

# An introduction to Bayesian Reasoning and its applications

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#### **Overview**

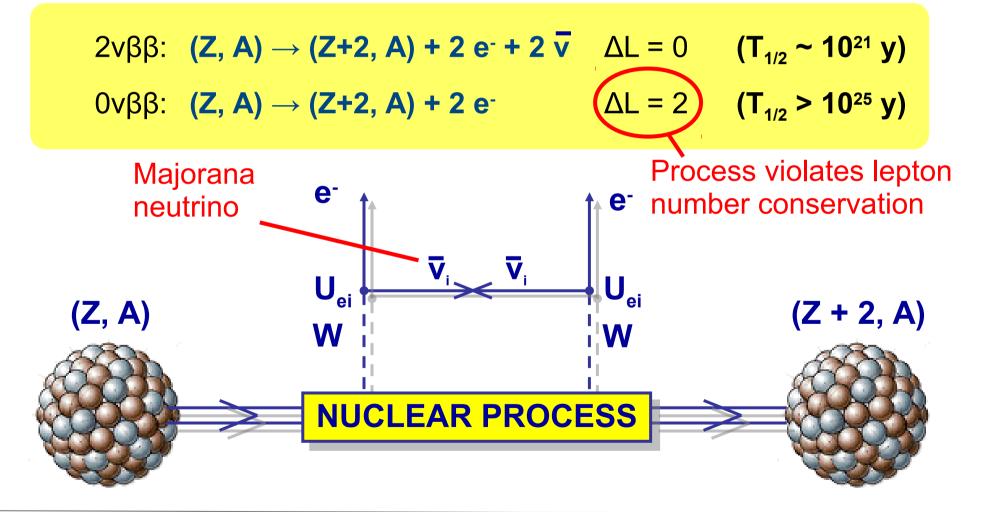
- A concrete example
- Scientific reasoning
- Probability and the Bayesian interpretation
- Parameter estimation
- A concrete example (continued)
- Model comparison
- Numerical method: MCMC
- Further examples
- Summary



## A concrete example

#### **Neutrinoless double beta-decay**

Rare nuclear transition (2<sup>nd</sup> order weak process):

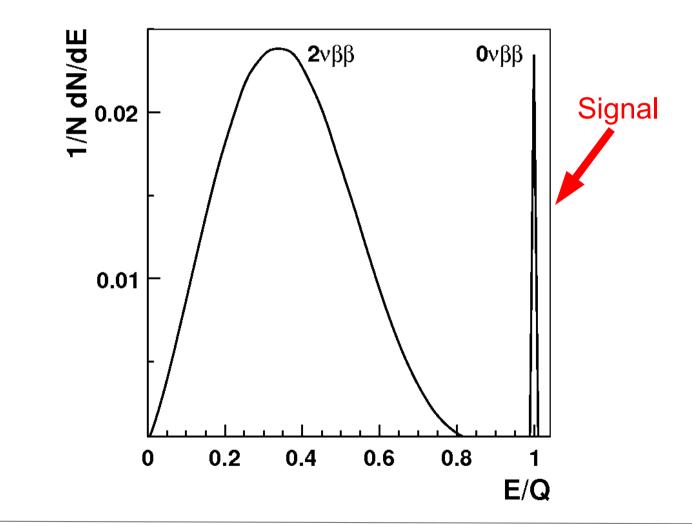




## A concrete example

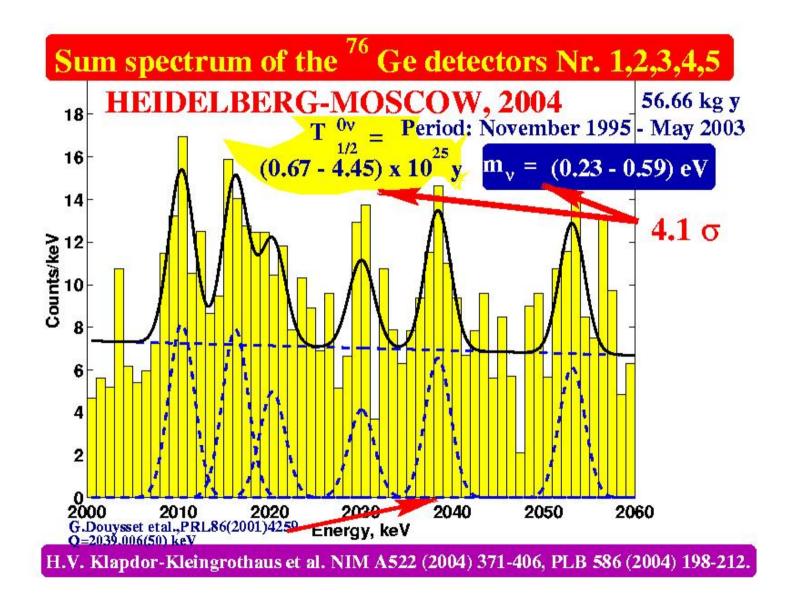
#### **Neutrinoless double beta-decay**

Searching for a single peak on top of a (flat) background...



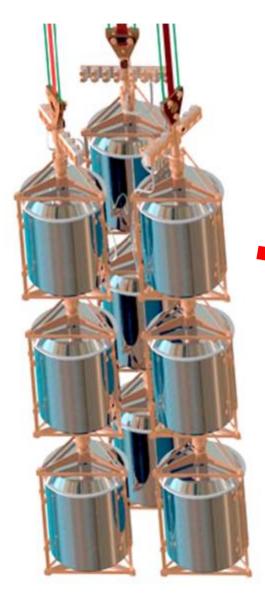
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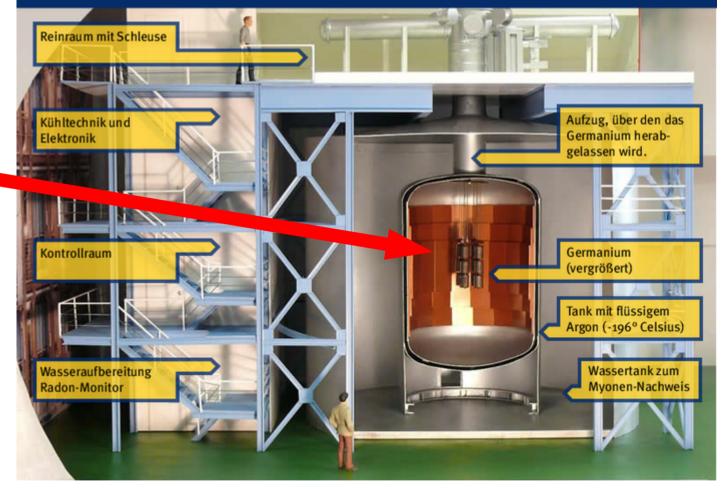




