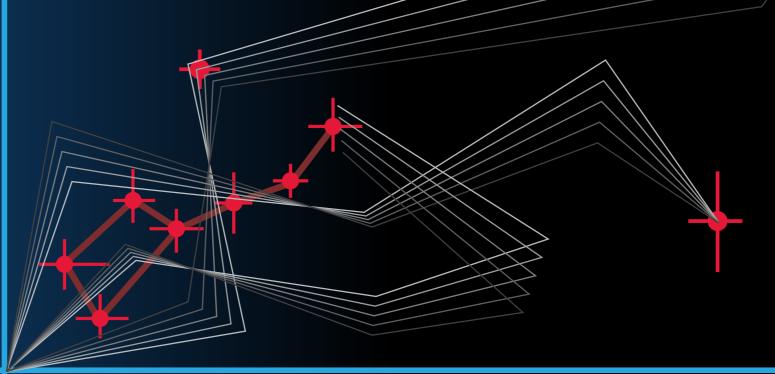


# Bayesian Model Comparison

Roberto Trotta - www.robertotrotta.com





Copenhagen PhD School Oct 6th-10th 2014

Imperial College London

#### Frequentist hypothesis testing



- Warning: frequentist hypothesis testing (e.g., likelihood ratio test) cannot be interpreted as a statement about the probability of the hypothesis!
- **Example:** to test the null hypothesis  $H_0$ :  $\theta = 0$ , draw n normally distributed points (with known variance  $\sigma^2$ ). The  $\chi^2$  is distributed as a chi-square distribution with (n-1) degrees of freedom (dof). Pick a significance level  $\alpha$  (or p-value, e.g.  $\alpha = 0.05$ ). If  $P(\chi^2 > \chi^2_{obs}) < \alpha$  reject the null hypothesis.
- This is a statement about the likelihood of observing data as extreme or more extreme than have been measured assuming the null hypothesis is correct.
- It is not a statement about the probability of the null hypothesis itself and cannot be interpreted as such! (or you'll make gross mistakes)
- The use of p-values implies that a hypothesis that may be true can be rejected because it has not predicted observable results that have not actually occurred. (Jeffreys, 1961)



## The significance of significance



- Important: A 2-sigma result does not wrongly reject the null hypothesis 5% of the time: at least 29% of 2-sigma results are wrong!
  - Take an equal mixture of H<sub>0</sub>, H<sub>1</sub>
  - Simulate data, perform hypothesis testing for H<sub>0</sub>
  - Select results rejecting H<sub>0</sub> at (or within a small range from) 1-α CL (this is the prescription by Fisher)
  - What fraction of those results did actually come from H<sub>0</sub> ("true nulls", should not have been rejected)?

p–value	$_{ m sigma}$	fraction of true nulls	lower bound
0.05	1.96	0.51	0.29
0.01	2.58	0.20	0.11
0.001	3.29	0.024	0.018

Recommended reading:

Sellke, Bayarri & Berger, The American Statistician, 55, 1 (2001)



Bayesian model comparison

#### Bayesian inference chain



- Select a model (parameters + priors)
- Compute observable quantities as a function of parameters
- Compare with available data
  - derive parameters constraints: PARAMETER INFERENCE
  - compute relative model probability: MODEL COMPARISON
- Go back and start again



#### The 3 levels of inference

#### Imperial College London

#### LEVEL 1

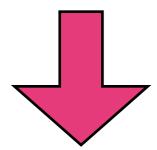
I have selected a model M and prior P(θ|M)

#### LEVEL 2

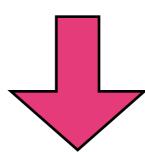
Actually, there are several possible models: M<sub>0</sub>, M<sub>1</sub>,...

#### LEVEL 3

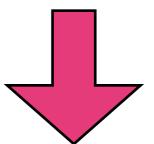
None of the models is clearly the best



$$P(\theta|d,M) = \frac{P(d|\theta,M)P(\theta|M)}{P(d|M)}$$



$$odds = \frac{P(M_0|d)}{P(M_1|d)}$$



$$P(\theta|d) = \sum_{i} P(M_i|d)P(\theta|d, M_i)$$

#### Parameter inference

(assumes M is the true model)

#### **Model comparison**

What is the relative plausibility of M<sub>0</sub>, M<sub>1</sub>,... in light of the data?

#### **Model averaging**

What is the inference on the parameters accounting for model uncertainty?



## Level 2: model comparison



$$P(\theta|d, M) = \frac{P(d|\theta, M)P(\theta|M)}{P(d|M)}$$

Bayesian evidence or model likelihood

The evidence is the integral of the likelihood over the prior:

$$P(d|M) = \int_{\Omega} d\theta P(d|\theta, M) P(\theta|M)$$

Bayes' Theorem delivers the model's posterior:

$$P(M|d) = \frac{P(d|M)P(M)}{P(d)}$$

When we are comparing two models:

The Bayes factor:

$$\frac{P(M_0|d)}{P(M_1|d)} = \frac{P(d|M_0)}{P(d|M_1)} \frac{P(M_0)}{P(M_1)}$$

$$B_{01} \equiv \frac{P(d|M_0)}{P(d|M_1)}$$



Posterior odds = Bayes factor × prior odds

#### Scale for the strength of evidence



• A (slightly modified) Jeffreys' scale to assess the strength of evidence (**Notice:** this is empirically calibrated!)

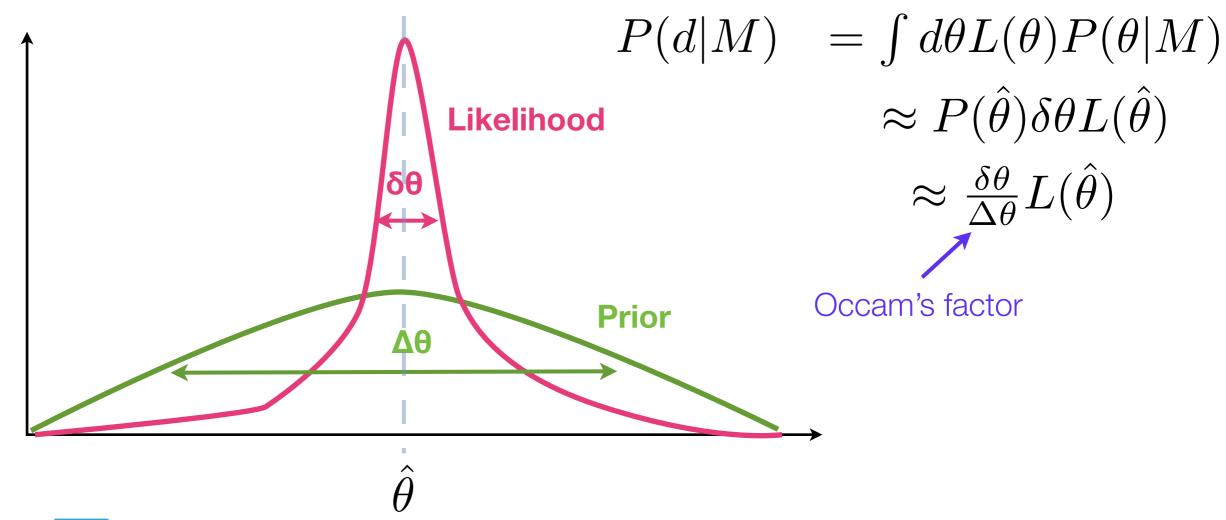
InB	relative odds	favoured model's probability	Interpretation
< 1.0	< 3:1	< 0.750	not worth mentioning
< 2.5	< 12:1	0.923	weak
< 5.0	< 150:1	0.993	moderate
> 5.0	> 150:1	> 0.993	strong



