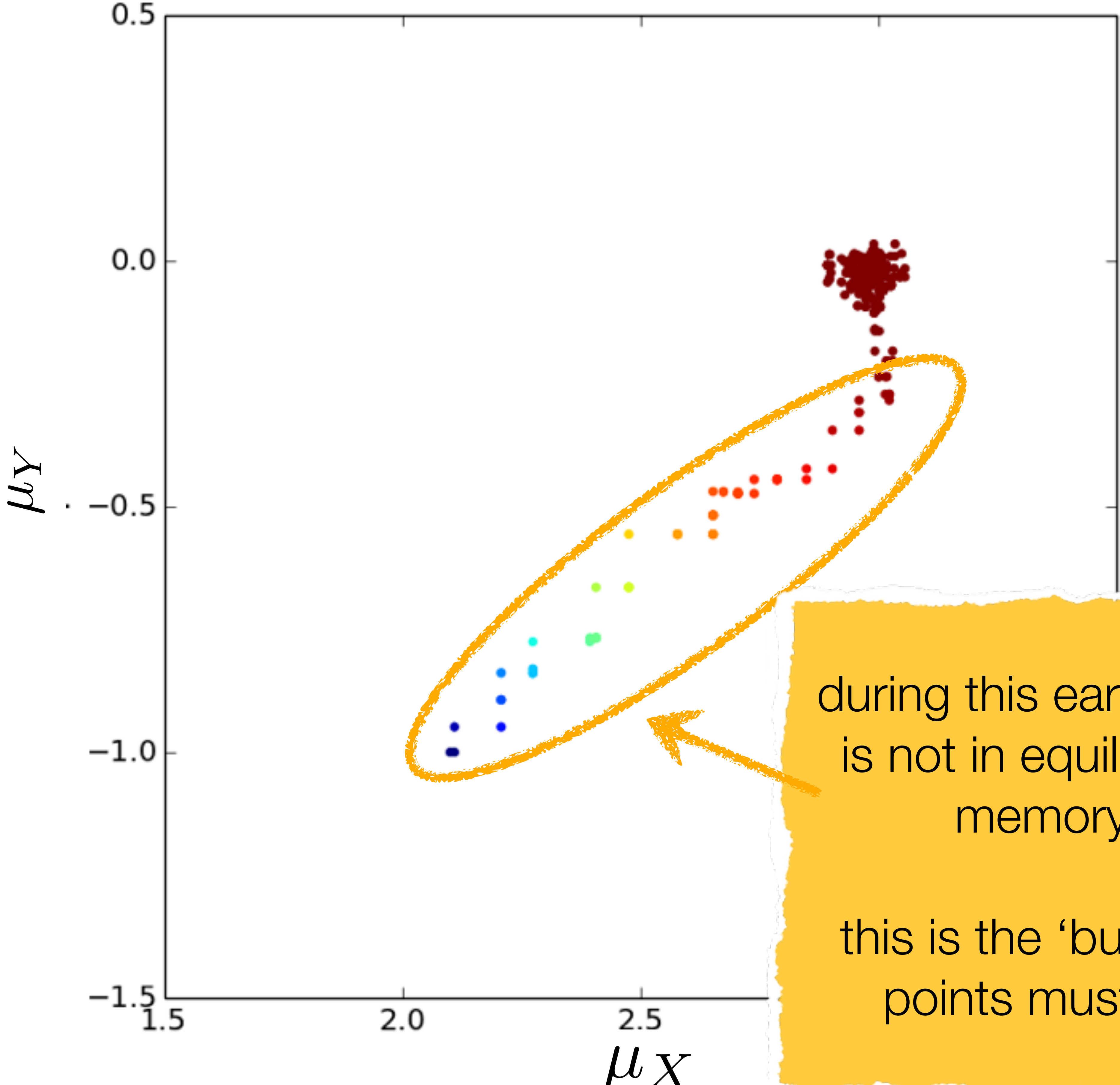
- This algorithm is a piece of cake to write, excellent for playing around to develop some intuition as to how the MCMC works