# **Example: GERDA**

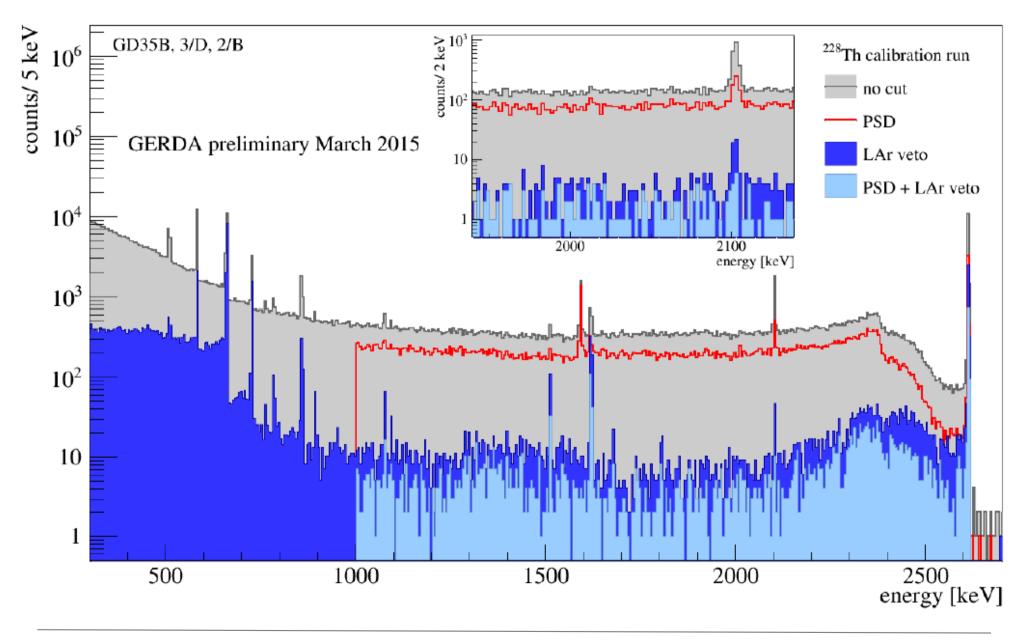


#### **GERDA-Experiment**





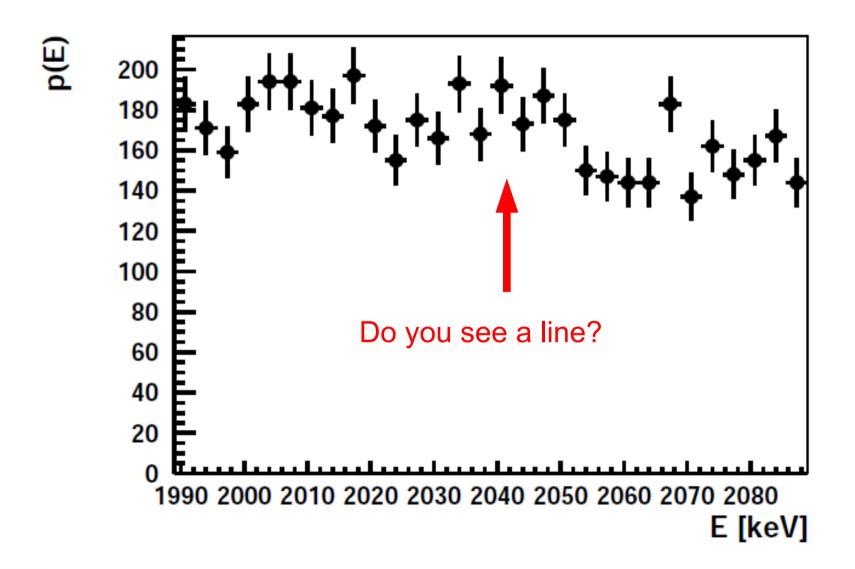
# **Example: GERDA**





The principle

#### **Neutrinoless double beta-decay**





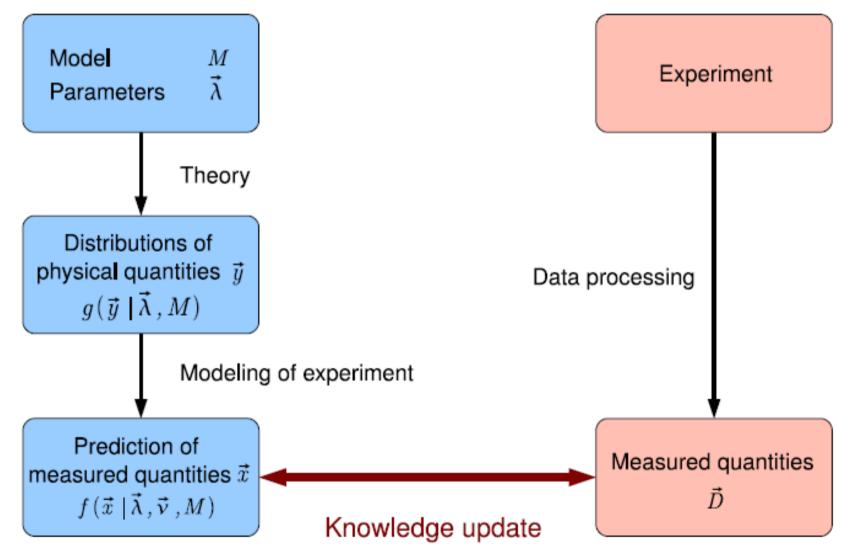
# **Typical questions**

## Major subjects of data analysis

- Model comparison: Which model describes the data best?
  - SM background only?
  - Does 0nubb + background describe the data better?
- Parameter estimation: Given a model, what are the values of its free parameters?
  - What is the rate of 0nubb?
  - What is the actual background level?
- Goodness-of-fit: Given a model, is it consistent with the data?
  - Does the background-only hypothesis describe the data reasonably well?



#### Ingredients





## **Deductive reasoning**

- Used when making predictions from a model
- Application in data analysis:
  - Premise P (model with parameters)  $\rightarrow$  Conclusion Q (observables)
  - Premise Q (observables) → Conclusion R (set of observations)
  - Thus: Premise P (model) → Conclusion R (set of observations)
- Given a model, the outcome is specified
- No need to argue, it's math!
- *Example:* Onubb + background model predicts a certain energy spectrum



## Inductive reasoning

- Used when choosing a model
- Application in data analysis:
  - Premise P (model with parameters)  $\rightarrow$  Conclusion R (set of observations)
  - Observe R, what does it say about P? Not much since it could have been P<sub>1</sub>→R, P<sub>2</sub>→R, P<sub>3</sub>→R, …
- Validity of model P?
  - If we know all models, and only P results in R, then we know that P is true.
  - Otherwise, can *not verify* the model.
  - Can try to *falsify* the model: if we observe something that contradicts the model, it can not be true
- Can we know which model is true? No!



## Truth and knowledge

- Plato: knowledge is justified true belief.
- Proposition P is known to be true if and only if
  - P is true.
  - P is believed to be true.
  - It is justified that P is believed to be true.
- But: we can not know the truth, so:

## Knowledge is justified belief

- This discussion is known as the Gettier problem
- Justification comes from experimental observations:
  - Derive predictions from model and test them
  - The more tests are passed, the greater the belief in the model

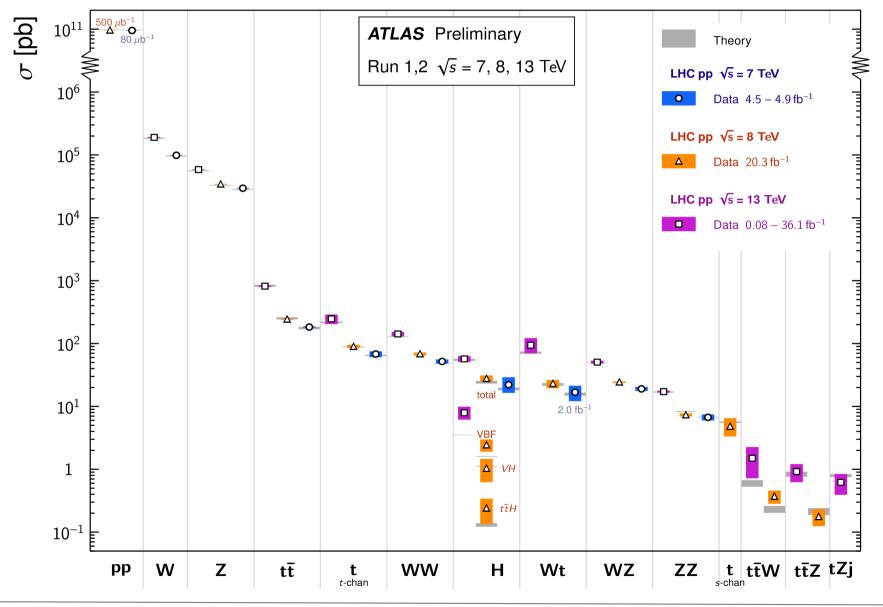
*Examples*: SM of particle physics, general relativity, ...



## SM vs. "tensions"



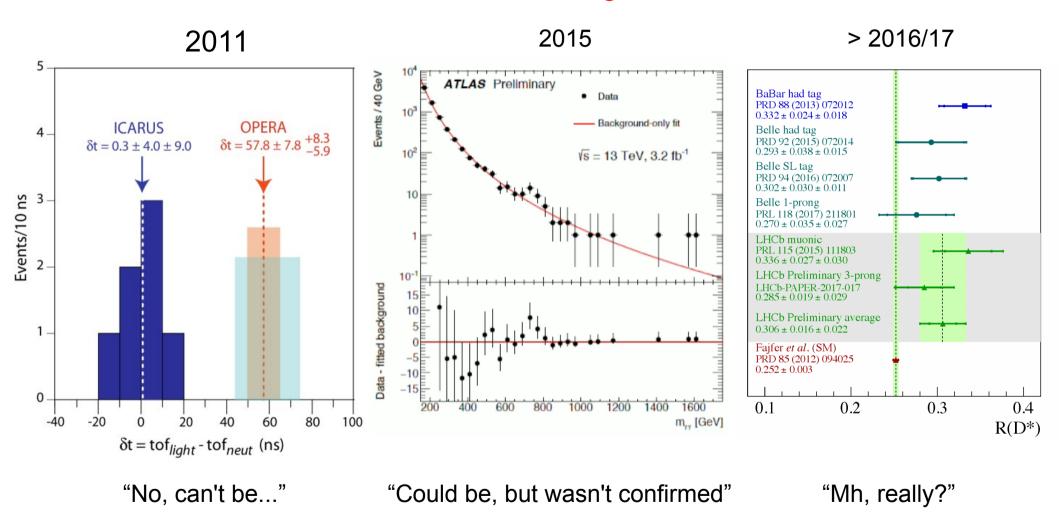
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SM vs. "tensions"

Is the SM wrong?





## **Application in science**

- How do we gain knowledge?
  - Set up models and specify their parameters (check arXiv.org!)
  - Derive (deductively) predictions from the models
  - Can not know all models, so can not verify a model
  - Good model: falsifiable, make predictions which can be proven wrong (Z' vs. SUSY vs. string theory)
  - Use data to gain knowledge about the models and parameters

Examples:

- Special relativity predicts time dilation. Atmospheric muons can thus be observed on the earth's surface.
- Neutrino postulation: Pauli was hesitant to publish his neutrino idea because he thought it would be difficult to discover.

#### Can we quantify the knowledge about a model? Yes, use probabilities



**Probability** 

### **Axioms and interpretation**

- Kolmogorov axioms: start from set S
  - 1. For each subset A, assign probability P(A) between 0 and 1
  - 2. Probability P(S) = 1
  - 3. For disjunct subsets A and B:

P(A or B) = P(A) + P(B)

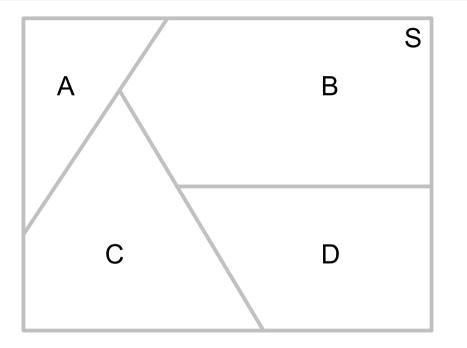
Nice mathematical formulation, but *meaningless*!

