Statistical techniques for data analysis in Cosmology

Numerical recipes (the “bible”)

Licia Verde
ICREA & ICC UB-IEEC

http://icc.ub.edu/~liciaverde
outline

• Lecture 1: Introduction Bayes vs Frequentists, priors, the importance of being Gaussian, modeling and statistical inference, some useful tools. Monte Carlo methods.

• Lecture 2 Different type of errors. Going beyond parameter fitting. Forecasting: Fisher matrix approach. Introduction to model selection. Real world effects

Conclusions.
What’s is all about

DATA

Models, models parameters

Measurement errors
Cosmic Variance

LCDM? w? etc…
Probabilities

Probability can be interpreted as a frequency

\[ P = \frac{n}{N} \]

Frequentists vs Bayesian

For Frequentists events are just frequencies of occurrence: probabilities are only defined as the quantities obtained in the limit when the number of independent trials tends to infinity.

Bayesians interpret probabilities as the degree of belief in a hypothesis: they use judgment, prior information, probability theory etc...

Bayesians and Frequentists often criticize each other; many physicists take a more pragmatic approach about what method to use.
Probabilities

Concept of Random variable $x$

Probability distribution $P(x)$

Properties of probability distribution:

1. $P(x)$ is a non-negative, real number for all real values of $x$.

2. $P(x)$ is normalized so that $\int dx P(x) = 1$

3. For mutually exclusive events $x_1$ and $x_2$, $P(x_1 + x_2) = P(x_1) + P(x_2)$ the probability of $x_1$ or $x_2$ to happen is the sum of the individual probabilities. $P(x_1 + x_2)$ is also written as $P(x_1 U x_2)$ or $P(x_1 OR x_2)$.

4. In general:
$$P(a, b) = P(a)P(b|a) ; \quad P(b, a) = P(b)P(a|b) \quad P(a, b) = P(b, a).$$

For independent events then $P(a, b) = P(a)P(b)$.

Ex. Produce examples of this last case
We might want to add:

\[ P(a) = \sum_b P(a, b) \]

Useful later when talking about marginalization
Bayes theorem

\[ P(H|D) = \frac{P(H)P(D|H)}{P(D)} \]

Fundamental difference here; “statistical INFERENCES”

Prior: how do you choose \( P(H) \)? Back to this later.
Drawbacks: Examples, discussion

\[ r \log r \]

\[ \tau \log \tau \quad \exp(-2 \tau) \]

comparing \( \mathcal{P}(x) \) with \( \mathcal{P}(f(x)) \):

\[ \mathcal{P}(f) = \mathcal{P}(x(f)) \left| \frac{df}{dx} \right|^{-1} \]
The importance of the prior

Priors are not generally bad!
Characterizing probability distributions

\[ \langle f(x) \rangle = \int dx f(x) \mathcal{P}(x) \]  

averages

\[ \hat{\mu}_m = \langle x^m \rangle \]  
moments

\[ \mu_m = \langle (x - \langle x \rangle)^m \rangle \]  
central moments

\[ \mu_2 \] is the variance, \[ \mu_3 \] is called the skewness, \[ \mu_4 \] is related to the kurtosis

Gaussian vs non-Gaussian
Characterizing probability distributions

Gaussian or Normal

The Normal Distribution

\( f(x) \)

\( \mu \)

\( X \)

kurtosis

skewness
Moments vs cumulants

For non-Gaussian distribution, the relation between central moments and cumulants for the first 6 orders is

\[
\begin{align*}
\mu_1 &= 0 \\
\mu_2 &= \kappa_2 \\
\mu_3 &= \kappa_3 \\
\mu_4 &= \kappa_4 + 3(\kappa_2)^2 \\
\mu_5 &= \kappa_5 + 10\kappa_3\kappa_2 \\
\mu_6 &= \kappa_6 + 15\kappa_4\kappa_2 + 10(\kappa_3)^2 + 15(\kappa_2)^3
\end{align*}
\]

