## **Statistics**

arXiv:0712.3028; arXiv:0911.3105 Numerical recipes (the "bible")

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There are 4 kinds of lies:

- 1. Lies
- 2. Damn Lies
- 3. Statistics
- 4. Bayesian Statistics

Ned Wright

# outline

- Introduction Bayes vs Frequentists
- priors
- modeling and statistical inference
- Monte Carlo methods.
- Different type of errors.
- Conclusions.

# What's is all about



#### Probabilities

Probability can be interpreted as a **frequency** 

$$\mathcal{P} = \frac{n}{N}$$

#### 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 (background)

Concept of Random variable x

Probability distribution  $\mathcal{P}(x)$ 

Properties of probability distribution:

- 1.  $\mathcal{P}(x)$  is a non negative, real number for all real values of x.
- 2.  $\mathcal{P}(x)$  is normalized so that  $\int dx \mathcal{P}(x) = 1$
- 3. For mutually exclusive events  $x_1$  and  $x_2$ ,  $\mathcal{P}(x_1 + x_2) = \mathcal{P}(x_1) + \mathcal{P}(x_2)$  the probability of  $x_1$  or  $x_2$  to happen is the sum of the individual probabilities.  $\mathcal{P}(x_1 + x_2)$  is also written as  $\mathcal{P}(x_1 U x_2)$  or  $\mathcal{P}(x_1 . OR. x_2)$ .
- 4. In general:

$$\mathcal{P}(a,b) = \mathcal{P}(a)\mathcal{P}(b|a) \hspace{0.2cm} ; \hspace{0.2cm} \mathcal{P}(b,a) = \mathcal{P}(b)\mathcal{P}(a|b) \hspace{0.2cm} \mathcal{P}(a,b) = \mathcal{P}(b,a).$$

For independent events then  $\mathcal{P}(a, b) = \mathcal{P}(a)\mathcal{P}(b)$ .

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**



#### From

 $\mathcal{P}(a,b) = \mathcal{P}(a)\mathcal{P}(b|a) \hspace{2mm} ; \hspace{2mm} \mathcal{P}(b,a) = \mathcal{P}(b)\mathcal{P}(a|b)$ 

Fundamental difference here; "statistical INFERENCE" Prior: how do you chose P(H)? Back to this later.

#### Drawbacks: Examples, discussion

- r log r
- $\tau \quad \log \tau \quad \exp(-2\tau)$

## 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!

## Random fields, probabilities and Cosmology

Average statistical properties Particulary important:  $\delta(\vec{x}) = \delta \rho(\vec{x}) / \rho$ 

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 <u>fair sample</u> 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



# 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.



# 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....

$$\chi^2 = \sum_i w_i [D_i - y(x_i | \vec{\alpha})]^2$$

you can show that the minimum variance weights are  $w_i = 1/\sigma_1^2$ .

And what if data are correlated?

$$\chi^2 = \sum_{ij} (D_i - y_i) F_{ij} (D_j - y_j) = (\vec{D} - \vec{y}) C^{-1} (\vec{D} - \vec{y})$$

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 v=n-m degrees of freedom # data points # data points #parameters

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

Incomplete gamma function

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

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

Number of parameters

σ	р	1	2	3	
1-σ	68.3%	1.00	2.30	3.53	
	90%	2.71	4.61	6.25	$\Delta \chi^2$
$2$ - $\sigma$	95.4%	4.00	6.17	8.02	
3-σ	99.73%	9.00	11.8	14.2	

Joint confidence levels

## Likelihoods

Remember Bayes ...  $\mathcal{P}(H|D) = \frac{\mathcal{P}(H)\mathcal{P}(D|H)}{\mathcal{P}(D)}$ 

set  $\mathcal{P}(D) = 1$  Back to this later

In many cases, can invoke the central limit theorem

a multi-variate Gaussian:

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

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

## **Confidence levels**

Bayesians  $\int_{R} \mathcal{P}(\vec{\alpha}|D) d\vec{\alpha} = 0.683... \text{ or } 0.95... \text{ or } ...$ 

Integrating over the hypothesis

Classical: likelihood ratio

$$-2\ln\left[\frac{\mathcal{L}(\vec{\alpha})}{\mathcal{L}_{max}}\right] \leq \text{threshold}$$



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

	$\Delta\chi^2$ as a Function of Confidence Level and Degrees of Freedom									
		ν								
	p	1	2	3	4	5	6			
<b></b>	68.3%	1.00	2.30	3.53	4.72	5.89	7.04			
	90%	2.71	4.61	6.25	7.78	9.24	10.6			
<b>→</b>	95.4%	4.00	6.17	8.02	9.70	11.3	12.8			
	99%	6.63	9.21	11.3	13.3	15.1	16.8			
	99.73%	9.00	11.8	14.2	16.3	18.2	20.1			
	99.99%	15.1	18.4	21.1	23.5	25.7	27.8			

Only for multivariate Gaussian with constant covariance

 $\frac{\delta}{reduced \chi}^{2}$ 

 $\chi^2$ 

 $-2\ln \int \chi^2$  From: "Numerical recipes" Ch. 15 If likelihood is Gaussian and Covariance is constant



Example: for multi-variate Gaussian

**Errors** 

# Marginalization

$$P(\alpha_1..\alpha_j|D) = \int d\alpha_{j+1}, ...d\alpha_m P(\vec{\alpha}|D)$$



## Other data sets

If independent, multiply the two likelihoods

(can use some of them as "priors")

Beware of inconsistent experiments!