• Law of total probability:

 $P(B) = \sum P(B|A_i) \cdot P(A_i)$ 



# Probability



P(A) ≥ 0, ...

 $A \cap B = \emptyset, \dots$ 

 $S = A \cup B \cup C \cup D$ 

$$P(S) = P(A) + P(B) + P(C) + P(D) = 1$$

$$\begin{bmatrix} A_1 & A_2 & A_5 & S \\ & & \\ & & \\ & & \\ B & & \\ & & \\ A_3 & & & \\ & & & & \\ & & & \\ & & &$$

P(A) ≥ 0, ...

 $P(B) = \sum P(B|A_{i}) \cdot P(A_{i})$  $= P(B|A_{1}) \cdot P(A_{1}) + P(B|A_{2}) \cdot P(A_{2})$  $+ P(B|A_{3}) \cdot P(A_{3}) + P(B|A_{4}) \cdot P(A_{4})$ 

+ 
$$P(B|A_5) \cdot P(A_5)$$



**Probability** 

### **Axioms and interpretation**

- Kolmogorov axioms: start from set S
  - 1. For each subset A, assign probability P(A) between 0 and 1
  - 2. Probability P(S) = 1
  - 3. For disjunct subsets A and B: P(A or B) = P(A) + P(B)
- Nice mathematical formulation, but meaningless!

#### **Bayesian interpretation**

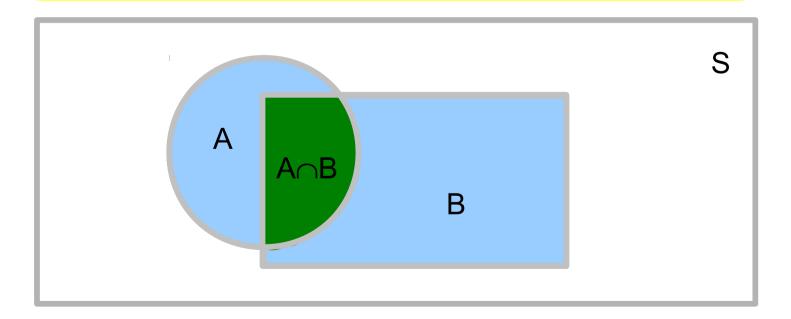
- Subsets correspond to hypotheses, i.e. a model with a particular value of the parameter. Example: SM and the electron mass
- Probability is understood as *degree-of-belief* (or *state-of-knowledge*) for this hypothesis to be true
- Interpretation fully consistent with Kolmogorov axioms



**Bayes' Theorem** 

#### **Bayes' Theorem**

$$\begin{split} P(A|B) \cdot P(B) &= P(A \wedge B) = P(B|A) \cdot P(A) \\ \Leftrightarrow \ P(A|B) &= \frac{P(B|A) \cdot P(A)}{P(B)} \\ \Leftrightarrow \ P(A|B) &= \frac{P(B|A) \cdot P(A)}{\sum P(B|A_i) \cdot P(A_i)} \end{split}$$





#### **Bayes' Theorem**

$$\begin{aligned} P(A|B) \cdot P(B) &= P(A \land B) = P(B|A) \cdot P(A) \\ \Leftrightarrow \ P(A|B) &= \frac{P(B|A) \cdot P(A)}{P(B)} \\ \Leftrightarrow \ P(A|B) &= \frac{P(B|A) \cdot P(A)}{\sum P(B|A_i) \cdot P(A_i)} \end{aligned}$$

#### • Here:

- $P(\text{theory}|\text{data}) \propto P(\text{data}|\text{theory}) \cdot P(\text{theory})$
- P(theory | data): *posterior probability* (induction)
- P(data | theory): probability of the data, likelihood (deduction)
  - P(theory): prior probability
  - In words: "My degree-of-belief of a model is x%", or

"The parameter values lie in an interval [a,b] with x% probability"



# A simple example

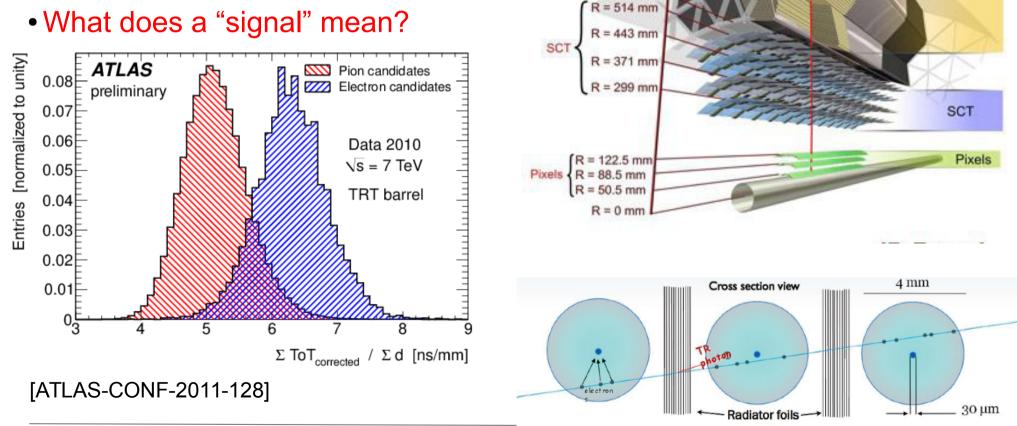
R = 1082 mm

R = 554 mr

TRT

## Particles in a TRT

- Particle identification based on transition radiation
- Distinguish between electrons and charged pions



TRT





#### Particles in a TRT

- Assume test beam measurement
- Test beam composition:
- p(electron) = 90%
- p(pion) = 10%

- Detection efficiencies:
- p(signal | electron) = 95%
- p(signal | pion) = 6%

## Your turn! What is p(electron | signal)?

Use Bayes' Theorem: P

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{\sum P(B|A_i) \cdot P(A_i)}$$

What are  $A_1$  and  $A_2$  and B?





### Particles in a TRT

- Assume test beam measurement
- Test beam composition:
- p(electron) = 90%
- p(pion) = 10%

• Detection efficiencies:

• p(signal | pion) = 6%

$$p(e|Signal|) = \frac{p(Signal|e) \cdot p(e)}{p(Signal|e) \cdot p(e) + p(Signal|\pi) \cdot p(\pi)}$$
$$p(\pi|Nosignal|) = \frac{p(Nosignal|\pi) \cdot p(\pi)}{p(Nosignal|e) \cdot p(e) + p(Nosignal|\pi) \cdot p(\pi)}$$



### **Particles in a TRT**

• Probabilities:

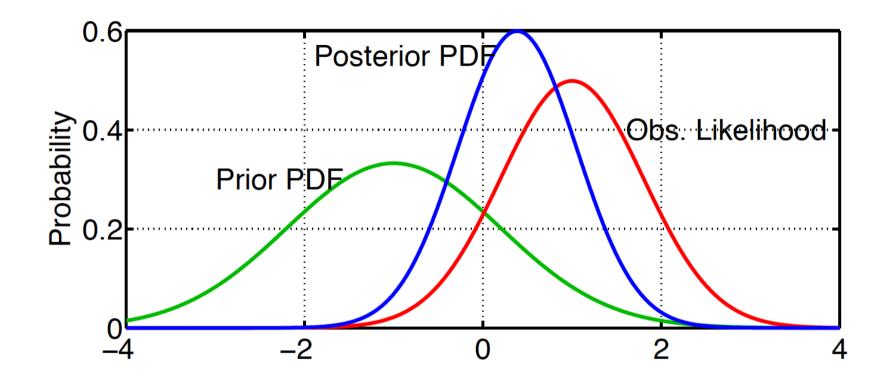
$$p(e|Signal) = \frac{0.95 \cdot 0.9}{0.95 \cdot 0.9 + 0.06 \cdot 0.10} = 0.993$$

$$p(\pi|Signal) = \frac{0.06 \cdot 0.10}{0.95 \cdot 0.9 + 0.06 \cdot 0.10} = 0.007$$

$$p(e|No signal) = \frac{0.05 \cdot 0.90}{0.05 \cdot 0.90 + 0.94 \cdot 0.10} = 0.312$$

$$p(\pi|No Signal) = \frac{0.94 \cdot 0.10}{0.05 \cdot 0.90 + 0.94 \cdot 0.10} = 0.676$$





"A Bayesian is one who, vaguely expecting a horse, and catching a glimpse of a donkey, strongly believes he has seen a mule"

Stephen Senn, Statistician & Bayesian Skeptic (mostly)



## Where does prior knowledge come from?

- Prior can come from
  - personal degree-of-belief (gut feeling),
  - theoretical considerations (how badly do you want SUSY to be true?),
  - auxiliary measurements, ...
  - ... good arguments ... (in the best case)
- Elegant update of knowledge: posterior of one experiment can be prior of another experiment. Natural way to combine measurements.