#### An automatic Occam's razor



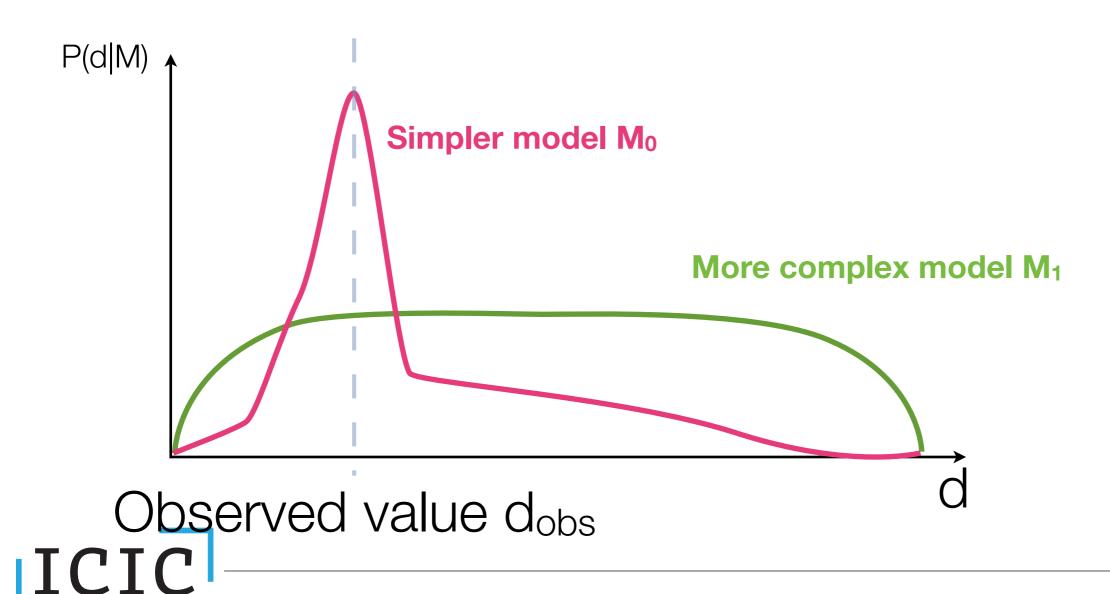
- Bayes factor balances quality of fit vs extra model complexity.
- It rewards highly predictive models, penalizing "wasted" parameter space





## The evidence as predictive probability

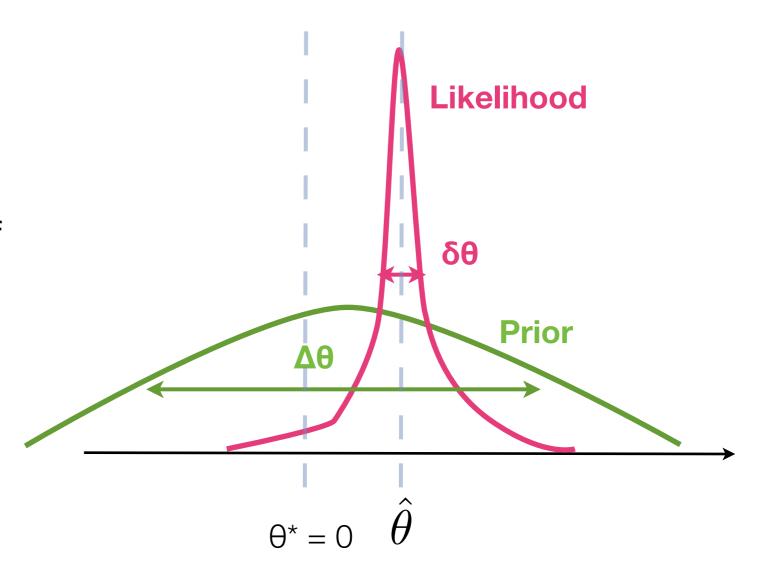
• The evidence can be understood as a function of d to give the predictive probability under the model M:



## Simple example: nested models

This happens often in practice: we have a more complex model, M<sub>1</sub> with prior P(θ|M<sub>1</sub>), which reduces to a simpler model (M<sub>0</sub>) for a certain value of the parameter, e.g. θ = θ\* = 0 (nested models)

 Is the extra complexity of M<sub>1</sub> warranted by the data?



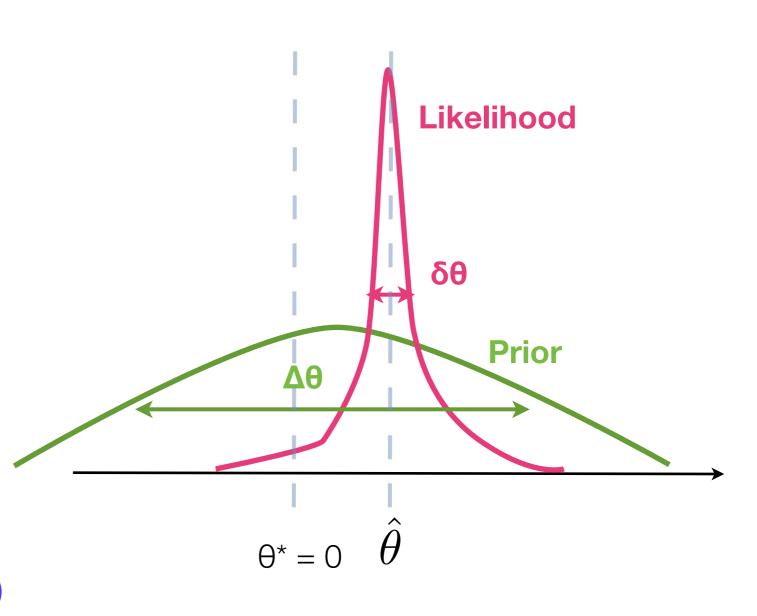
## Simple example: nested models

Define:  $\lambda \equiv \frac{\hat{\theta} - \theta^*}{\delta \theta}$ 

For "informative" data:

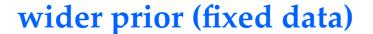
$$\ln B_{01} \approx \ln \frac{\Delta \theta}{\delta \theta} - \frac{\lambda^2}{2}$$

wasted parameter space (favours simpler model) mismatch of prediction with observed data (favours more complex model)



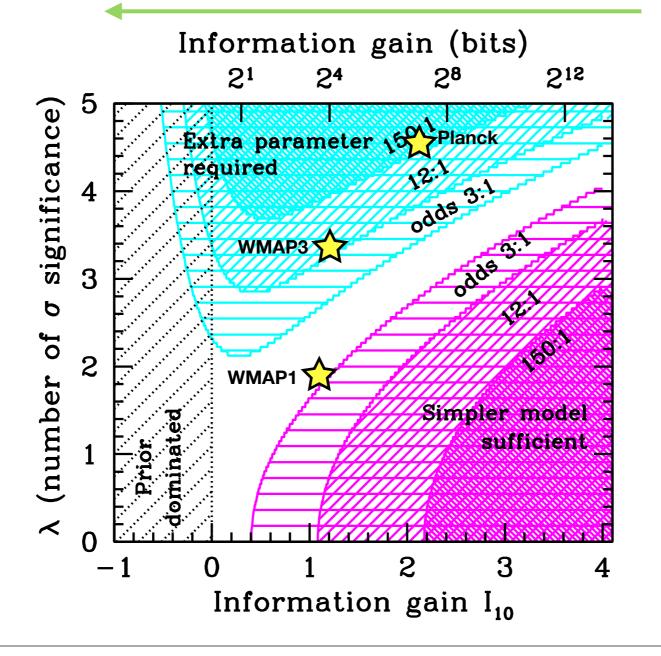
#### The rough guide to model comparison





Trotta (2008)

larger sample (fixed prior and significance)



 $\Delta\theta$  = Prior width  $\delta\theta$  = Likelihood width

$$I_{10} \equiv \log_{10} \frac{\Delta \theta}{\delta \theta}$$



#### Information criteria

- Several information criteria exist for approximate model comparison
   k = number of fitted parameters
   N = number of data points,
  - $-2 \ln(L_{max}) = best-fit chi-squared$
- Akaike Information Criterium (AIC):  $AIC \equiv -2 \ln \mathcal{L}_{\max} + 2k$
- Bayesian Information Criterium (BIC): BIC  $\equiv -2 \ln \mathcal{L}_{\max} + k \ln N$
- Deviance Information Criterium (DIC):  $\mathrm{DIC} \equiv -2\widehat{D_{\mathrm{KL}}} + 2\mathcal{C}_b$

#### Notes on information criteria



- The best model is the one which minimizes the AIC/BIC/DIC
- Warning: AIC and BIC penalize models differently as a function of the number of data points N.
  - For N>7 BIC has a more strong penalty for models with a larger number of free parameters k.
- BIC is an approximation to the full Bayesian evidence with a default Gaussian prior equivalent to 1/N-th of the data in the large N limit.
- DIC takes into account whether parameters are measured or not (via the Bayesian complexity, see later).
- When possible, computation of the Bayesian evidence is preferable (with explicit prior specification).