For a Gaussian distribution all moments of order higher than 2 are specified by \(\mu_1\) and \(\mu_2\)
Generating function

\[ Z(k) = \langle \exp(ikx) \rangle = \int dx \exp(ikx) \mathcal{P}(x) \]

\[ Z(k) = \sum_{n=0}^{\infty} \frac{(ik)^n}{n!} \hat{\mu}_n \]

\[ \hat{\mu}_n = (-i^n) \frac{d^n}{dk^n} Z(k) \big|_{k=0} \]

Check that:

**cumulants** are obtained by doing the same operation on \( \ln Z \).
Central limit theorem

Let $n$ be the number of events. The probability distribution $P(x_i)$ is such that $<x_i> = 0$ for simplicity.

Let $Y$ be their sum. What is $P(Y)$?

$$Z_Y(k) = \sum_{m=0}^{\infty} \left[ \frac{(ik)^m}{m!} \mu^m \right]^n \approx \left( 1 - \frac{1}{2} \frac{k^2 <x^2>}{n} + ... \right)^n$$

For $n \to \infty$ then $Z_Y(k) \to \exp[-1/2k^2 <x^2>]$.

$$P(Y) = \frac{1}{\sqrt{2\pi} <x^2>} \exp \left[ -\frac{1}{2} \frac{Y^2}{<x^2>} \right]$$
There are exceptions:

Cauchy distribution

\[ P(x) = \frac{1}{\pi \sigma (1 + [(x - \bar{x})/\sigma]^2)^{-1}}. \]
The Poisson distribution

\[ \mathcal{P}_1 = \rho \delta V \quad \mathcal{P}_0 = 1 - \rho \delta V. \]

\[ Z(k) = \sum_n \mathcal{P}_n \exp(ikn) = 1 + \rho \delta V (\exp(ik) - 1) \]

\[ Z(k) = (1 + \rho \delta V (\exp(ik) - 1))^{V/\delta V} \sim \exp[\rho V (\exp(ik) - 1)]. \]

substitution \( \rho V \rightarrow \lambda \).

\[ Z(k) = \exp[\lambda (\exp(ik) - 1)] = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \exp(-\lambda) \exp(ikn). \]

\[ \mathcal{P}_n = \frac{\lambda^n}{n!} \exp[-\lambda] \]
The importance of Gaussian

Analytic
Simplicity
Inflation
and the central limit theorem
Random fields, probabilities and Cosmology

Average statistical properties
Particular important: \( \delta(x) = \delta \rho(x)/\rho \)

Ensamble: all the possible realizations of the true underlying Universe

Inference: examples

The Cosmological principle: models of the universe are homogeneous on average; in widely separated regions of the Universe the density field has the same statistical properties

A crucial assumption: we see a fair sample of the Universe

Ergodicity then follows: averaging over many realizations is equivalent to averaging over a large(enough) volume

Tools… statistics! Correlation functions etc…
Big advantage of being Bayesian

- Urn example
  (in reality NOT transparent)

Cosmic variance
Gaussian random fields

If $\delta$ is a Gaussian random field with average 0, its probability distribution is given by:

$$P_n(\delta_1, \cdots, \delta_n) = \frac{\sqrt{\text{Det} C^{-1}}}{(2\pi)^{n/2}} \exp \left[ -\frac{1}{2} \delta^T C^{-1} \delta \right]$$

$C_{ij} = \langle \delta_i \delta_j \rangle$.

Multi-variate Gaussian

Useful (back to this later)

Fourier!