P(Model | Data 1) ~ P(Data 1 | Model) x P(Model)

- and P(Model | Data 2) ~ P(Data 2 | Model) x P'(Model)
- with P' = P(Model | Data 1) = P(Data 1 | Model) x P(Model)
- → P(Model | Data 2) ~ P(Data 2 | Model) x P(Data 1 | Model) x P(Model)
   = P(Model | Data 1 + Data 2)





## Criticism

- Priors are subjective
  - Yes, but it is made explicit
  - Objective Bayesian movement, try to find objective priors
  - reference priors minimize the "information"
- Prior depends on parametrization (lifetime  $\tau$  vs. decay constant  $\lambda = 1/\tau$ )
  - Jeffreys prior invariant under reparameterization

## Remarks

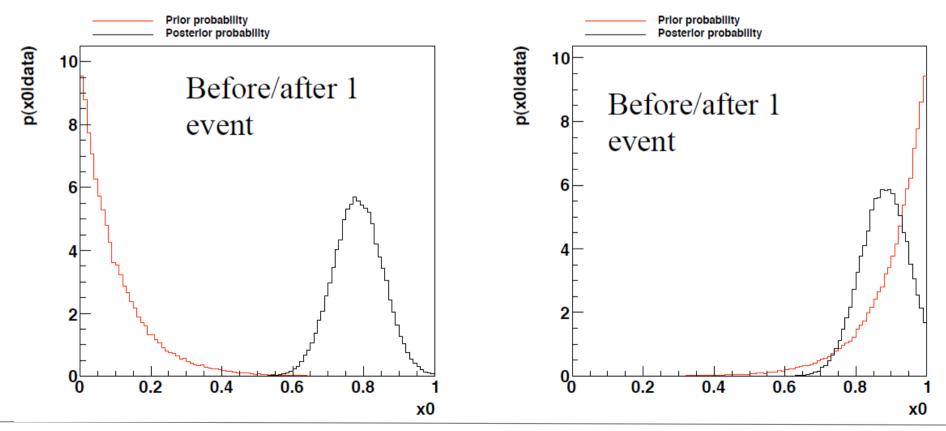
- Choice of (initial) prior should not play a strong role.
- Difficult to formulate a single prior for a collaboration of ~3.000 people
- Practical solution: subjunctive priors. Requote your result under different prior assumptions ("the optimist", "the pessimist", "the ignorant", ...)
- Write down your prior!



Impact of priors

#### **Two different priors**

- Model: Gaussian with (unknown) mean value between 0 and 1 (truth: 0.75), and width of 0.1
- Start with two different priors (optimistic / pessimistic).
- $\rightarrow$  Slightly different posteriors after one event.



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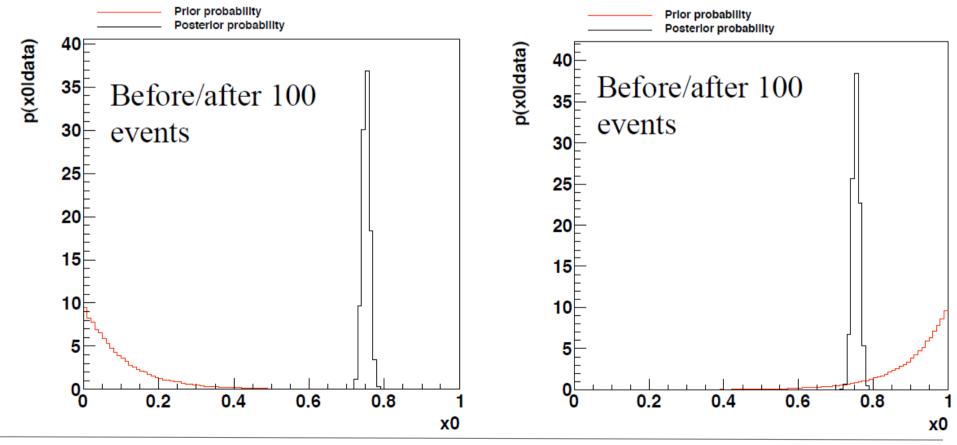


Impact of priors

#### **Two different priors**

Model: Gaussian with (unknown) mean value between 0 and 1 (truth: 0.75), and width of 0.1

 $\rightarrow$  About the same posterior after 100 events



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# Parameter estimation

### **Parameter estimation**

- Full solution: posterior probability (nothing more than that, but difficult to write down in a paper)
- For papers/talks: summarize posterior using point and interval estimates
- Common point estimators:
  - Maximum posterior probability (global mode)
  - Maximum of marginalized probability (local mode)
  - Mean value of marginalized probability
  - Median of marginalized probability:

$$p(\lambda_i|D) = \int \prod_{i\neq j} d\lambda_j p(\vec{\lambda}|D)$$



# **Parameter estimation**

### **Parameter estimation**

- Common interval estimates:
  - Smallest (set of) interval(s) covering 68% probability
  - (Central interval) 16% 84% quantile
  - Standard deviation of marginalized posterior (a la Gauß)
  - Upper (lower) limits: 99%, 95%, 90% (1%, 5%, 10%) quantiles

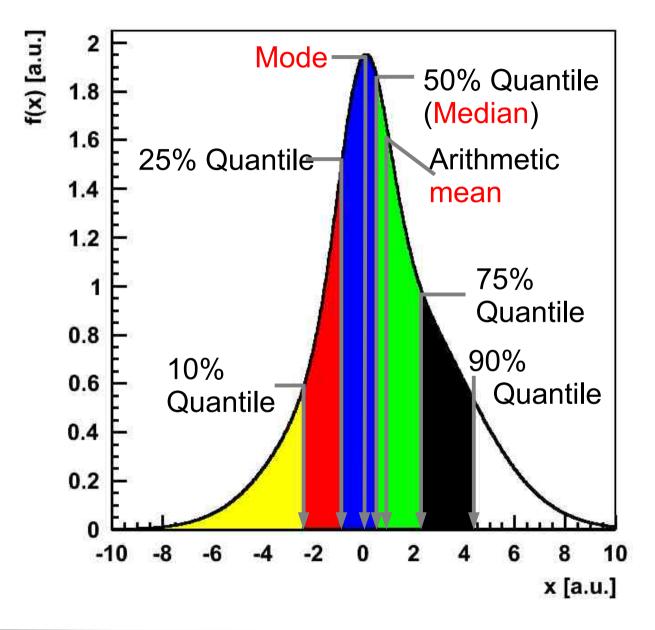
#### • Practical suggesstion:

Choose such that point estimator lies inside the estimated interval!

Mean	$\leftrightarrow$	Standard deviation
Mode	$\leftrightarrow$	Smallest interval
Median	$\leftrightarrow$	Central interval

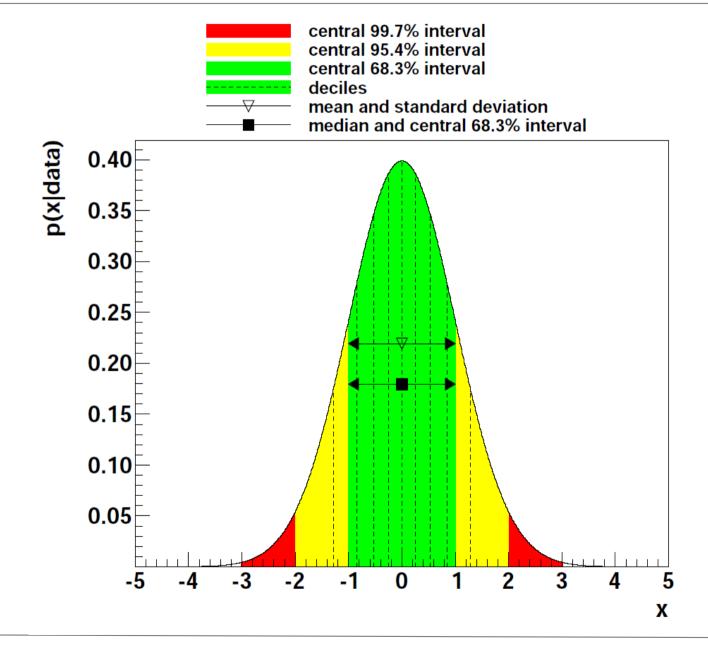
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# **Parameter estimation**