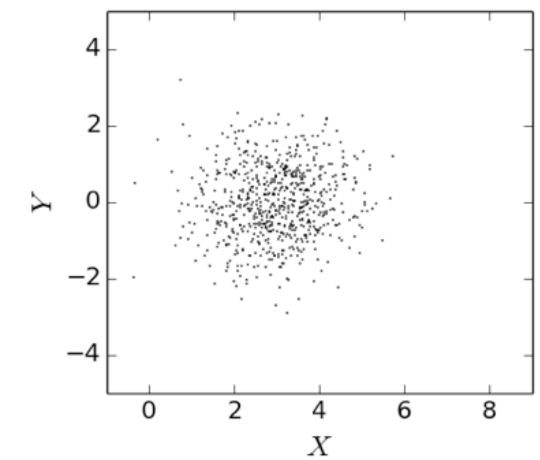
- The problem is that fine-tunning the chain when the number of parameters is large is highly non-trivial! (there's no way of guessing it a priori)

- This is solved by MCMC implementations like ***emcee*** (in Python, Foreman-Mackey et al. 2013) that use algorithms more sophisticated than Metropolis-Hastings, with very few free parameters


0.5
0.0
0.5
−1.0
−1.5
1.5
2.0
2.5
3.0
3.5
μ_Y
μ_X


4
2
0
−2
−4
0
2
4
6
8
Y
X



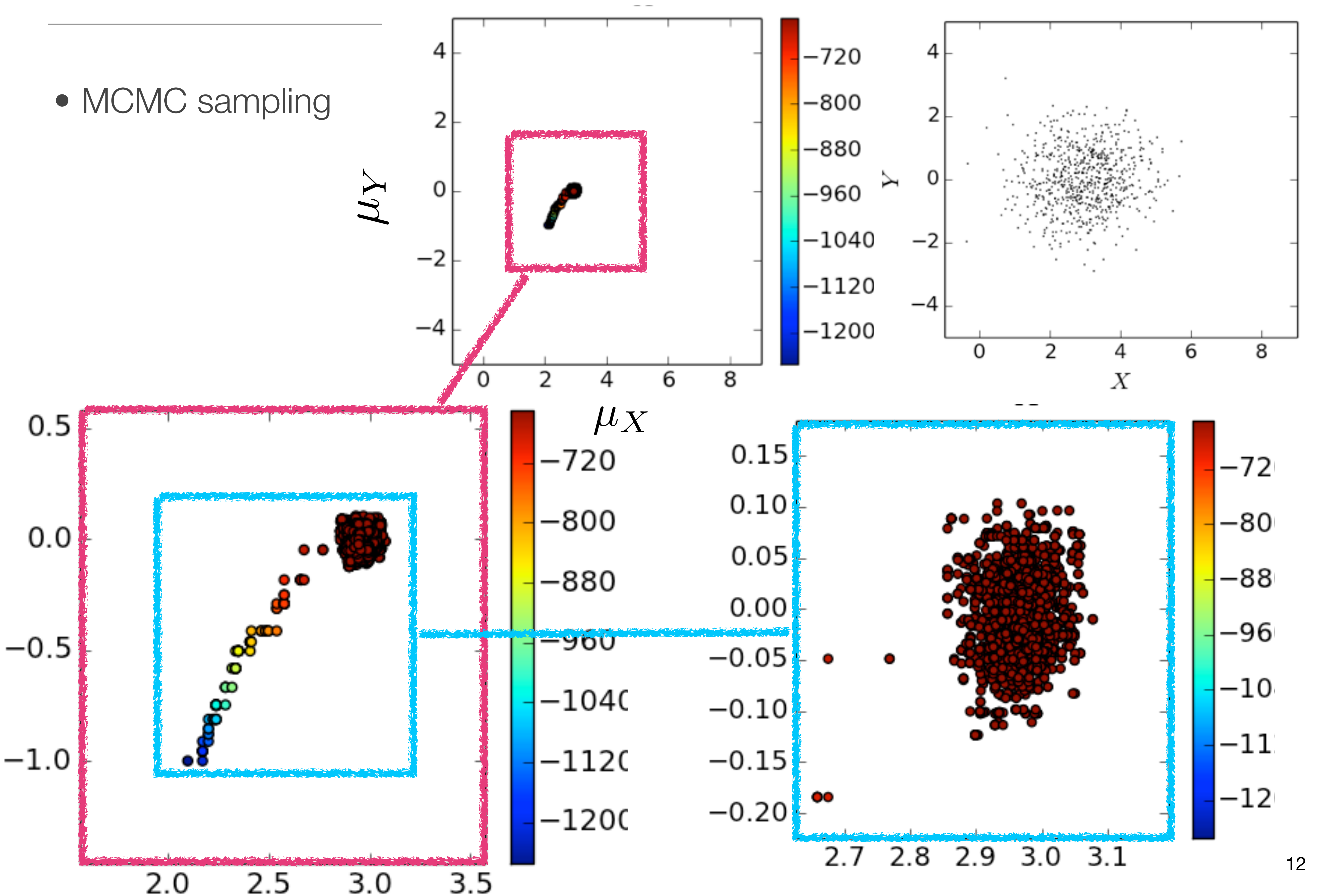


during this early stage the chain is not in equilibrium yet, it has memory of its path