## Computing the evidence



evidence: 
$$P(d|M) = \int_{\Omega} d\theta P(d|\theta, M) P(\theta|M)$$

Bayes factor: 
$$B_{01}\equiv rac{P(d|M_0)}{P(d|M_1)}$$

- Usually computational demanding: multi-dimensional integral!
- Several techniques available:
  - Brute force: thermodynamic integration
  - Laplace approximation: approximate the likelihood to second order around maximum gives Gaussian integrals (for normal prior). Can be inaccurate.
  - Savage-Dickey density ratio: good for nested models, gives the Bayes factor
  - Nested sampling: clever & efficient, can be used generally



## The Savage-Dickey density ratio

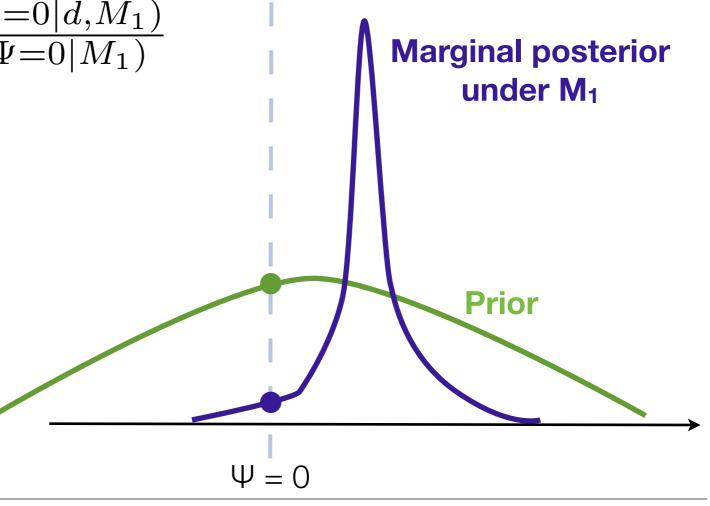


- This methods works for nested models and gives the Bayes factor analytically.
- Assumptions: nested models ( $M_1$  with parameters  $\theta$ , $\Psi$  reduces to  $M_0$  for e.g.  $\Psi$  =0) and separable priors (i.e. the prior  $P(\theta,\Psi|M_1)$  is uncorrelated with  $P(\theta|M_0)$ )
- Result:

Advantages:

$$B_{01} = \frac{P(\Psi=0|d, M_1)}{P(\Psi=0|M_1)}$$

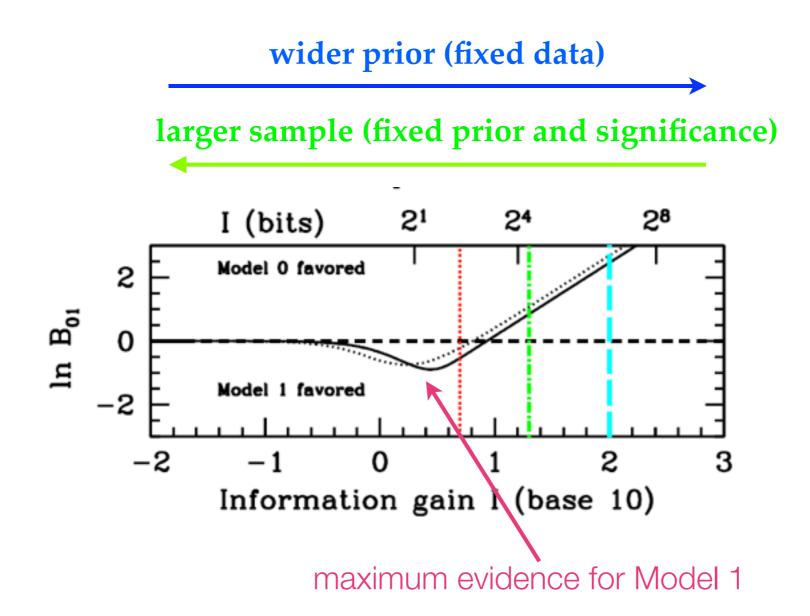
- analytical
- often accurate
- clarifies the role of prior
- does not rely on Gaussianity





#### "Prior-free" evidence bounds

• What if we do not know how to set the prior? For nested models, we can still choose a prior that will maximise the support for the more complex model:



#### Maximum evidence for a detection

 The absolute upper bound: put all prior mass for the alternative onto the observed maximum likelihood value. Then

$$B < \exp(-\chi^2/2)$$

• More reasonable class of priors: symmetric and unimodal around  $\Psi=0$ , then  $(\alpha = \text{significance level})$ 

$$B < \frac{-1}{\exp(1)\alpha \ln \alpha}$$

# If the upper bound is small, no other choice of prior will make the extra parameter significant.

Sellke, Bayarri & Berger, The American Statistician, 55, 1 (2001)

# How to interpret the "number of sigma's"



α	sigma	Absolute bound on InB (B)	"Reasonable" bound on InB (B)
0.05	2	2.0 (7:1) weak	0.9 (3:1) undecided
0.003	3	4.5 (90:1) moderate	3.0 (21:1) moderate
0.0003	3.6	6.48 (650:1) strong	5.0 (150:1) strong





# Rule of thumb: interpret a n-sigma result as a (n-1)-sigma result

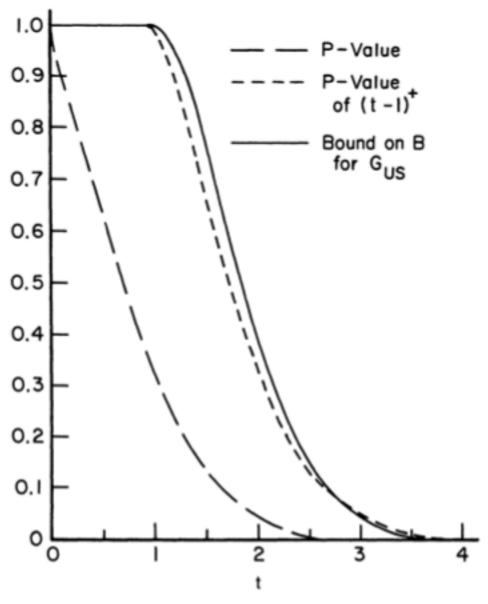
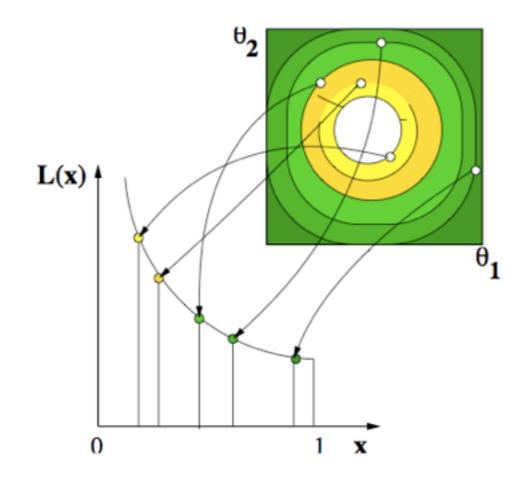


Figure 4. Comparison of B(x, Gus) and P Values.