Property n1: a Gaussian random field in Fourier space is still Gaussian
Property n2

\[ P(\text{Re}\delta_k, \text{Im}\delta_k)d\text{Re}\delta_kd\text{Im}\delta_k = \frac{1}{2\pi\sigma_k^2} \exp \left[ -\frac{\text{Re}\delta_k^2 + \text{Im}\delta_k^2}{2\sigma_k^2} \right] d\text{Re}\delta_kd\text{Im}\delta_k \]

Real and imaginary parts of the coefficients are randomly distributed
And mutually independent

Property n3: the phases of the Fourier modes are random

\[ P(|\delta_k|, \phi_k)d|\delta_k|d\phi_k = \frac{1}{2\pi\sigma_k^2} \exp \left[ -\frac{|\delta_k|^2}{2\sigma_k^2} \right] |\delta_k|d|\delta_k|d\phi_k \]

that is \(|\delta_k|\) follows a Rayleigh distribution.

From here the name Gaussian random phases

Important property: \(\sigma_k^2\) or \(\langle \delta_i\delta_j \rangle\) completely specifies your Gaussian random field
follows that the probability that the amplitude is above a certain threshold $X$

$$P(|\delta_k|^2 > X) = \int_{\sqrt{X}}^{\infty} \frac{1}{\sigma_k^2} \exp \left[ - \frac{|\delta_k|^2}{2\sigma_k^2} \right] |\delta_k| d|\delta_k| = \exp \left[ - \frac{X}{\langle |\delta_k|^2 \rangle} \right].$$

Is the density field Gaussian?

Today no way

In the beginning?

Now you can generate a Gaussian random field!
Brief digression

Useful tools:

Fourier transform of overdensity field

\[
\delta_{\vec{k}} = A \int d^3r \delta(\vec{r}) \exp[-i\vec{k} \cdot \vec{r}]
\]

\[
\delta(\vec{r}) = B \int d^3k \delta_{\vec{k}} \exp[i\vec{k} \cdot \vec{r}]
\]

\[
\delta^D(\vec{k}) = BA \int d^3r \exp[\pm i\vec{k} \cdot \vec{r}]
\]

Here I chose the convention \( A = 1, \ B = 1/(2\pi)^3 \), but always beware
(2-point) Correlation function

\[ \xi(x) = \langle \delta(\vec{r})\delta(\vec{r} + \vec{x}) \rangle = \int < \delta_{\vec{k}} \delta_{\vec{k}'} > \exp[i\vec{k} \cdot \vec{r}] \exp[i\vec{k}' \cdot (\vec{r} + \vec{x})] \, d^3 k \, d^3 k' \]

isotropy \( \xi(|x|) \)

Power spectrum

\[ < \delta_{\vec{k}} \delta_{\vec{k}'} > = (2\pi)^3 P(k) \delta^D(\vec{k} + \vec{k}') \]

isotropy \( P(k) \)

Since \( \delta(\vec{r}) \) is real, we have that \( \delta^*_{\vec{k}} = \delta_{-\vec{k}} \)
This implies:

$$< \delta_k \delta^*_k '> = (2\pi)^3 \int d^3 x \xi(x) \exp[-i \vec{k} \cdot \vec{x}] \delta^d(\vec{k} - \vec{k}')$$

Fourier transform pairs

$$\xi(x) = \frac{1}{(2\pi)^3} \int P(k) \exp[i \vec{k} \cdot \vec{r}] d^3 k$$

$$P(k) = \int \xi(x) \exp[-i \vec{k} \cdot \vec{x}] d^3 x$$

They contain the same information!
variance

\[ \sigma^2 = \langle \delta^2(x) \rangle = \xi(0) = \frac{1}{(2\pi)^3} \int P(k) d^3k \]

\[ \sigma^2 = \int \Delta^2(k) d \ln k \text{ where } \Delta^2(k) = \frac{1}{(2\pi)^3} k^3 P(k) \]

Independent of FT conventions!