this is the ‘burn-in’ stage, this points must be discarded

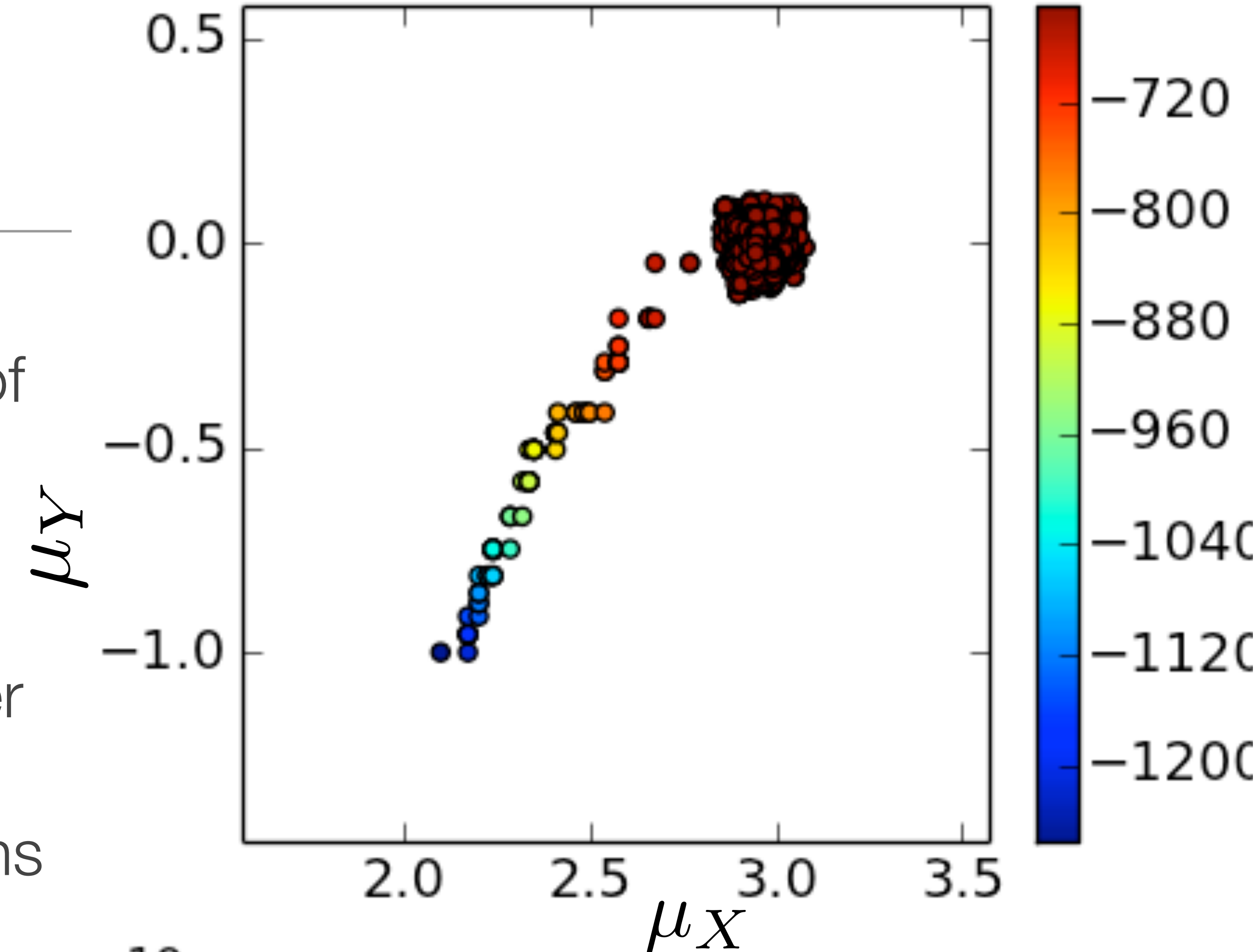
A two-parameter problem

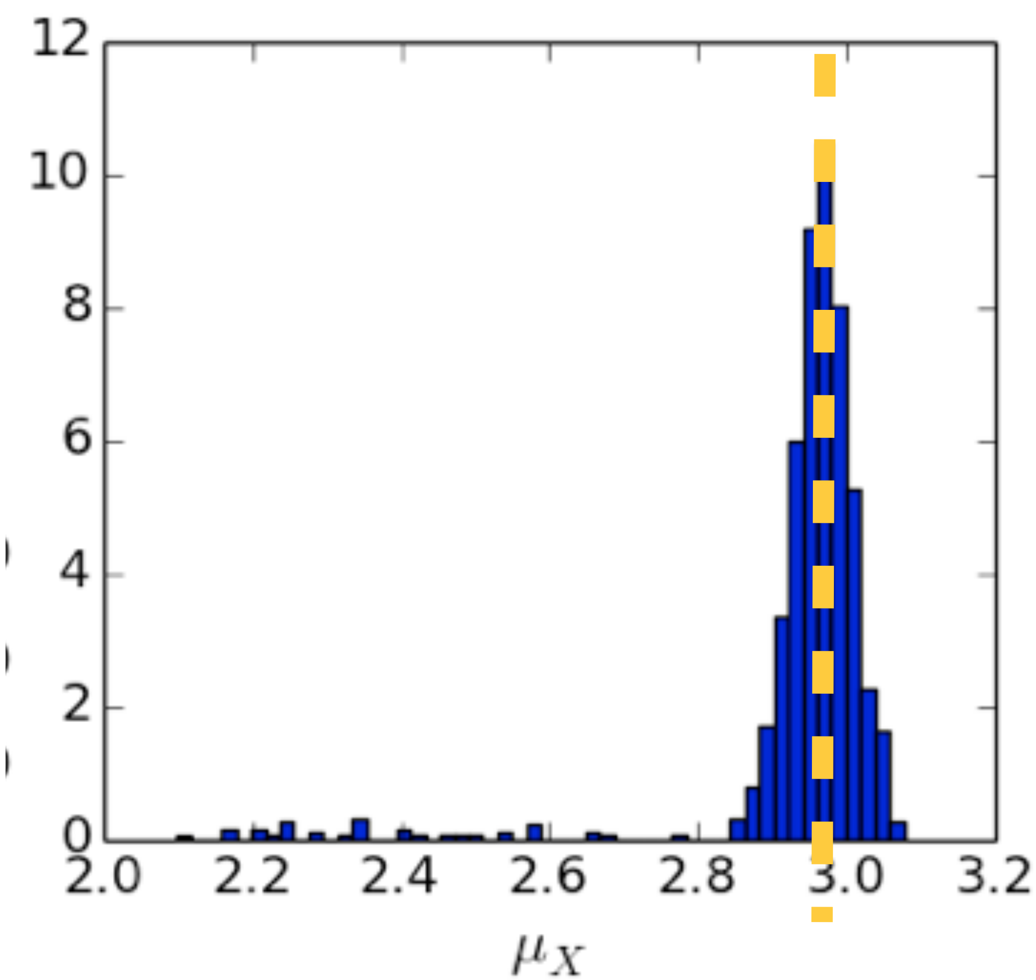