#### Nested sampling



- Perhaps the method to compute the evidence
- At the same time, it delivers samples from the posterior: it is a highly efficient sampler! (much better than MCMC in tricky situations)
- Invented by John Skilling in 2005: the gist is to convert a n-dimensional integral in a 1D integral that can be done easily.

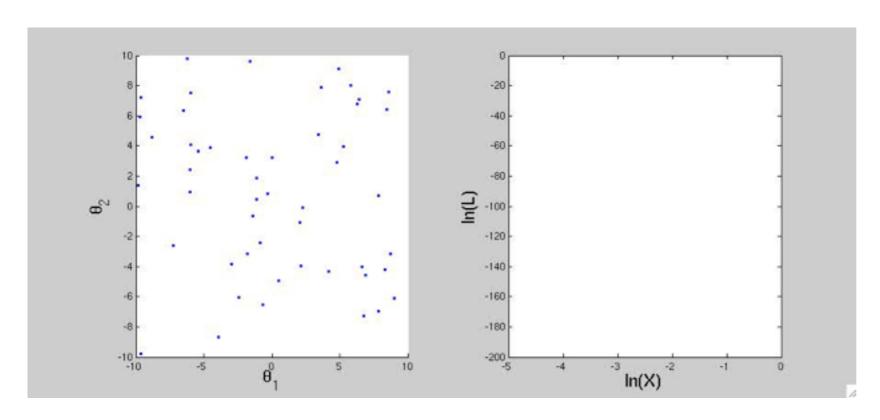


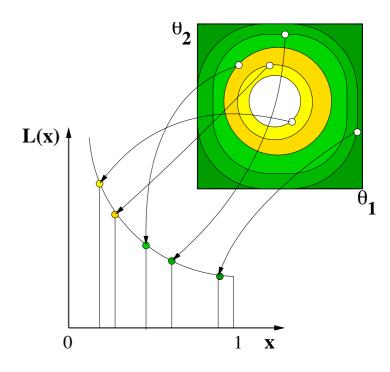
Liddle et al (2006)



#### Nested sampling







(animation courtesy of David Parkinson)

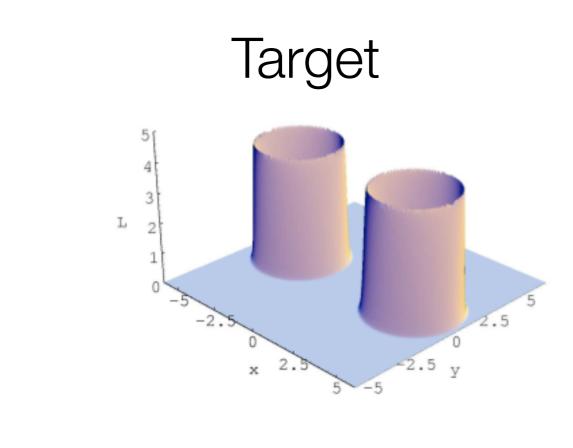
An algorithm originally aimed primarily at the Bayesian evidence computation (Skilling, 2006):

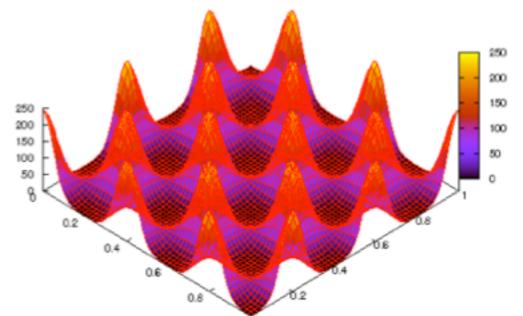
$$X(\lambda) = \int_{\mathcal{L}(\theta) > \lambda} P(\theta) d\theta$$
$$P(d) = \int_{0}^{1} d\theta L(\theta) P(\theta) = \int_{0}^{1} L(X) dX$$



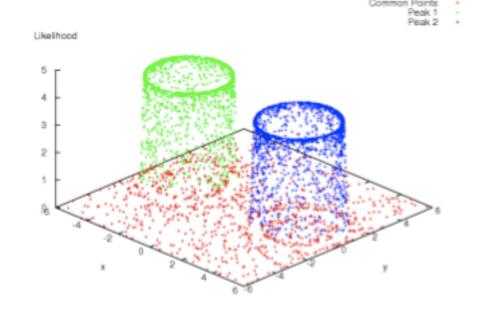
# The MultiNest algorithm

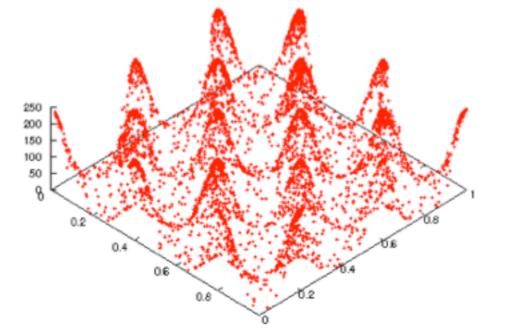
Feroz & Hobson (2007)





#### Reconstructed

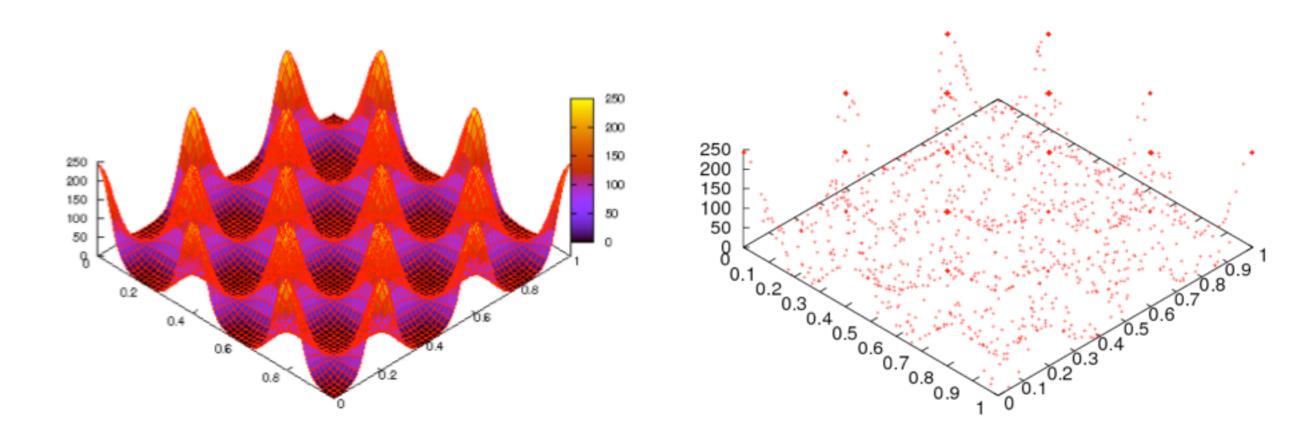




## The egg-box example



MultiNest reconstruction of the egg-box posterior:

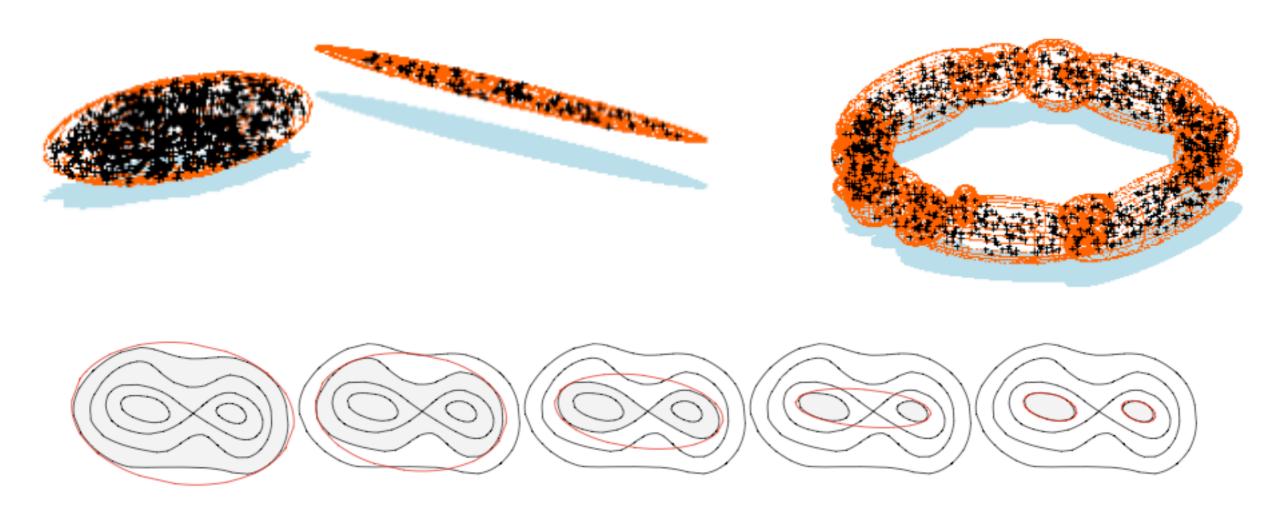




## Ellipsoidal decomposition



#### Unimodal distribution Multimodal distribution

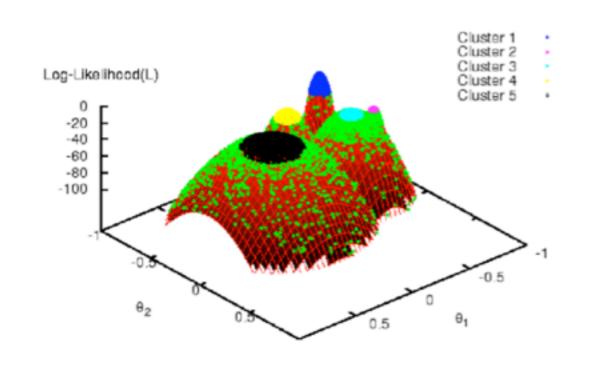




Courtesy Mike Hobson

#### Multinest: Efficiency





#### Gaussian mixture model:

True evidence: log(E) = -5.27

**Multinest:** 

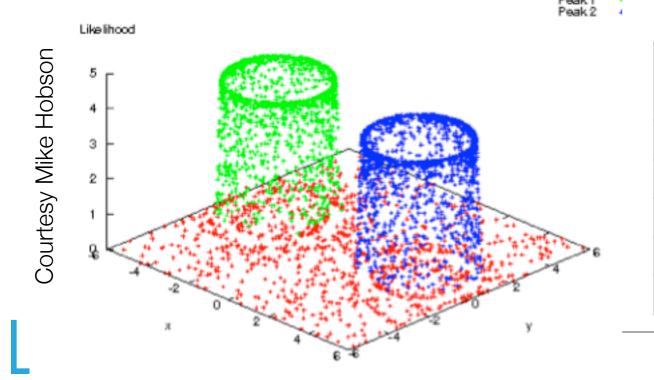
Reconstruction:  $log(E) = -5.33 \pm 0.11$ 

Likelihood evaluations ~ 10<sup>4</sup>

#### Thermodynamic integration:

Reconstruction:  $log(E) = -5.24 \pm 0.12$ 

Likelihood evaluations ~ 10<sup>6</sup>



D	Ν	efficiency	likes per dimension
2	7000	70%	83
5	18000	51%	7
10	53000	34%	3
20	255000	15%	1.8
30	753000	8%	1.6

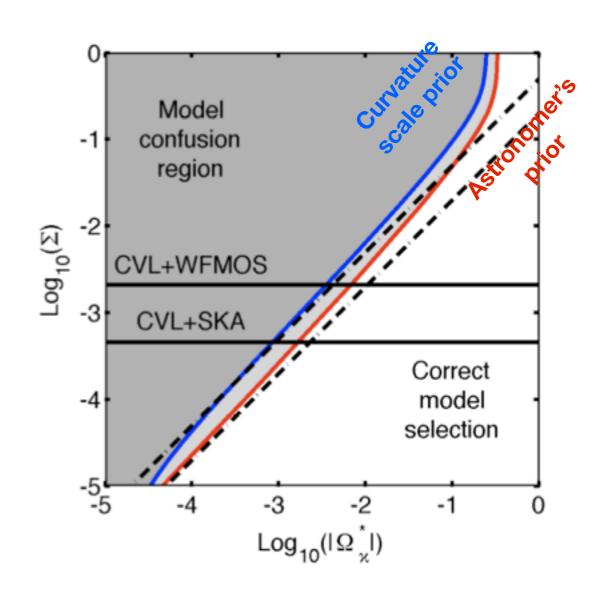
### Application: the spatial curvature



- Is the Universe spatially flat? (Vardanyan, Trotta and Silk, 2009)
- A three-way model comparison:  $\Omega_k = 0 \text{ vs } \Omega_k < 0 \text{ vs } \Omega_k > 0$  (with either the Astronomer's prior or

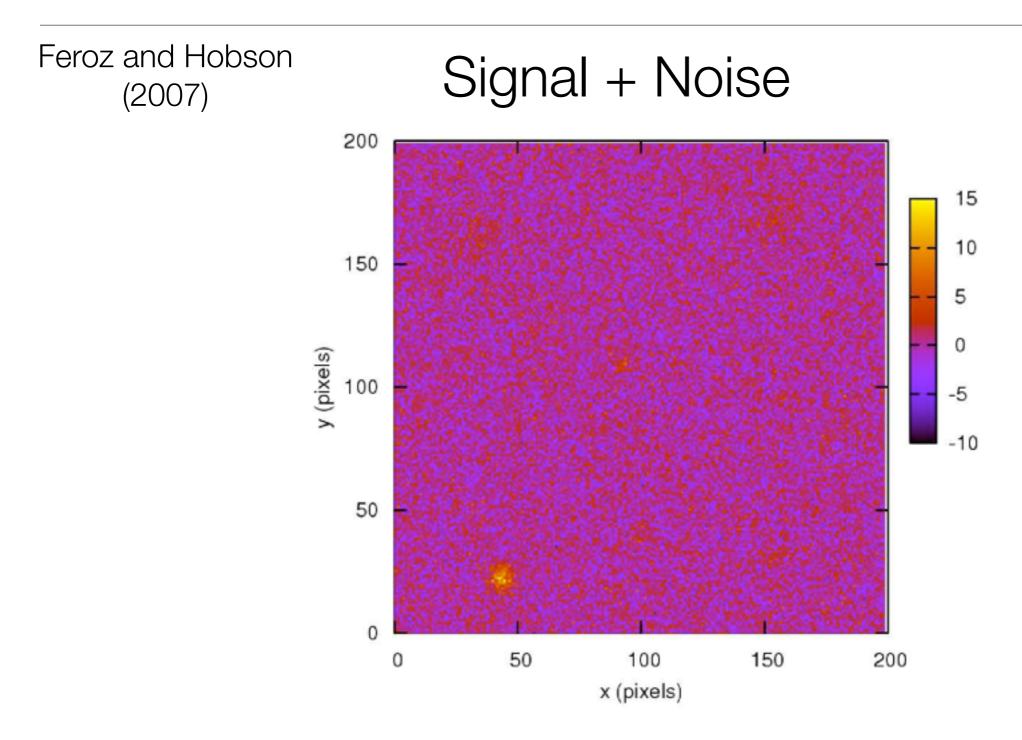
(with either the Astronomer's prior or Curvature scale prior)