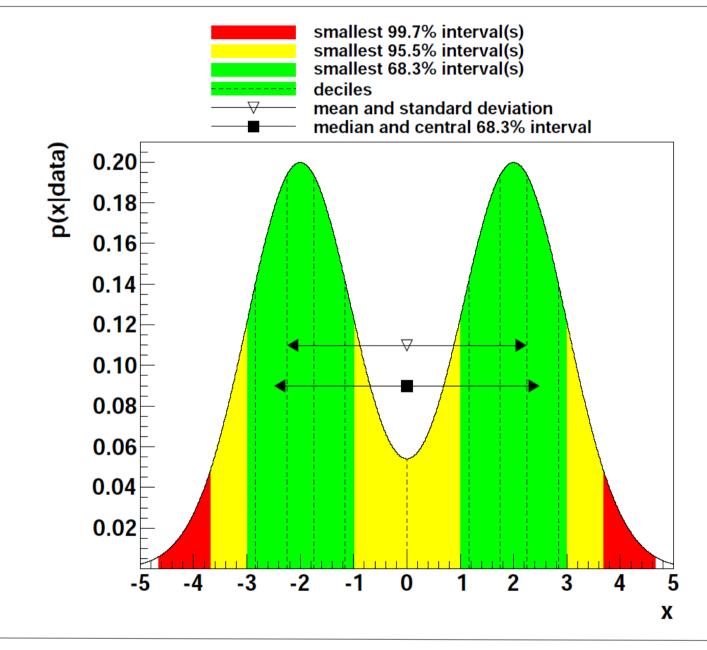


# A 1-dim Gaussian



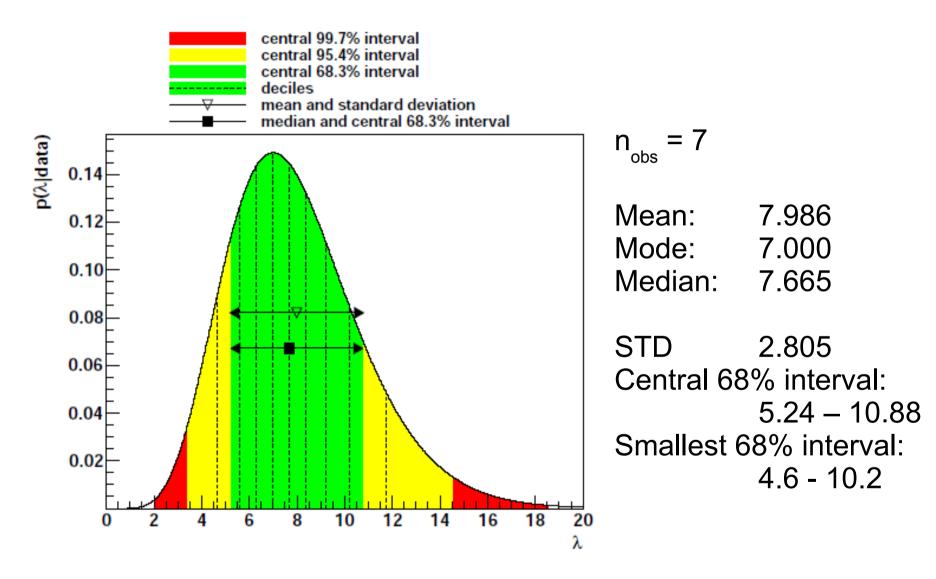


# A bimodal distribution



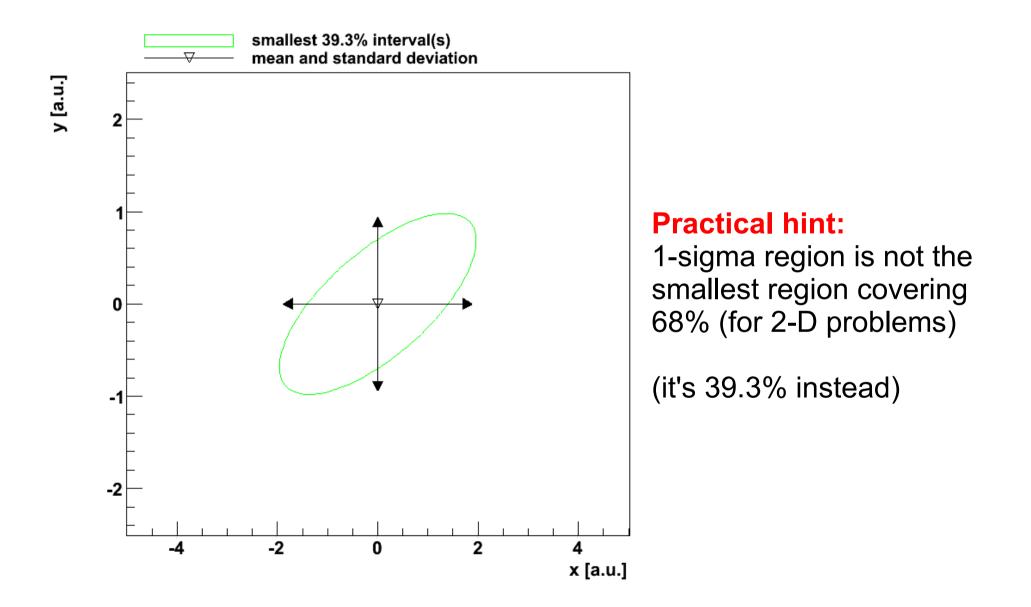


# **Example: Poisson**

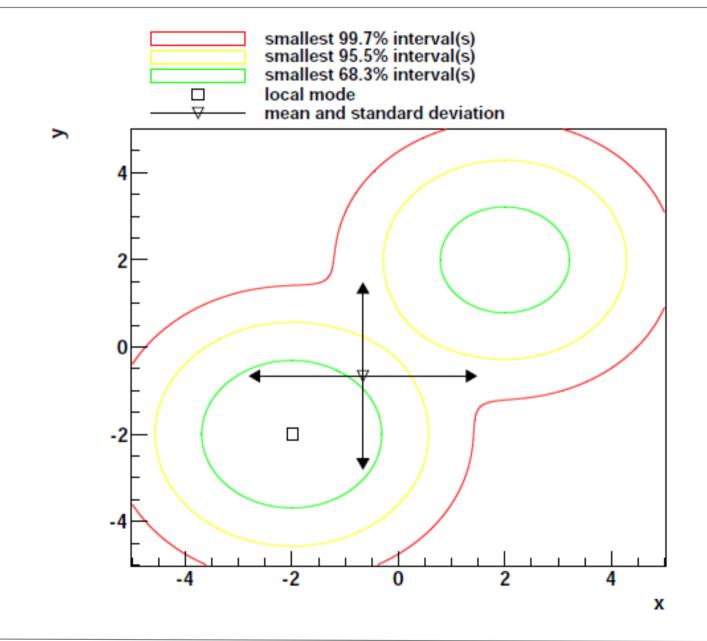




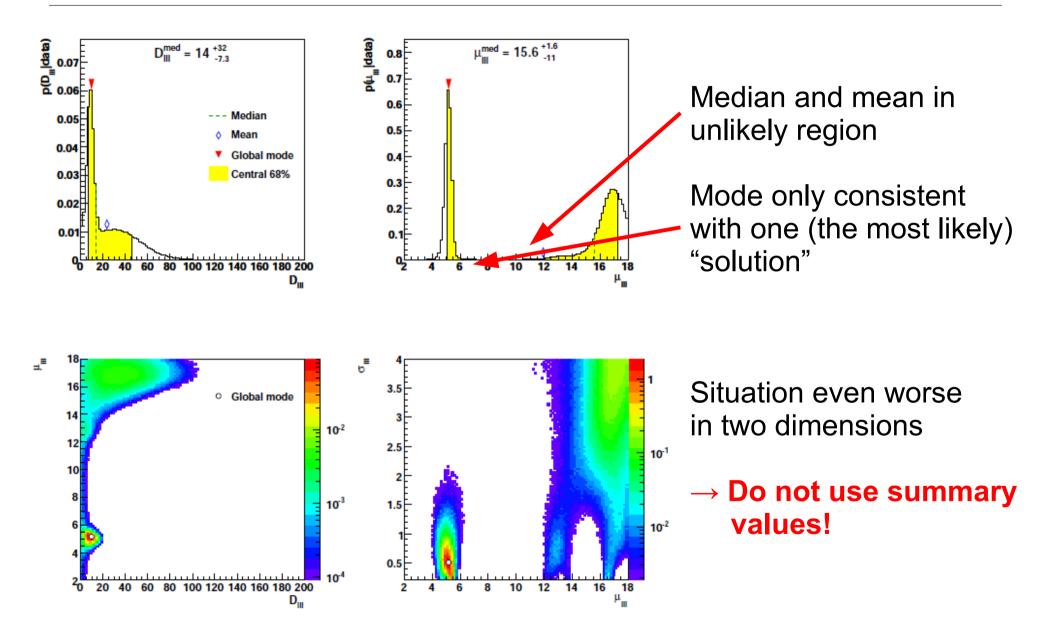




technische universitä 2D bimodal distribution



# technische universität Highly non-Gaussian

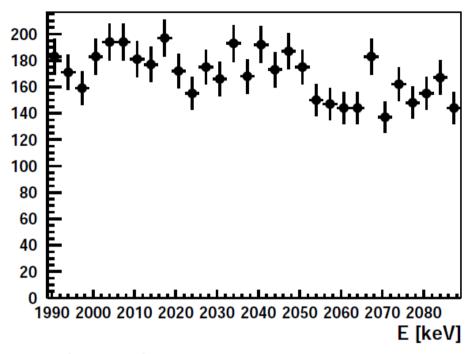


# tu technische univer ditätmore complex) example

p(E)

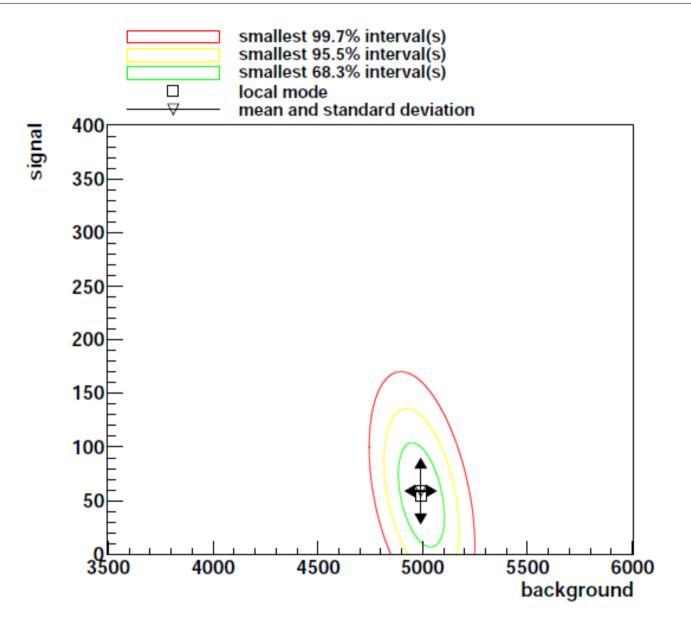
### **Concrete model**

- Data:
  - Binned, number of events
- Shapes:
  - Background linearly decreasing
  - Signal: Gaussian at fixed position
- Statistical model:
  - Independent Poisson fluctuations
  - Parameter 1: background strength, Gaussian prior
  - Parameter 2: signal strength, exponentially decreasing prior
- Fit procedure
  - Template fit: scale signal and background shapes until sum of templates matches data