- MCMC sampling

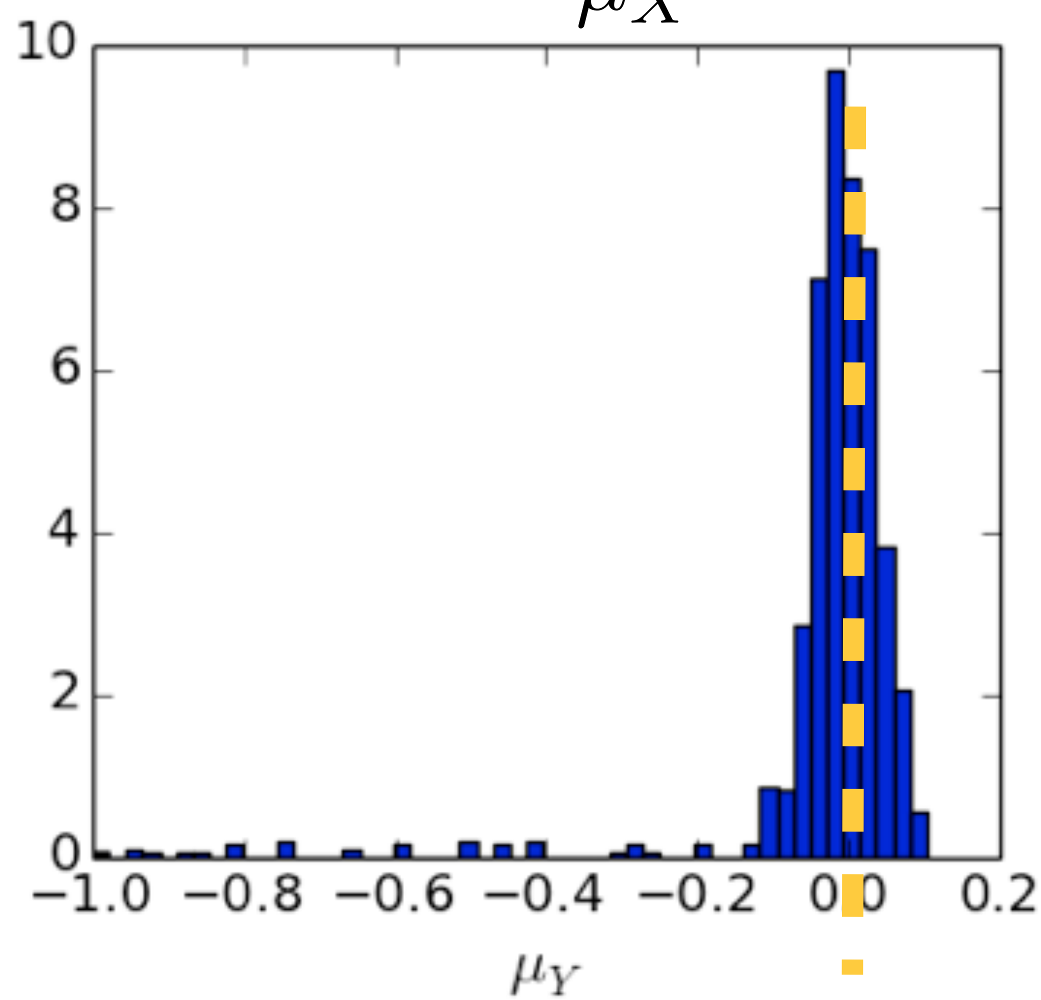


MCMC samples

- The set of points obtained in the final Markov Chain is a random realization of the Posterior PDF
- The mode of the histogram gives the most probable value of each parameter
- The percentiles give the credible regions