- Result: odds range from moderate evidence (lnB = 4) for flatness to undecided (lnB = 0.4) depending on the choice of prior
- Probability(infinite Universe) = 98%
   (Astronomer's prior)
   Probability(infinite Universe) = 45%
   (Curvature scale prior)
- Upper bound: odds of 49:1 at best for n ≠ 1 (Gordon and Trotta 2007)





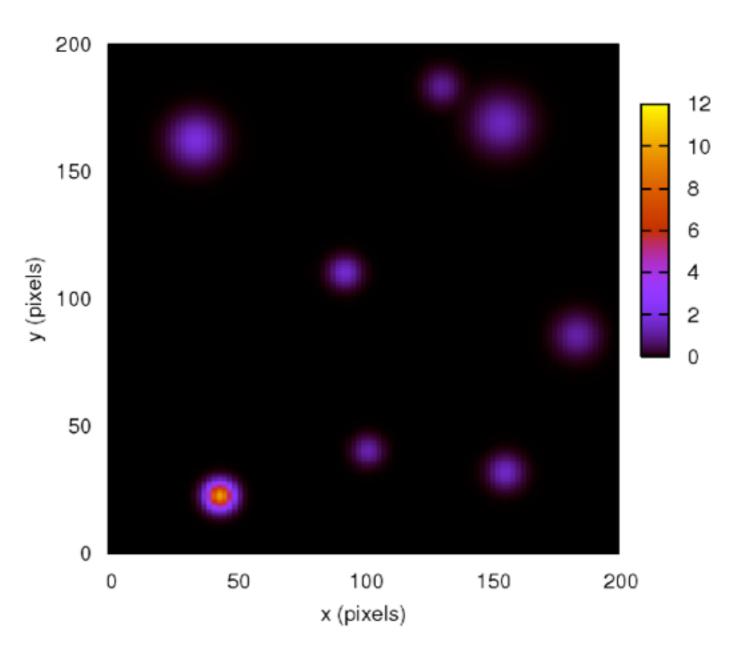
# A "simple" example: how many sources?



# A "simple" example: how many sources?

Feroz and Hobson (2007)

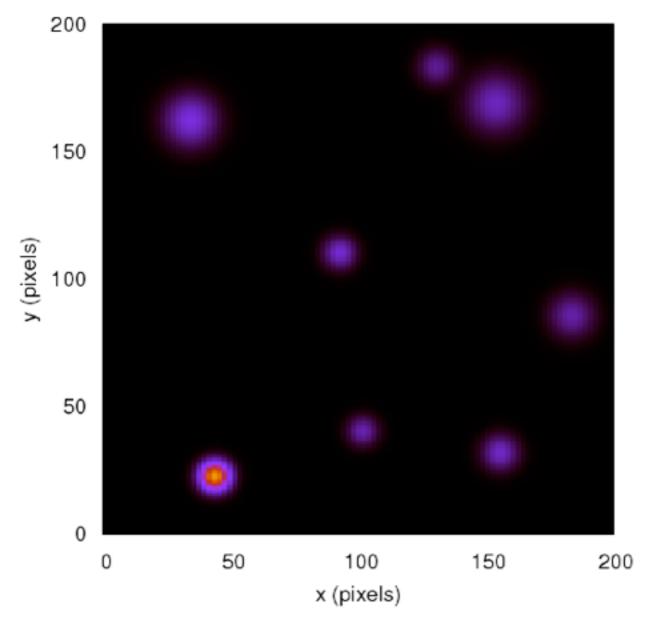
### Signal: 8 sources



# A "simple" example: how many sources?

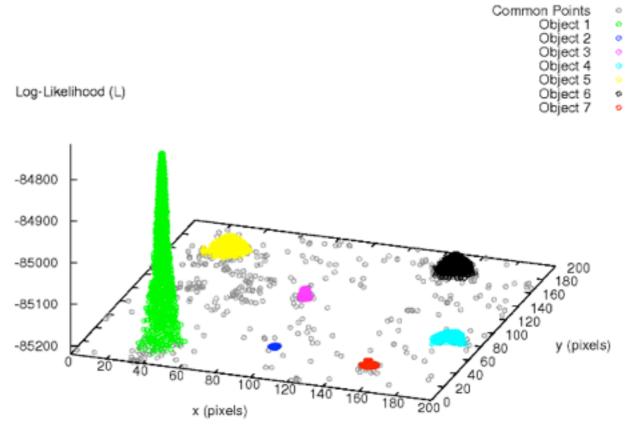
Imperial College London

Feroz and Hobson (2007)

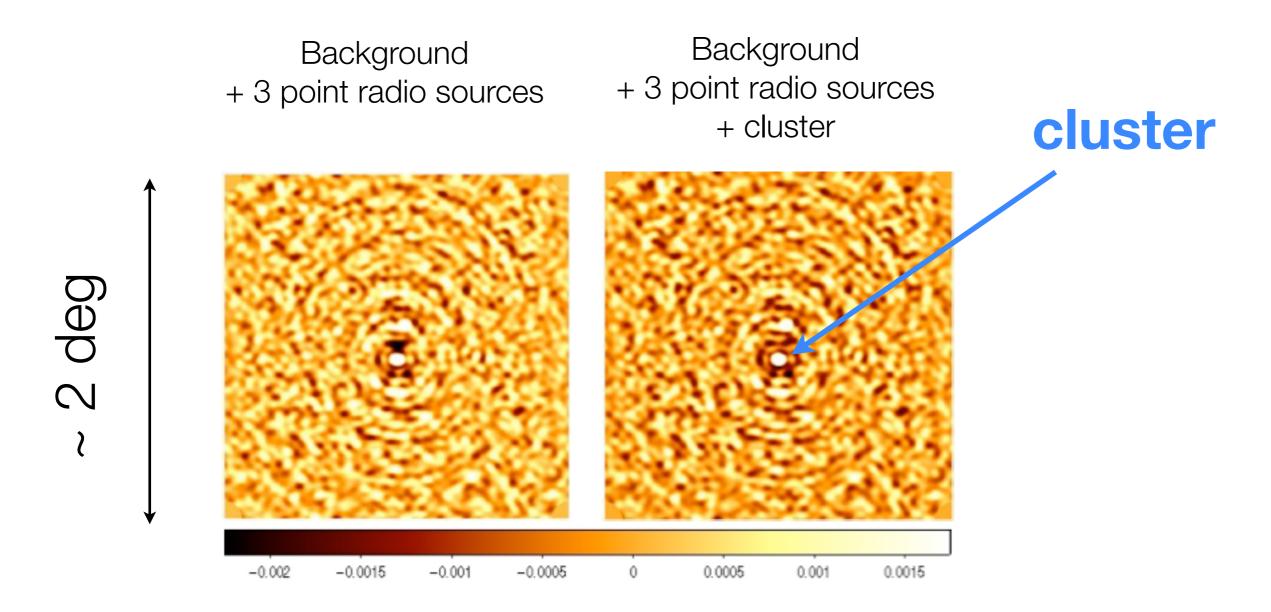


#### Bayesian reconstruction

7 out of 8 objects correctly identified. Mistake happens because 2 objects very close.