PS on what scale?
Filters

Two typical choices

\[ f = \frac{1}{(2\pi)^{3/2} R_G^3} \exp[-1/2x^2/R_G^2] \quad \text{Gaussian} \rightarrow f_k = \exp[-k^2 R_G^2/2] \]

\[ f = \frac{1}{(4\pi) R_T^3} \Theta(x/R_T) \quad \text{TopHat} \rightarrow f_k = \frac{3}{(kR_T)^3} \left[ \sin(kR_T) - kR_T \cos(kR_T) \right] \]

roughly \( R_T \simeq \sqrt{5} R_G \)

Remember:

Convolution in real space is multiplication in Fourier space

Multiplication in real space in convolution in Fourier space
exercise

Consider a multi variate gaussian

\[ P(\delta_1..\delta_n) = \frac{1}{(2\pi)^{n/2}\text{det}C^{1/2}} \exp\left[-\frac{1}{2}\delta^T C^{-1} \delta\right] \]

Where \( C_{ij} = \langle \delta_i \delta_j \rangle \) is the covariance. Show that if the \( \delta_i \) are Fourier modes then \( C_{ij} \) is diagonal.

For Gaussian fields the k-modes are independent. Consequences…
The importance of the power spectrum

\[ P(k) = A \left( \frac{k}{k_0} \right)^n \]

Spectral index

generalize

\[ P(k) = A \left( \frac{k}{k_0} \right)^{n(k_0) + \frac{1}{2} \frac{dn}{d \ln k} \ln (k/k_0)} \]

Running of the Spectral index

Beware of the pivot:

\[ A(k_1) = A(k_0) \left( \frac{k}{k_0} \right)^{n(k_0) + \frac{1}{2} \frac{dn}{d \ln k} \ln (k_1/k_0)} \]
End of digression: Back to Moments vs cumulants

For non-Gaussian distribution, the relation between central moments and cumulants for the first 6 orders is

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\begin{align*}
\mu_1 &= 0 \\
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\end{align*}
\]

For a Gaussian distribution all moments of order higher than 2 are specified by \( \mu_1 \) and \( \mu_2 \)
Wick’s theorem
Is a method of reducing high-order derivatives to a combinatorics problem used in QFT.

Cumulant expansion theorem
Example:

\[
\langle \delta_1 \ldots \delta_6 \rangle = \langle \delta_1 \delta_2 \rangle_{\text{conn.}} \langle \delta_3 \delta_4 \rangle_{\text{conn.}} \langle \delta_5 \delta_6 \rangle_{\text{conn.}} + \ldots 15 \text{ terms} \\
+ \langle \delta_1 \delta_2 \rangle_{\text{conn.}} \langle \delta_3 \delta_4 \delta_5 \delta_6 \rangle_{\text{conn.}} + \ldots 15 \text{ terms} \\
+ \langle \delta_1 \delta_2 \delta_3 \rangle_{\text{conn.}} \langle \delta_4 \delta_5 \delta_6 \rangle_{\text{conn.}} + \ldots 10 \text{ terms} \\
+ \langle \delta_1 \ldots \delta_6 \rangle_{\text{conn.}}
\]
Modeling of data and Statistical inference

Read numerical recipes chapter 15, read it again, then when you have to apply all this, read it again.

example

Fit this with a line

Need a “figure of merit”

Least squares….
What you want:

- Best fit parameters
- Error estimates on the parameters
- A statistical measure of the goodness of fit (possibly)

Bayesian: “what is the probability that a particular set of parameters is correct?”

Figure of merit: “given a set of parameters this is the probability of occurrence of the data”
Least squares fit….

\[ \chi^2 = \sum_i w_i [D_i - y(x_i | \alpha')]^2 \]

you can show that the minimum variance weights are \( w_i = 1/\sigma_i^2 \).

And what if data are correlated?

\[ \chi^2 = \sum_{ij} (D_i - y_i) F_{ij} (D_j - y_j) = (\tilde{D} - \bar{y}) C^{-1} (\tilde{D} - \bar{y}) \]

In general: chi-squared
Goodness of fit?