Lv, Protopapas, Jimenez, 2013

Useful trick for Gaussian likelihoods

e.g. marginalizing over point source amplitude

$$P(\alpha_{1}..\alpha_{m-1}|D) = \int \frac{dA}{(2\pi)^{\frac{m}{2}} ||C||^{\frac{1}{2}}} e^{\left[-\frac{1}{2}(C_{i}-(\hat{C}_{i}+AP_{i}))\Sigma_{ij}^{-1}(C_{j}-(\hat{C}_{j}+AP_{j}))\right]} \\ \times \frac{1}{\sqrt{2\pi\sigma^{2}}} \exp\left[-\frac{1}{2}\frac{(A-\hat{A})^{2}}{\sigma^{2}}\right]$$

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  $A \longrightarrow A - C_2/C_3$ 

result 
$$\propto \exp[-1/2(C_1 - C_2^2/C_3)]$$

## 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 Madrid?

 $\sum_{i=1}^{N} rac{h_i}{N}$  If N is very large this is untractable soo... r

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

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:

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

You can show that:

The estimator is unbiased and you can quantify the variance of the estimator: The error shrinks like S<sup>1/2</sup>

# Very simple example: A dumb approximation of $\pi$



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 remakably 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

# history



# Monte Carlo methods

a) Monte Carlo error estimation

Back to parameter estimation and confidence regions

Conceptual interpretation in cosmology



There could be infinitely many realizations (hypothetical data sets)  $D_1, D_2, ...$ 

Each one with best fit parameters  $\alpha_1, \alpha_2, ...$ 

Expect:  $< lpha_i > = lpha_{ ext{true}}$ 

If I knew the distribution of  $\alpha_i - lpha_{ ext{true}}$  That'd be all I need

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

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 <a href="http://cg.scs.carleton.ca/~luc/mbookindex.html">http://cg.scs.carleton.ca/~luc/mbookindex.html</a>
- 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



MCMC gives approximated, correlated samples from the target distribution

### Monte Carlo Markov Chains

### http://cosmologist.info/cosmomc/

#### **Cosmological MonteCarlo**



Google" Custom Search Get help: Search

NEW: (May 08) Support for UNION supernovae, equal-likelihood limits, WMAP5-format chains, more confidence limits (Mar/Apr 08) Support for WMAP5, CMB SZ templates, new reionization model (Feb 08) Latest ACBAR data, CAMB update, option to use as a generic sampler

See the <u>ReadMe</u> file for program documentation and download. Also the <u>CosmoloGUI</u> documentation.

## Markov Chain Monte Carlo (MCMC)

Standard in CMB analyses (publicly available COSMOMC)



Generate random draws from the posterior that are a fair sample of the probability(Likelihood) surface



Adding external data sets is often very easy

Operationally (Metropolis-Hastings):

1. Start at a random location in parameter space:  $\alpha_i^{\text{old}} \mathcal{L}^{\text{old}}$ 2. Try to take a random step in parameter space:  $\alpha_{\cdot}^{\text{new}} \beta_{\cdot}^{\text{new}}$ 3a. If  $\underline{\int}^{\text{new}} \geq \underline{\int}^{\text{old}} = Accept (take and save) the step,$ "new"--> "old" and go to 2.If  $x \ge \frac{\int_{-\infty}^{\infty} do$  not take the step (i.e. save "old")  $\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dc$  and go to 2. If  $x < \frac{\hat{\mathcal{L}}^{new}}{\hat{\Gamma}^{old}}$  do as in 3a.

**KEEP GOING....** 

"Take a random step"

The probability distribution of the step is the "proposal 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





### The importance of stepsize



Take a random step

For statisticians: transition operators

Detailed balance: (beware of boundaries....)

Detailed balance means  $\rightarrow x \rightarrow x'$  and  $\rightarrow x' \rightarrow x$  are equally probable:



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 
$$ar{y}^j = rac{1}{N}\sum_{i=1}^N y_i^j,$$

Vector with parameters value

Mean of distrib.

$$\bar{y} = \frac{1}{NM} \sum_{ij=1}^{NM} y_i^j \,.$$

3734

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**



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 azimutally 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

-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

### Errors, what errors?





# Statistical vs systematic errors



Statistics can tell you how to deal with statistical errors

As a data set grows, the statistical errors shrink; systematic errors do not shrink

You' ve got a problem.

Rumsfeld can help:

There are known knowns. These are things we know that we know. There are known unknowns. That is to say, there are things that we know we don't know. But there are also unknown unknowns. There are things we don't know we don't know. Donald Rumsfeld

Jokes aside: some interesting literature has appeared

# Key concepts today

- Probability
- Bayes theorem
- Modeling of data and statistical inference
- Likelihoods and chisquare
- Confidence levels; confidence regions
- Monte Carlo methods
- Monte-Carlo errors
- MCMC
- Errors, what errors?

# Exercise(s)

Monte Carlo integration

 $\pi$ 

A multi-dimensional Gaussian (compare to analytics)

Write your own MCMC

#### Simple example: H(z)

For a flat universe, generic equation of state parameter for dark energy

$$H(z) = H_0 (1+z)^{3/2} \sqrt{\Omega_m + \Omega_{vac} \exp\left[3\int_0^z \frac{w(z')}{(1+z')} dz'\right]};$$
(5)

for a non-flat Universe, equation of state parameter for dark energy given by the  $w_0, w_a$  parameterization:

$$H(z) = H_0 \left\{ \Omega_m (1+z)^3 + \Omega_k (1+z)^2 + \Omega_{vac} (1+z)^{3(1+w_0+w_a)} \exp[-3w_a z/(1+z)] \right\}^{1/2};$$
(6)

of course for a flat  $\Lambda$ CDM model we have:

$$H(z) = H_0 \sqrt{\Omega_m (1+z)^3 + (1-\Omega_m)}.$$
(7)

#### H(z) data from:

http://www.physics-astronomy.unibo.it/en/research/areas/astrophysics/ cosmology-with-cosmic-chronometers