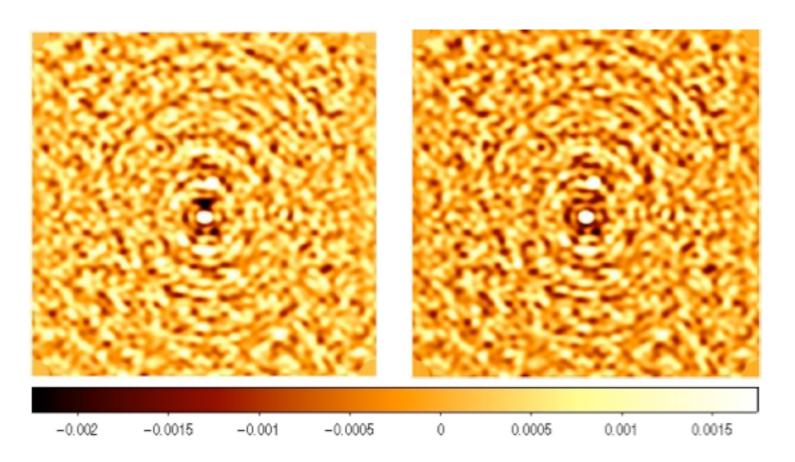
# Cluster detection from Sunyaev-Zeldovich effect in cosmic microwave background maps



Feroz et al 2009

Background + 3 point radio sources

Background + 3 point radio sources + cluster



Bayesian model comparison:

R = P(cluster | data)/P(no cluster | data)

$$R = 0.35 \pm 0.05$$

$$R \sim 10^{33}$$

Cluster parameters also recovered (position, temperature, profile, etc)

# The cosmological concordance model



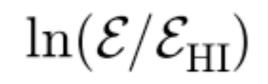
Competing model	$\Delta N_p$	$r = \ln B$	Ref	Data	Outcome
Initial conditions Isocurvature modes					
CDM isocurvature + arbitrary correlations Neutrino entropy + arbitrary correlations Neutrino velocity + arbitrary correlations	+1 +4 +1 +4 +1 +4	$-7.6$ $-1.0$ $[-2.5, -6.5]^p$ $-1.0$ $[-2.5, -6.5]^p$ $-1.0$	[58] [46] [60] [46] [60] [46]	WMAP3+, LSS WMAP1+, LSS, SN Ia WMAP3+, LSS WMAP1+, LSS, SN Ia WMAP3+, LSS WMAP1+, LSS, SN Ia	Strong evidence for adiabaticity Undecided Moderate to strong evidence for adiabaticity Undecided Moderate to strong evidence for adiabaticity Undecided
Primordial power spectr No tilt $(n_s = 1)$	rum -1	$+0.4$ $[-1.1, -0.6]^p$ $-0.7$ $-0.9$ $[-0.7, -1.7]^{p,d}$ $-2.0$ $-2.6$ $-2.9$ $< -3.9^c$	[47] [51] [58] [70] [186] [185] [70] [58] [65]	WMAP1+, LSS WMAP1+, LSS WMAP1+, LSS WMAP1+ WMAP3+ WMAP3+, LSS WMAP3+, LSS WMAP3+, LSS WMAP3+, LSS	Undecided Undecided Undecided Undecided Undecided $n_s = 1$ weakly disfavoured $n_s = 1$ weakly disfavoured $n_s = 1$ moderately disfavoured $n_s = 1$ moderately disfavoured Moderate evidence at best against $n_s \neq 1$
Running Running of running	+1 +2	$[-0.6, 1.0]^{p,d}$ $< 0.2^c$ $< 0.4^c$	[186] [166] [166]	WMAP3+, LSS WMAP3+, LSS WMAP3+, LSS	No evidence for running Running not required Not required
Large scales cut-off	+2	$[1.3, 2.2]^{p,d}$	[186]	WMAP3+, LSS	Weak support for a cut-off
Matter-energy content Non-flat Universe	+1	-3.8 -3.4	[70] [58]	WMAP3+, HST WMAP3+, LSS, HST	Flat Universe moderately favoured Flat Universe moderately favoured
Coupled neutrinos	+1	-0.7	[193]	WMAP3+, LSS	No evidence for non-SM neutrinos
Dark energy sector $w(z) = w_{\text{eff}} \neq -1$	+1	$[-1.3, -2.7]^p$ -3.0 -1.1 $[-0.2, -1]^p$ $[-1.6, -2.3]^d$	[187] [50] [51] [188] [189]	SN Ia SN Ia WMAP1+, LSS, SN Ia SN Ia, BAO, WMAP3 SN Ia, GRB	Weak to moderate support for $\Lambda$ Moderate support for $\Lambda$ Weak support for $\Lambda$ Undecided Weak support for $\Lambda$
$w(z) = w_0 + w_1 z$	+2	$[-1.5, -3.4]^p$ -6.0 -1.8	[187] [50] [188]	SN Ia SN Ia SN Ia, BAO, WMAP3	Weak to moderate support for $\Lambda$ Strong support for $\Lambda$ Weak support for $\Lambda$
$w(z) = w_0 + w_a(1 - a)$	+2	-1.1 [-1.2, -2.6] <sup>d</sup>	[188] [189]	SN Ia, BAO, WMAP3 SN Ia, GRB	Weak support for $\Lambda$ Weak to moderate support for $\Lambda$
Reionization history No reionization ( $\tau = 0$ ) No reionization and no tilt	-1 -2	-2.6 -10.3	[70] [70]	WMAP3+, HST WMAP3+, HST	$\tau \neq 0$ moderately favoured Strongly disfavoured
)O)					

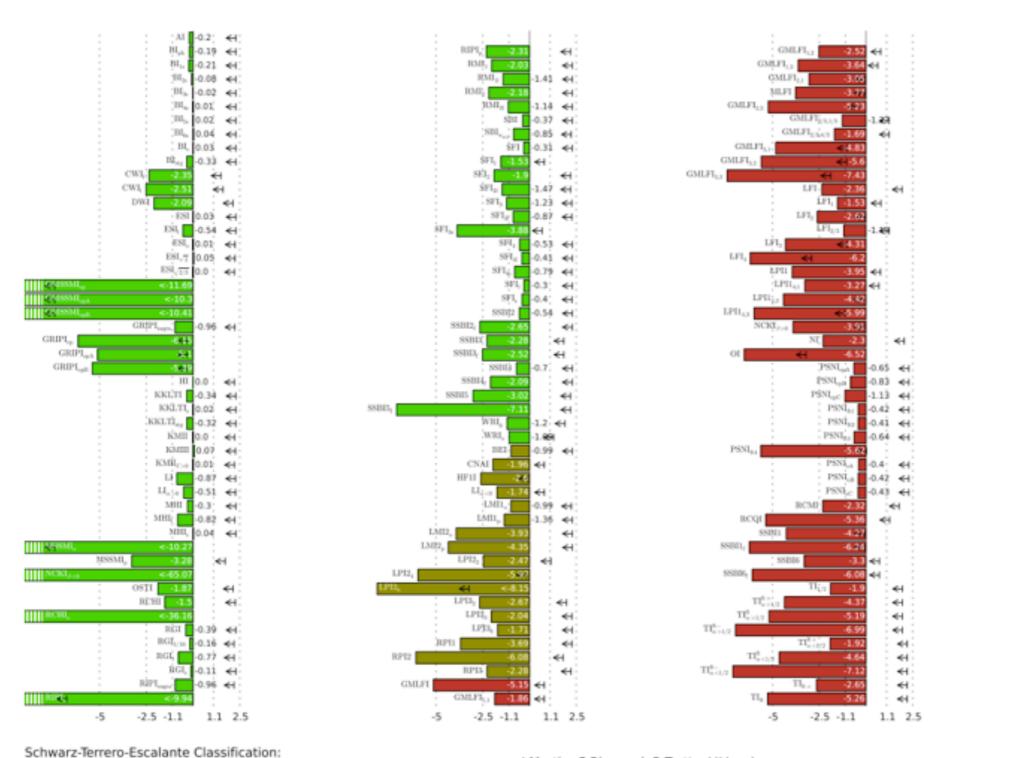
from Trotta (2008)