If all is Gaussian, the probability of $\chi^2$ at the minimum follows a $\chi^2$ distribution, with $\nu=n-m$ degrees of freedom

\[
P(\chi^2 < \hat{\chi}^2, \nu) = P(\nu/2, \hat{\chi}^2/2) = \Gamma(\nu/2, \hat{\chi}^2/2)
\]

Incomplete gamma function

\[
Q = 1 - P(\nu/2, \hat{\chi}^2/2)
\]

Goodness of fit if evaluated at the best fit
Too small $Q$?

a) Model is wrong! Try again…

b) Real errors are larger

c) non-Gaussian

In general Monte-Carlo simulate….

Too large $Q$?

a) Errors overestimated

b) Neglected covariance?

c) Non-Gaussian (almost never..)

P.S chi-by-eye?
Confidence regions

If $m$ is the number of fitted parameters for which you want to plot the joint confidence region and $p$ is the confidence limit desired, find the $\Delta \chi^2$ such that the probability of a chi-Square variable with $m$ degrees of freedom being less than $\Delta \chi^2$ is $p$. Use the Q function above.
Confidence regions

<table>
<thead>
<tr>
<th>$\sigma$</th>
<th>$p$</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-(\sigma)</td>
<td>68.3%</td>
<td>1.00</td>
<td>2.30</td>
<td>3.53</td>
</tr>
<tr>
<td>2-(\sigma)</td>
<td>95.4%</td>
<td>4.00</td>
<td>6.17</td>
<td>8.02</td>
</tr>
<tr>
<td>3-(\sigma)</td>
<td>99.73%</td>
<td>9.00</td>
<td>11.8</td>
<td>14.2</td>
</tr>
</tbody>
</table>

$\Delta \chi^2$
Likelihoods

Remember Bayes …

\[ P(H|D) = \frac{P(H)P(D|H)}{P(D)} \]

set \( P(D) = 1 \)  Back to this later

In many cases, can invoke the central limit theorem

a multi-variate Gaussian:

\[
\mathcal{L} = \frac{1}{(2\pi)^{n/2}|\text{det}C|^{1/2}} \exp \left[ -\frac{1}{2} \sum_{ij} (D - y)_i C_{ij}^{-1} (D - y)_j \right]
\]

where \( C_{ij} = \langle (D_i - y_i)(D_j - y_j) \rangle \) is the covariance matrix.
Confidence levels

Bayesians

\[ \int_R P(\alpha|D) d\alpha = 0.683 \ldots \text{ or } 0.95 \ldots \text{ or } \ldots \]

Integrating over the hypothesis

Classical: likelihood ratio

\[ -2 \ln \left( \frac{\mathcal{L}(\alpha)}{\mathcal{L}_{\max}} \right) \leq \text{threshold} \]
In higher dimensions....
Questions for you

• in what simple case can you make an easy identification of the likelihood ratio with the chi-square?

• In what case can you make an easy identification between the two approaches?
There is a BIG difference between $\chi^2$ & reduced $\chi^2$

Only for multivariate Gaussian with constant covariance
\[-2 \ln L = \chi^2\]

If likelihood is **Gaussian** and **Covariance is constant**

Example: for multi-variate Gaussian

Errors
Marginalization

\[ P(\alpha_1, \ldots, \alpha_j | D) = \int d\alpha_{j+1}, \ldots, d\alpha_m P(\bar{\alpha} | D) \]
Other data sets

If independent, multiply the two likelihoods

(can use some of them as “priors”)

Beware of inconsistent experiments!
Spergel 2007
Useful trick for Gaussian likelihoods

e.g. marginalizing over point source amplitude

\[
P(\alpha_1..\alpha_{m-1}|D)=\int \frac{dA}{(2\pi)^{m/2}||C||^{1/2}} e^{-\frac{1}{2}(C_i-(\hat{C}_i+AP_i))\Sigma_{ij}^{-1}(C_j-(\hat{C}_j+AP_j))} \\
\times \frac{1}{\sqrt{2\pi}\sigma^2} \exp \left[-\frac{1}{2} \frac{(A-\hat{A})^2}{\sigma^2}\right]
\]