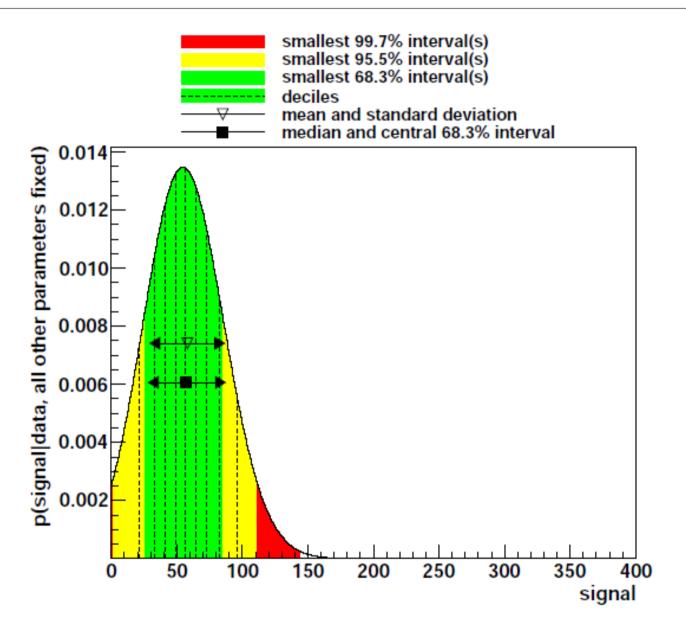




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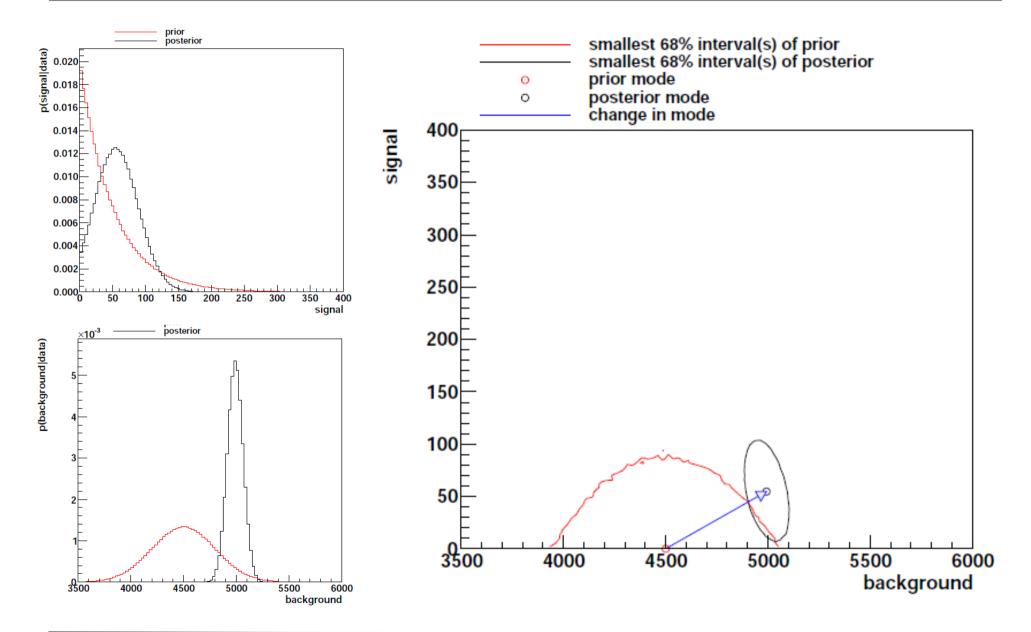






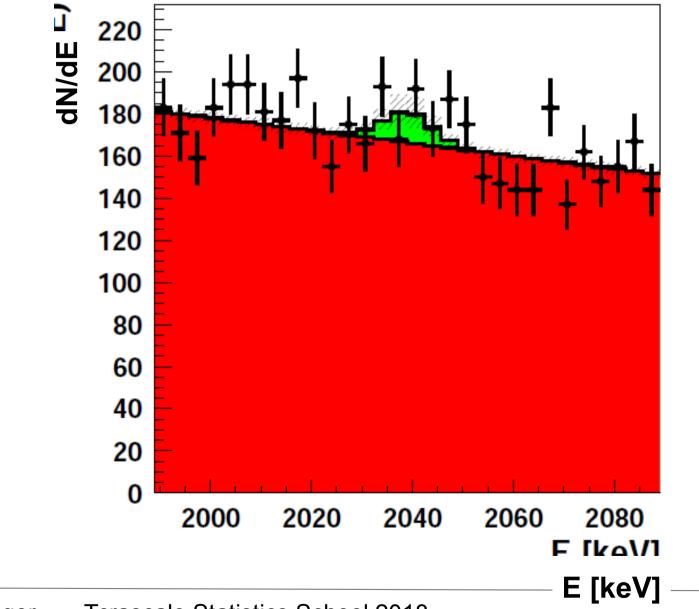


# Update of knowledge









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## Syst. uncertainties

### **Nuisance parameters**

- Model = Physics model (+ par.) × Detector model (+ nuisance par.)
- Associate nuisance parameters to sources of systematic uncertainties, e.g.
  - Collider: Luminosity uncertainty (1 parameter)
  - Calorimeter: jet energy resolution (typically 3 parameters)
  - Reconstructed objects: reconstruction efficiency (*n* parameters)
  - Different physics models ?
  - ...
- Is it justified to use a nuisance parameter? Discrete vs. continuous par.
- Choose appropriate prior (typically Gaussian, sometimes flat)
- Marginalize w.r.t. all nuisance parameters
  - Remove nuisance parameter from the final answer
  - Combine systematic and statistical uncertainties



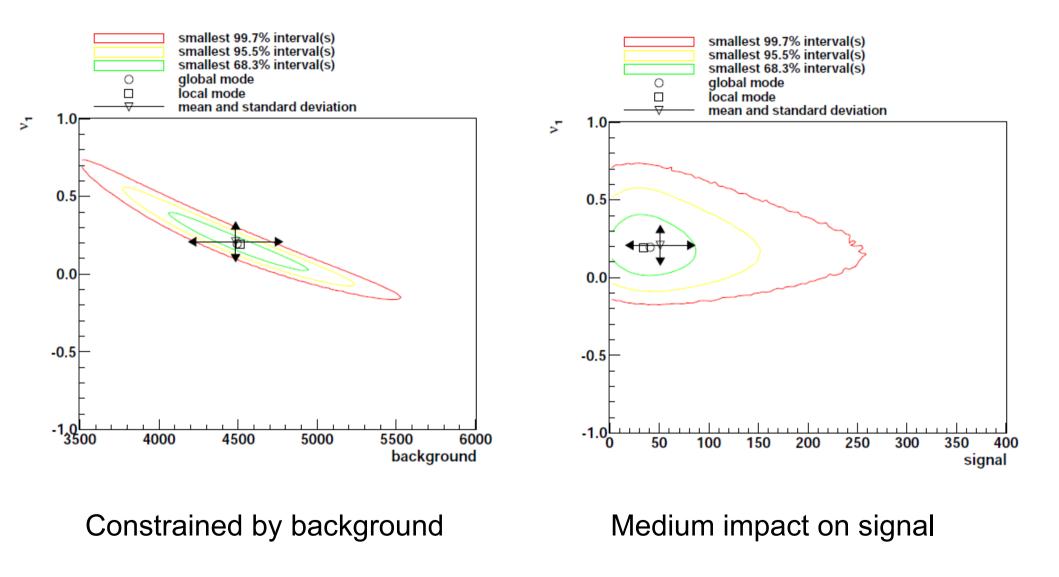


### **Systematic uncertainties**

- Add two uncertainties:
  - Systematic 1: 10% uncertainty on signal and background yield
  - Systematic 2: 60% uncertainty on signal yield
- Priors:
  - Gaussian with mean value of 0 and width of 1 sigma



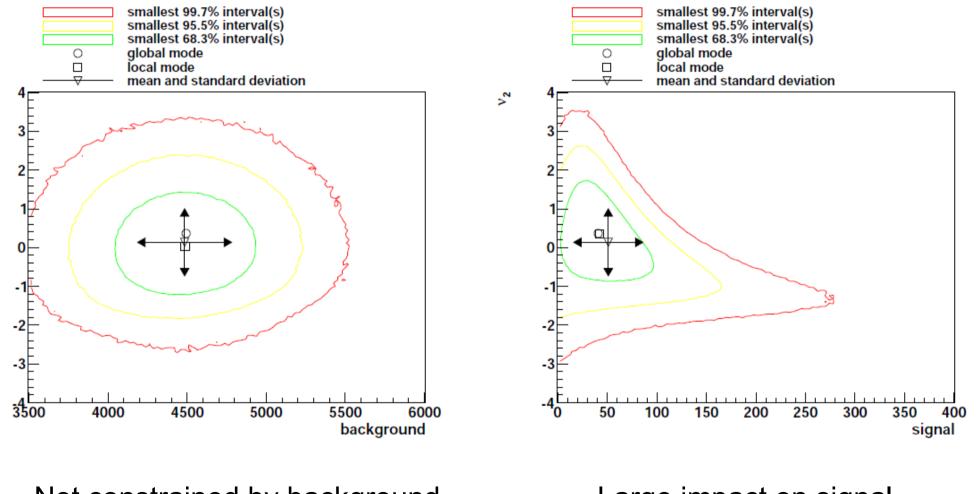
Systematic 1





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### Systematic 2



#### Not constrained by background

Large impact on signal



### **Comparing different models**

- Assume you have a full set of models which all describe the data D
- Start with the naïve Bayes ansatz:
  - Assign a probability to all models  $M_i: 0 \le P(M_i) \le 1$
  - If you have all models, then the sum of probabilities is 1:  $\sum P(M_i) = 1$
  - Next, use Bayes' theorem to calculate the probability for each model:

 $P(M_i|D) = P(D|M_i) \cdot P(M_i) / P(D) ,$ where P(D) =  $\sum P(D|M_i) \cdot P(M_i)$ 

• If the model has free parameters  $\lambda$ , then integrate them out

 $P(M|D) = \int p(M,\lambda|D) d\lambda$ 



### Model comparison

### **Comparing different models**

- Naïve Bayes ansatz (continues):
  - The last term can be calculated as

 $p(M_i,\lambda|D) = p(D|M_i,\lambda) \cdot P(M_i,\lambda) / \sum \int p(D|M_i,\lambda) \cdot P(M_i,\lambda) d\lambda$ 

- Note that there is no distinction between a model and a model with parameters (composite hypothesis)
- Example: A. Caldwell and K. Kröninger, "Signal discovery in sparse spectra: A Bayesian analysis", Phys. Rev. D 74 (2006) 092003



### **Comparing different models**

- Bayes factors:
  - Assume posterior probabilites for two models M<sub>1</sub> and M<sub>2</sub>:

 $p(M_1|D) = p(D|M_1) \cdot P(M_1) / (p(D|M_1) \cdot P(M_1) + p(D|M_2) \cdot P(M_2))$ 

• Calculate the posterior odds:

 $p(M_1|D) / p(M_2|D) = p(D|M_1) \cdot P(M_1) / p(D|M_2) \cdot P(M_2)$ 

• The ratio

 $B_{12} = p(D|M_1) / p(D|M_2)$ 

is referred to as Bayes factor.



### **Comparing different models**

- Bayes factors (continued):
  - So we find

"posterior odds" = "Bayes factor" times "prior odds"

- Traditionally, for a null hypothesis  $H_0$  and an alternative hypothesis  $H_1$ , the ratio  $B_{10}$  gives evidence against the null hypothesis. Large values of  $B_{10}$  are an indication that the hypothesis  $H_0$  is wrong in favour of  $H_1$
- Bayes factors do not rely on the priors.
- If the models do not have any free parameters, then the Bayes factors are likelihood ratios. Otherwise, the parameters have to be integrated out.



### Model comparison

### **Comparing different models**

- Bayes factors (continued):
  - Rough scales:

 $B_{12} = p(D|M_1) / p(D|M_2)$ 

B <sub>10</sub>	Evidence against $H_0$
< 1	none
1 – 3.2	Not worth mentioning
3.2 - 10	substantial
10 - 100	strong
> 100	decisive

• Of course, somebody just made that up. Depends on application.



### Occam's razor

- Principle that an explaination should not be unnecessarily complicated, i.e. chose the simpler models of the two if both describe the data reasonably well.
- Intuitively clear, although the more complex model could still be true.
- Bayesian reasoning includes Occam's razor: the prior probabilities for complex models are typically smaller than for complex ones, and thus are the posterior probabilities.
- Assume a simple model M<sub>1</sub> and a complex one M<sub>2</sub> with constant priors for

their parameters

 $p(\lambda_i) = 1 / c_i (c_i > 1),$ 

and equal prior probabilities for the models themselves, i.e.

 $p(M_1) = p(M_2) = 0.5.$ 



### **Occam's razor**

• Then we find

$$p(\vec{\lambda}, M_1 | \vec{D}) = \frac{p(\vec{D} | \vec{\lambda}, M_1) \cdot p(\vec{\lambda}, M_1)}{\int d\vec{\lambda} \, p(\vec{D} | \vec{\lambda}, M_1) \cdot p(\vec{\lambda}, M_1) + \int d\vec{\lambda} \, p(\vec{D} | \vec{\lambda}, M_2) \cdot p(\vec{\lambda}, M_2)}$$
  
$$= \frac{p(\vec{D} | \vec{\lambda}, M_1) \cdot 0.5 \cdot \prod_{i=1}^{N_1} 1/c_i}{\int d\vec{\lambda} \, p(\vec{D} | \vec{\lambda}, M_1) \cdot 0.5 \cdot \prod_{i=1}^{N_1} 1/c_i + \int d\vec{\lambda} \, p(\vec{D} | \vec{\lambda}, M_2) \cdot 0.5 \cdot \prod_{i=1}^{N_2} 1/c_i}$$

 ${\scriptstyle \bullet}$  So the posterior probability for  $\rm M_{_1}$  will increase, the more parameters we add.



# **Computational steps**

### **Numerical issues**

- Point estimate:
  - Maximization of posterior
  - Typical tool: Minuit
  - Also: Simulated annealing
- Calculation of marginal distributions:
  - Analytical solutions usually difficult
  - Numerical integration methods, e.g. VEGAS
  - Sampling methods:
    - Hit&miss, simple Monte Carlo, ...
    - Importance sampling
    - Markov Chain Monte Carlo (MCMC)
      - Revolution of Bayesian computation

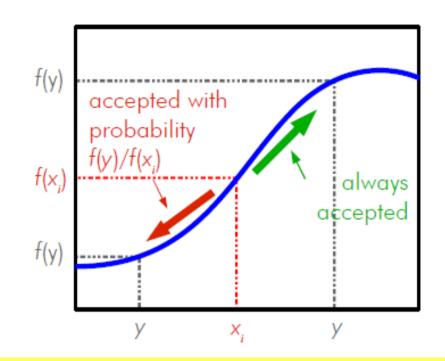


MCMC

### How does MCMC work?

- Output of Bayesian analyses are posterior probability densities, i.e., functions of an arbitrary number of parameters (dimensions).
- Sampling large dimensional functions is difficult.
- Idea: use random walk heading towards region of larger values (probabilities)
- Metropolis algorithm

N. Metropolis *et al.*, J. Chem. Phys. 21 (1953) 1087.



- Start at some randomly chosen x<sub>i</sub>
- Randomly generate y around x<sub>i</sub>
- If  $f(y) > f(x_i)$  set  $x_{i+1} = y$
- If  $f(y) < f(x_i)$  set  $x_{i+1} = y$  with prob.  $p=f(y)/f(x_i)$
- If y is not accepted set  $x_{i+1} = x_i$
- Start over



MCMC

### **MCMC for Bayesian inference**

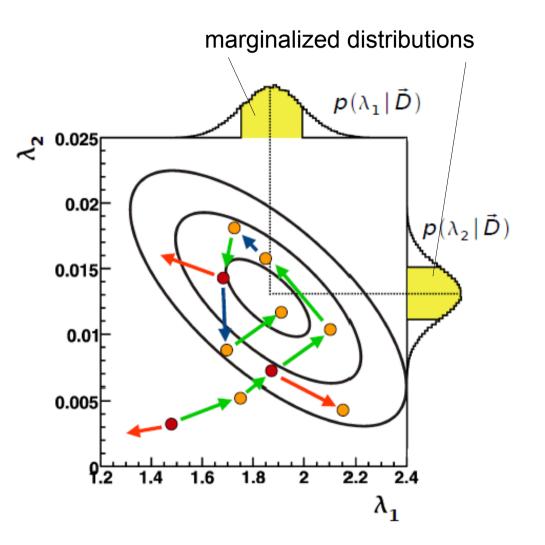
• Use MCMC to sample the posterior probability, i.e.

 $\boldsymbol{f}(\vec{\lambda}) = \boldsymbol{p}(\vec{D} \mid \vec{\lambda}) \, \boldsymbol{p}_{0}(\vec{\lambda})$ 

Marginalization of posterior:

 $\boldsymbol{p}(\lambda_i \,|\, \vec{\boldsymbol{D}}) = \int \boldsymbol{p}(\vec{\boldsymbol{D}} \,|\, \vec{\lambda}) \, \boldsymbol{p}_0(\vec{\lambda}) \boldsymbol{d} \, \vec{\lambda}_{j \neq i}$ 

- Fill a histogram with just one coordinate while sampling
- Error propagation: calculate any function of the parameters while sampling
- Point estimate: find mode while sampling



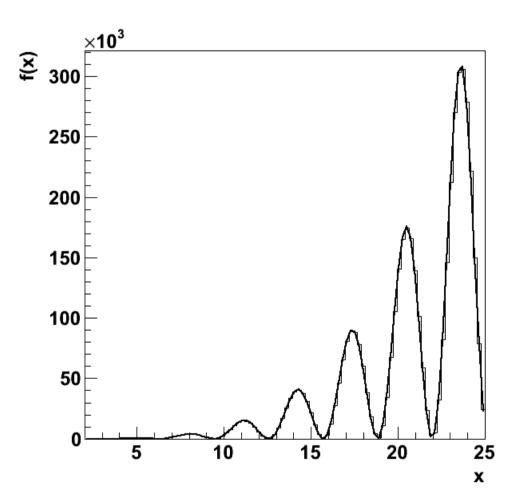


### Does it work?

• Test MCMC on a function:

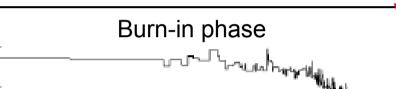
 $f(x) = x^4 \sin(x^2)$ 

- Compare MCMC distribution to analytic function
- Several minima/maxima are no problem.
- Different orders of magnitude are no problem.
- But: need to make sure that these chains converge towards the true distribution