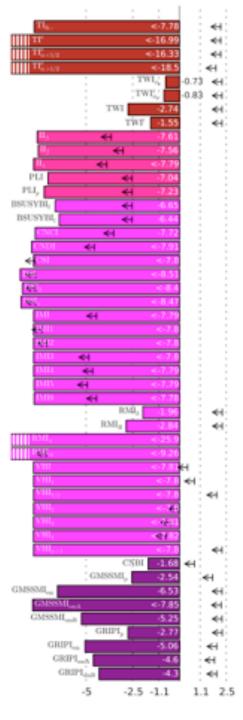


InB < 0: favours ΛCDM

# Bayesian model comparison of 193 models Higgs inflation as reference model







#### Model complexity



- "Number of free parameters" is a relative concept. The relevant scale is set by the prior range
- How many parameters can the data support, regardless of whether their detection is significant?
- Bayesian complexity or effective number of parameters:

$$C_b = \overline{\chi^2(\theta)} - \chi^2(\widehat{\theta})$$
$$= \sum_i \frac{1}{1 + (\sigma_i/\Sigma_i)^2}$$

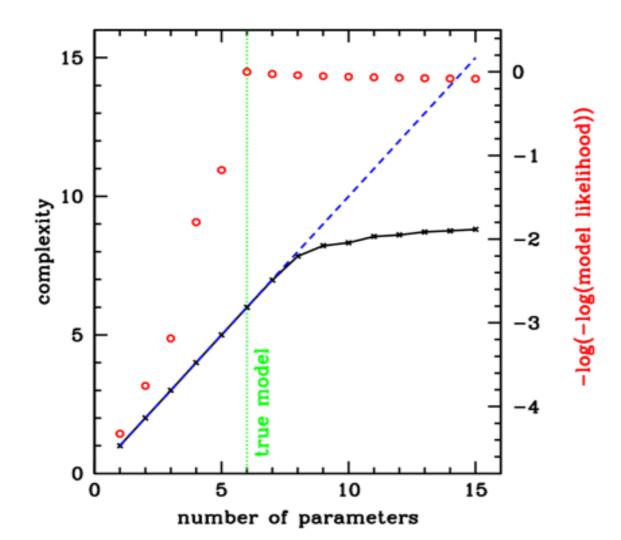
Kunz, RT & Parkinson, astro-ph/0602378, Phys. Rev. D 74, 023503 (2006) Following Spiegelhalter et al (2002)



Data generated from a model with n = 6:

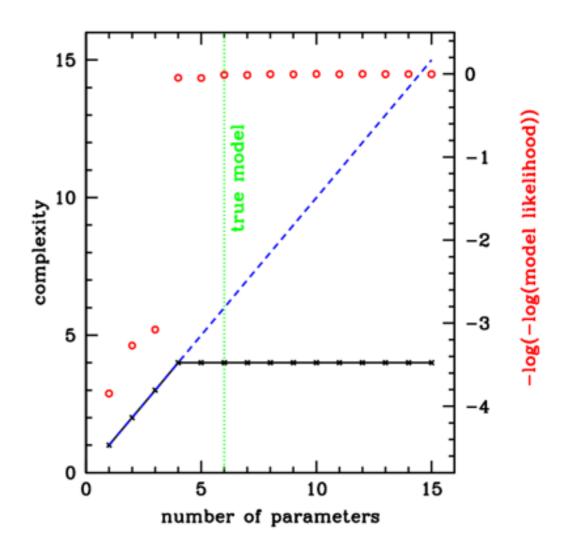
GOOD DATA

Max supported complexity ~ 9



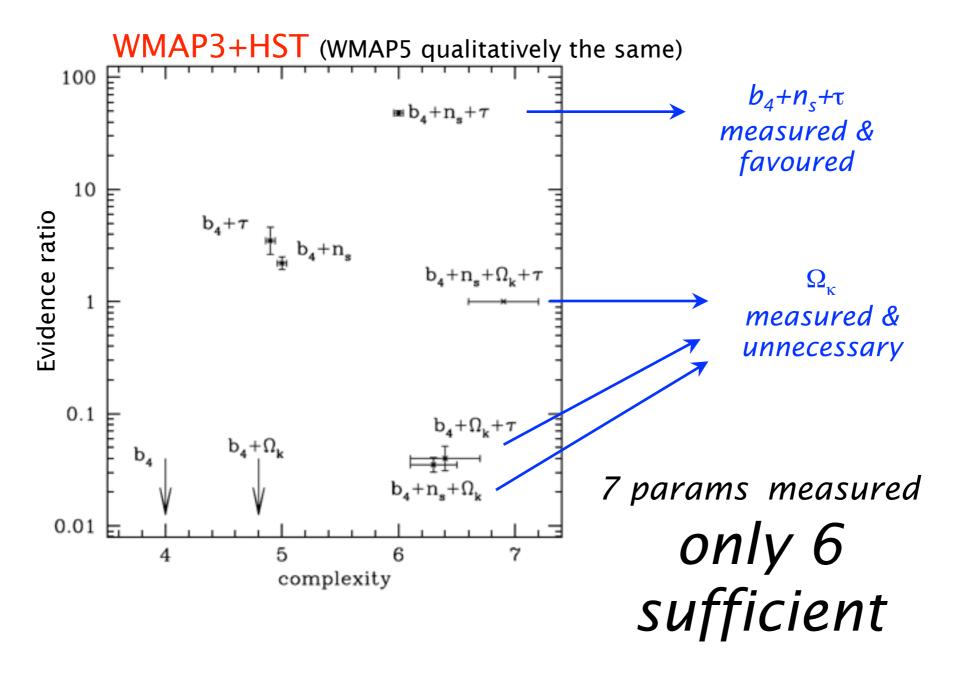
INSUFFICIENT DATA

Max supported complexity ~ 4





# How many parameters does the CMB need?





# Liddle et al (2007)

# Bayesian Model-averaging

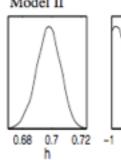


#### $P(\theta|d) = \sum_{i} P(\theta|d,M_i)P(M_i|d)$

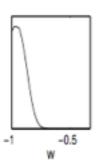
An application to dark energy:



0.2 <sub>Ω</sub> 0.3



Model IV

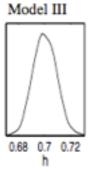


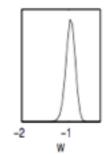
0.68 0.7 0.72

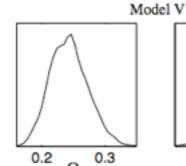
0

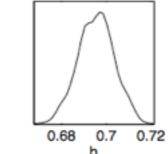
-1

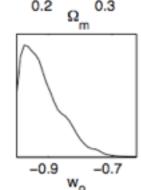


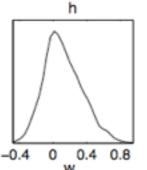




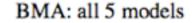


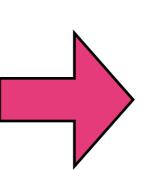


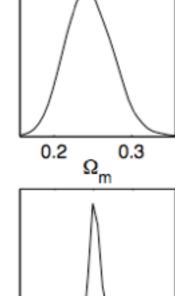




#### Model averaged inferences

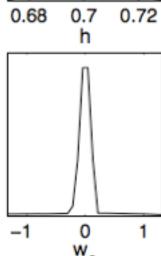






-1.2 -1 -0.8







#### Key points



- Bayesian model comparison extends parameter inference to the space of models
- The Bayesian evidence (model likelihood) represents the change in the degree of belief in the model after we have seen the data
- Models are rewarded for their predictivity (automatic Occam's razor)
- Prior specification is for model comparison a key ingredient of the model building step. If the prior cannot be meaningfully set, then the physics in the model is probably not good enough.
- Bayesian model complexity can help (together with the Bayesian evidence) in assessing model performance.