The trick is to recognize that this integral can be written as:

\[
P(\alpha_1..\alpha_{m-1}|D) = C_0 \exp \left[-\frac{1}{2}C_1 - 2C_2A + C_3A^2\right] dA
\]

substitution \( A \rightarrow A - C_2/C_3 \)

result \( \propto \exp[-1/2(C_1 - C_2^2/C_3)] \).
Observation of N clusters is Poisson

\[ \mathcal{P} = \prod_{i=1}^{N} \left[ e_i^{n_i} \exp(-e_i) / n_i! \right] \]

\( n_i \) is the number of clusters observed in the \( i \)-th experimental bin

\( e_i = I(x) \delta x_i \)  ... expected  .......

Experimental bin (mass, SZ decrement, X-ray lum, z…)

Define \( C \equiv -2 \ln \mathcal{P} = 2 \left( E - \sum_{i=1}^{N} \ln I_i \right) \)

E is the total expected number of clusters in a given model

\( \Delta C \) Between 2 different models is chisquared-distributed!
question

Have used the product of Poisson distributions so have assumed independent processes...

Clusters are clustered...
Monte Carlo methods
Monte Carlo methods

a) Monte Carlo error estimation

b) Monte Carlo Markov Chains
Your brain does it!

Spot the differences…
Intro to: Monte Carlo

Simple problem: what’s the mean of a large number of objects?

What’s the mean height of people in La Palma?

$$\frac{\sum_{i=1}^{N} h_i}{N}$$

If N is very large this is untractable soo…

$$\sim \frac{\sum_{i=1}^{n} h_i}{n}$$

If n<<N but still a fair sample, great!

In probability:

$$\int f(x)P(x)dx \sim \frac{1}{S} \sum_{S} f(x^s)$$

if $x^s \sim P(x)$

In Bayesian inference:

$$p(x|D) = \int P(x|\theta, D)P(\theta|D)d\theta \sim \frac{1}{S} \sum P(x|\theta^s, D)$$

if $\theta^s \sim P(\theta|D)$
You can show that:

The estimator is unbiased
and you can quantify the variance of the estimator:
The error shrinks like $S^{1/2}$
Very simple example:

A dumb approximation of $\pi$

4 times the red area

$$P(x,y) = \begin{cases} 
1 & 0 < x < 1 \text{ and } 0 < y < 1 \\
0 & \text{otherwise}
\end{cases}$$

$$\pi = 4 \int \int I((x^2 + y^2) < 1) P(x,y) \, dx \, dy$$

octave:1> S=12; a=rand(S,2); 4*mean(sum(a.*a,2)<1)
an = 3.3333
octave:2> S=1e7; a=rand(S,2); 4*mean(sum(a.*a,2)<1)
an = 3.1418

There are better ways to compute $\pi$, so use mcmc only when right to use…
Historical note

Enrico Fermi (1901–1954) took great delight in astonishing his colleagues with his remarkably accurate predictions of experimental results... he revealed that his "guesses" were really derived from the statistical sampling techniques that he used to calculate with whenever insomnia struck in the wee morning hours!

—The beginning of the Monte Carlo method,
N. Metropolis
Monte Carlo methods

a) Monte Carlo error estimation

Back to parameter estimation and confidence regions

Conceptual interpretation in cosmology

\[ \alpha_{\text{true}} \quad \text{Set of parameters known only to Mother Nature} \]

\[ \alpha \quad \text{Observable universe} \]

\[ \text{Measurement (with its errors)} \]

Do

\[ \text{Measured data} \quad \text{analysis} \rightarrow \alpha_0 \]

NOT a unique realization of \[ \alpha_{\text{true}} \]

You (the experimenter)

Can see

want
There could be infinitely many realizations (hypothetical data sets) \(D_1, D_2, \ldots\)

Each one with best fit parameters \(\alpha_1, \alpha_2, \ldots\)

Expect: \(\langle \alpha_i \rangle = \alpha_{\text{true}}\)

If I knew the distribution of \(\alpha_i - \alpha_{\text{true}}\) That’d be all I need

Trick: say that (hope) \(\alpha_0 \sim \alpha_{\text{true}}\)

In many cases we can simulate the distribution of \(\alpha_i - \alpha_0\)

Make many synthetic realizations of universes where \(\alpha_0\) is the truth; mimic the observational process in all these mock universes, estimate the best fit parameters from each; map \(\alpha_S - \alpha_0\) Very important tool
How to sample from the probability distribution?