MCMC





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### Convergence

8

2

0

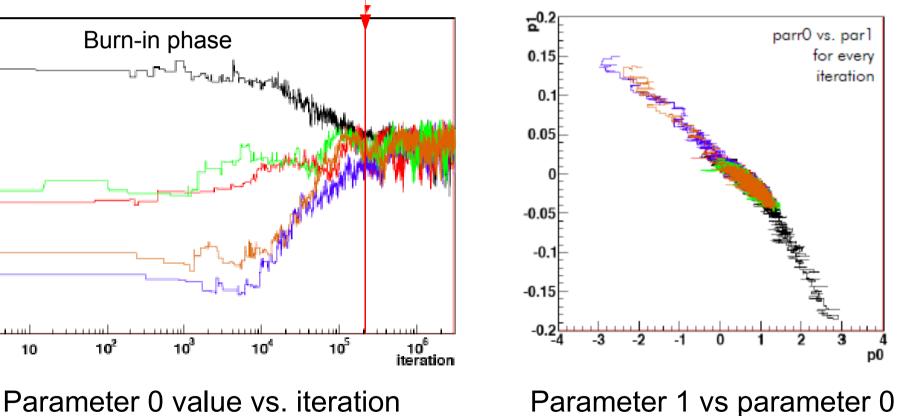
-1

- This is where it get's difficult...
- Add a burn-in phase

• Use multiple chains

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MCMC



BAT

### **Bayesian Analysis Toolkit**

- Tool for Bayesian inference written in C++
- Based on the ROOT-core functionality, interface to RooStats
- Uses MCMC for the calculation of the posterior probability
- Full control over convergence, automatic adjustment of step size
- Further algorithms: interface to CUBA, Minuit; importance sampling, simulated annealing, ...
- Pre-defined models: histogram fitter, template fitter, tool for combination of measurements, ...
- Web page: http://www.mppmu.mpg.de/bat/
- Contact: bat@mppmu.mpg.de
- Paper on BAT:

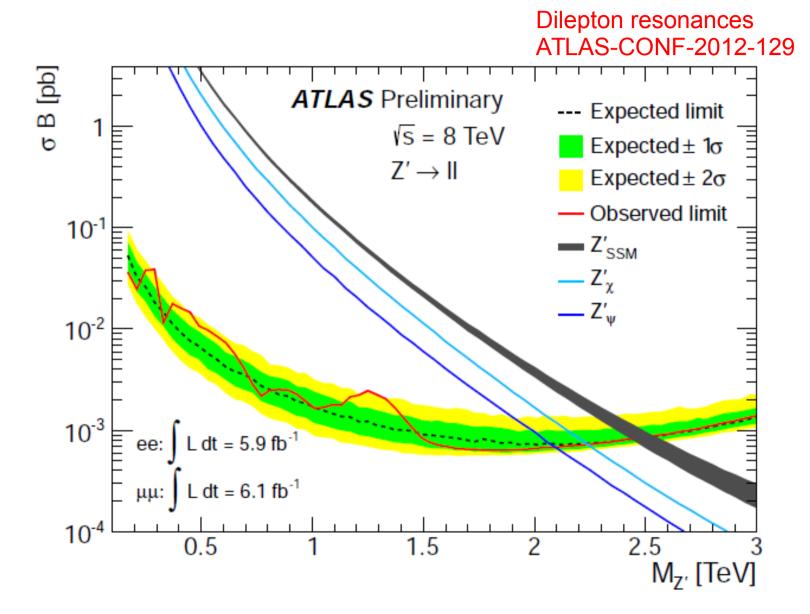
A. Caldwell, D. Kollar, K. Kröninger, BAT - The Bayesian Analysis Toolkit Comp. Phys. Comm. 180 (2009) 2197-2209 [arXiv:0808.2552].



https://github.com/bat/bat



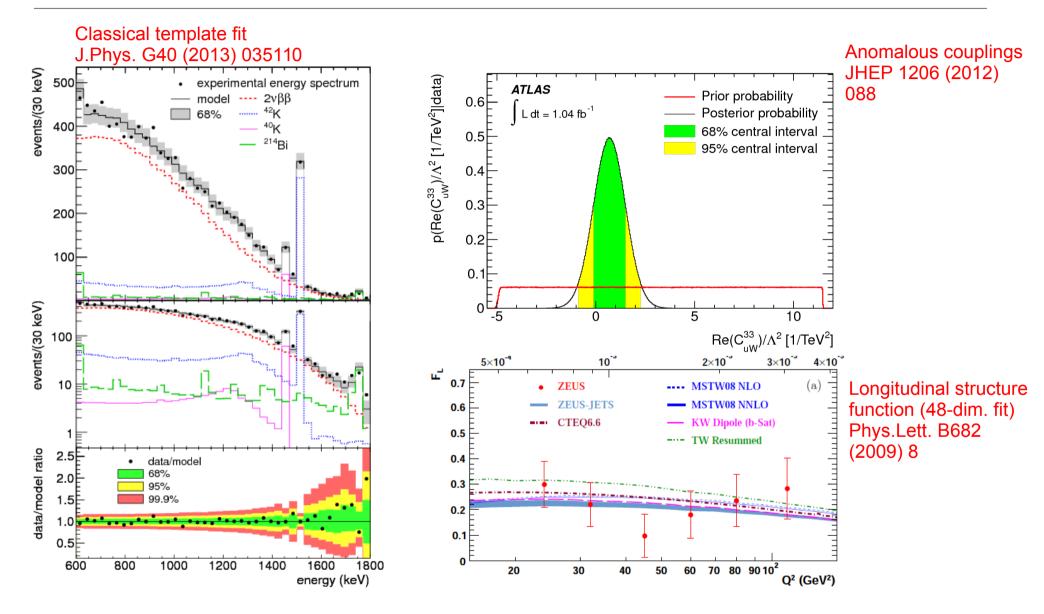




Kevin Kröninger - Terascale Statistics School 2018







#### Kevin Kröninger - Terascale Statistics School 2018

### Rare b-meson decays

dortmund

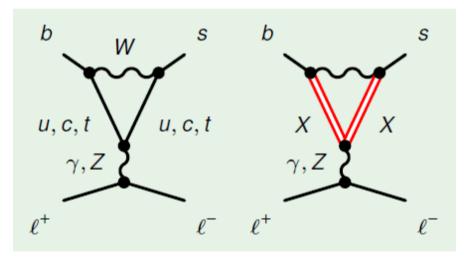
Tree-level FCNC forbidden in the SM

technische universität

- Effective field theory: add eff. operators to Lagrangian
- Similar to Fermi's four-point interaction
- Physics case: search for non-SM contributions
- Model parameters:
  - 3 Wilson coefficients
  - •25 nuisance parameters
- Input:
  - 59 measurements from BaBar, Belle, CDF, LHCb
  - Theory calculations, quark masses, CKM parameters, ...
- Numerically difficult ~ impossible with MCMC

# A complex example







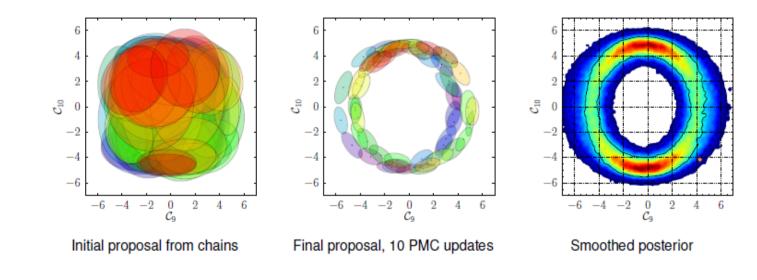
# A complex example

### **Rare b-meson decays**

Use MCMC plus population MC

	Pro	Con
MCMC	local exploration, learns on the fly	trapped in local maxima
PMC	massive parallelization, yields normalization, multiple modes OK	very sensitive to initialization

• Dominant contribution:  $BR(B \rightarrow Kll) \propto |C_9|^2 + |C_{10}|^2$ 



Frederic Beaujean *et al.* JHEP 08(2012)030

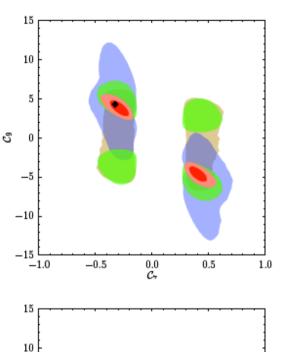


# A complex example

### **Rare b-meson decays**

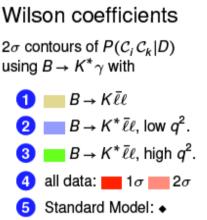
- Posterior probability well sampled
- No hint for new physics
- Showed necessity to implement new numerical algorithms
- Example:
  - F. Beaujean *et al.*, *Initializing adaptive importance sampling with Markov chains*, arXiv:1304.7808

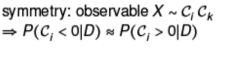
Frederic Beaujean *et al.* JHEP 08(2012)030

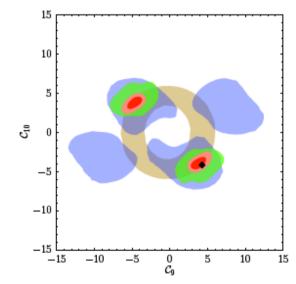


0.5

1.0







5

-5

-10

-15

-1.0

-0.5

0.0

 $C_7$ 

<u></u>2



Summary

### Summary

- Knowledge is justified belief
- Bayesian probability is degree-of-belief
- Bayes' theorem allows easy update of knowledge
- Everything else is about math and numerical methods:
  - Parameter (point and interval) estimation
  - Treatment of systematic uncertainties
  - Calculation of marginalized distributions
  - Also: model comparison and goodness-of-fit (not covered)
- Numerical methods necessary for complex fit with a large number of parameters