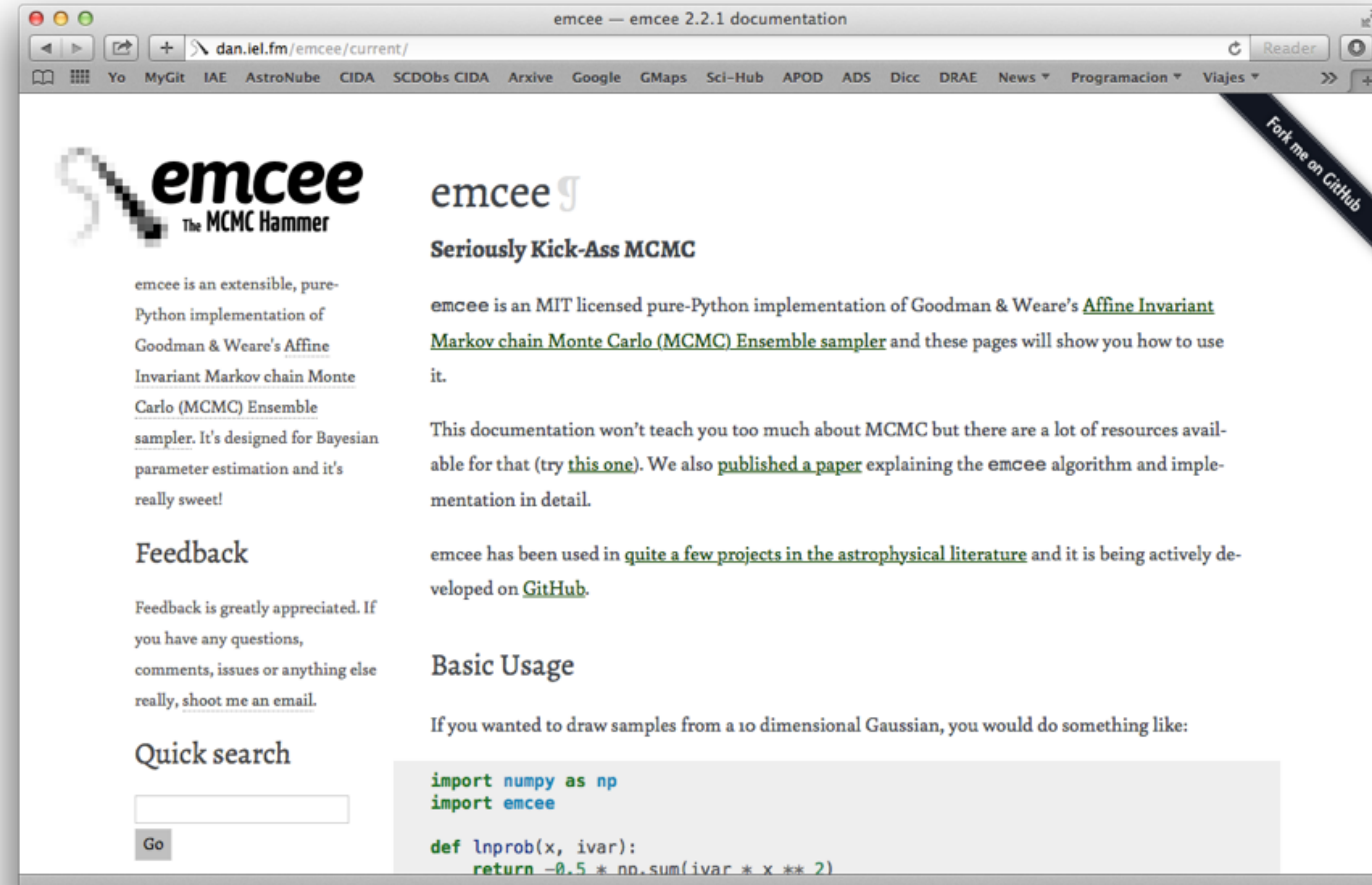






Suggested MCMC sampler: **emcee** (Python)

- Foreman-Mackey et al. 2013



More Suggested Bibliography

- Hogg, Bovy & Lang (2010)

Data analysis recipes:
Fitting a model to data*

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Approximate Bayesian Computation (ABC)

Approximate Bayesian Computation (ABC)

- Option for cases where there's no analytic likelihood, but there is enough knowledge about the problem to do forward modelling

Basic ABC algorithm

For the observed data $y_{1:n}$, prior $\pi(\theta)$ and distance function ρ:

Algorithm*

1. Sample θ^* from prior $\pi(\theta)$
2. Generate $x_{1:n}$ from forward process $f(y \mid \theta^*)$
3. Accept θ^* if $\rho(y_{1:n}, x_{1:n}) < \epsilon$
4. Return to step 1

Generates a sample from an approximation of the posterior:

$$f(x_{1:n} \mid \rho(y_{1:n}, x_{1:n}, \theta) < \epsilon) \cdot \pi(\theta) \approx f(y_{1:n} \mid \theta)\pi(\theta) \propto \pi(\theta \mid y_{1:n})$$

*Introduced in Pritchard et al. (1999) (population genetics)

"Though there be no such thing as Chance in the world; our ignorance of the real cause of any event has the same influence on the understanding"

-David Hume (1748)