• For some well known univariate probability distributions there are numerical routines http://cg.scs.carleton.ca/~luc/rnbookindex.html

• In other cases there may be numerical techniques to sample $P(x)$ [more later]

• Importance sampling: (if you know how to sample from $Q$ but not from $P$)

$$
\int f(x)P(x)dx = \int f(x) \frac{P(x)}{Q(x)} Q(x)dx \sim \frac{1}{S} \sum_{s=1}^{S} f(x^s) \frac{P(x^s)}{Q(x^s)} \text{ if } x^s \sim Q(x)
$$

Some $Q$ are more suitable for $P$ than others…. 
Monte Carlo Markov Chains

So you have a higher-dimensional probability distribution, you want to sample in a way proportional to it, with a random walk.

Start at an arbitrary point

Goal: density of points proportional to the probability

Take Markov steps

Burn-in

MCMC gives approximated, correlated samples from the target distribution.
b) Monte Carlo Markov Chains

http://cosmologist.info/cosmomc/

Using software as black box is ALWAYS a BAD idea
Grid-based approach

Operationally:

e.g., 2 params: 10 x 10

What if you have (say) 6 parameters?

You’ve got a problem!

b) Monte Carlo Markov Chains
Explore likelihood surface

$\Omega_m$

$\sigma_8$

6 params, 20 pixels/dim
= $6.7 \times 10^7$ evals
say 1.6 s/eval
~1200 days!
Markov Chain Monte Carlo (MCMC)

Standard in CMB analyses (publicly available COSMOMC)

Simulate

Bayes

Genera are a fair sample of the likelihood surface
Markov Chain Monte Carlo (MCMC)

Random walk in parameter space

At each step, sample one point in parameter space

The density of sampled points $\propto$ posterior distribution

FAST: before $10^7$ likelihood evaluations, now $< 10^5$

marginalization is easy: just project points and recompute their density

Adding external data sets is often very easy
Operationally (Metropolis-Hastings):

1. Start at a random location in parameter space: \( \alpha^\text{old}_i \) \( \mathcal{L}^\text{old} \)

2. Try to **take a random step** in parameter space: \( \alpha^\text{new}_i \) \( \mathcal{L}^\text{new} \)

3a. If \( \mathcal{L}^\text{new} \geq \mathcal{L}^\text{old} \) Accept (take and save) the step, “new” --> “old” and go to 2.

3b. If \( \mathcal{L}^\text{new} < \mathcal{L}^\text{old} \) Draw a random number \( x \) uniform in 0,1

    If \( x \geq \frac{\mathcal{L}^\text{new}}{\mathcal{L}^\text{old}} \) do not take the step (i.e. save “old”) and go to 2.

    If \( x < \frac{\mathcal{L}^\text{new}}{\mathcal{L}^\text{old}} \) do as in 3a.

KEEP GOING....
“Take a random step”

The probability distribution of the step is the “**propositional distribution**”, which you should not change once the chain has started.

The proposal distribution (the step-size) is crucial to the MCMC efficiency.

Steps too small step poor mixing

Steps too big step poor acceptance rate

“**fair sample of the likelihood surface**”, remember?
## The importance of stepsize

<table>
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<tr>
<th>Step size</th>
<th>Likelihood</th>
<th>Acceptance Rate</th>
</tr>
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<tr>
<td>$\sigma(0.1)$</td>
<td>99.8% accepts</td>
<td></td>
</tr>
<tr>
<td>$\sigma(1)$</td>
<td>68.4% accepts</td>
<td></td>
</tr>
<tr>
<td>$\sigma(100)$</td>
<td>0.5% accepts</td>
<td></td>
</tr>
</tbody>
</table>

The diagrams show the step number on the x-axis and the likelihood on the y-axis. The step sizes of $\sigma(0.1)$, $\sigma(1)$, and $\sigma(100)$ are depicted, with corresponding acceptance rates indicated. Each step size results in different exploration patterns, highlighting the importance of choosing an appropriate step size to balance exploration and acceptance.

- Poor exploration is observed for all step sizes, indicating the need for a more strategic approach to step size selection.

[Graphs showing step sizes and corresponding likelihoods]

- Step number

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### Diagram Notes

- The step size selection directly impacts the exploration of the likelihood space.
- Higher step sizes ($\sigma(100)$) lead to less exploration and fewer acceptances.
- Lower step sizes ($\sigma(0.1)$) result in more acceptance but less effective exploration.

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**Understanding Step Sizes**: The selection of step sizes is crucial for the effective exploration of the likelihood space, ensuring a balance between acceptance and exploration for optimal results.
The importance of stepsize
Take a random step

For statisticians: transition operators

Detailed balance: (beware of boundaries....)
When the MCMC has forgotten about the starting location and has well explored the parameter space, you’re ready to do parameter estimation.

**USE a MIXING and CONVERGENCE criterion!!!**
Gelmans and Rubin convergence

Recommended: start 4 to 8 chains at well separated points
M chains, N elements

Chain mean
\[ \bar{y}^j = \frac{1}{N} \sum_{i=1}^{N} y_i^j, \]

Vector with parameters value

Mean of distrib.
\[ \bar{y} = \frac{1}{NM} \sum_{ij=1}^{NM} y_i^j. \]

Variance between chains
\[ B_n = \frac{1}{M-1} \sum_{j=1}^{M} (\bar{y}^j - \bar{y})^2 \]

And within
\[ W = \frac{1}{M(N-1)} \sum_{ij} (y_i^j - \bar{y}^j)^2 \]

\[ \hat{R} = \frac{\frac{N-1}{N} W + B_n \left( 1 + \frac{1}{M} \right)}{W} \]

Always >1 by construction
Require <1.03
Unconverged chains are just nonsense
Metropolis-Hastings is NOT the only implementation,

Other options are:
Gibbs Sampler
Rejection method
Hamiltonian Monte-Carlo
Simulated annealing (though you do not get an MCMC)
Beware of DEGENERACIES

Reparameterization. e.g., Kosowsky et al. 2002

\[ \theta_A = \frac{r_s(a_{dec})}{D_A(a_{dec})} \]
Even “better”:

Cosmomc has the option of computing the covariance for the parameters. Find the axis of the multi dim. degeneracies, perform a rotation and re-scaling to obtain azimuthally symmetric contours.

An improve MCMC efficiency by factor of up to 10

It is still a linear operation.
Where’s the prior?
Once you have the MCMC output:

- The density of points in parameter space gives you the posterior distribution.
- To obtain the marginalized distribution, just project the points.
- To obtain confidence intervals, integrate the “likelihood” surface and compute where e.g. 68.3% of points lie.
- To each point in parameter space sampled by the MCMC give a weight proportional to the number of times it was saved in the chain.
- To add to the analysis another dataset (that does not require extra parameters) renormalize the weight by the “likelihood” of the new data set. No need to re-run!

**warning:** if new data set is not consistent with the old one --> nonsense
Key concepts today

• Random fields and cosmology
• Probability
• Bayes theorem
• Gaussian distributions (and not)
• Modeling of data and statistical inference
• Likelihoods and chi squared
• Confidence levels; confidence regions
• Monte Carlo methods
• Monte-Carlo errors
• MCMC