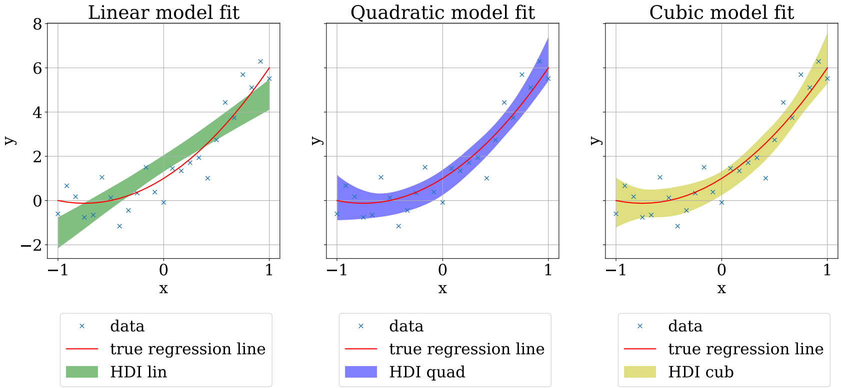
Bayesian model selection

Seminar physics760 – Computational Physics



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19.03.2021

Introduction

Bayes' Theorem – a quick reminder

$$\text{prob}(\boldsymbol{\theta}|y) = p(\boldsymbol{\theta}|y) = \frac{p(y|\boldsymbol{\theta}) \cdot p(\boldsymbol{\theta})}{p(y)}$$

with

- *posterior* $p(\boldsymbol{\theta}|y)$
- *likelihood* $p(y|\boldsymbol{\theta})$
- *prior* $p(\boldsymbol{\theta})$
- *marginal likelihood* $p(y) = \int_{-\infty}^{+\infty} \mathrm{d}\boldsymbol{\theta} p(y|\boldsymbol{\theta}) p(\boldsymbol{\theta})$

This can be used for *model selection* (?)

Table of Contents

1. Theory
   - Parameter estimation
   - Model comparison

2. Methods
   - Monte-Carlo-Sampling
   - Savage-Dickey-Density-Ratio (SDDR)

3. Examples
   - Coin Flip
   - Fitting a polynomial of unknown degree

4. Summary

Parameter estimation

JAN and MARIUS already talked about this, so here we only sketch the basics again

$$\textit{marginal posterior } p(\theta_i|y,M) = \int p(\boldsymbol{\theta}|y,M) \prod_{j\neq i} \mathrm{d}\theta_j \tag{1}$$

$$\begin{aligned} \text{best fit value(s) } p(\theta|y,M) = \max \Leftrightarrow \theta = \hat{\theta} \\ \langle\theta\rangle = \int_{-\infty}^{\infty} \mathrm{d}\theta p(\theta|y,M) \cdot \theta \end{aligned} \tag{2}$$

[Sivia and Skilling 2006]

Model comparison

BAYES factor

$$p(M_i|y) = \frac{p(M_i) \cdot p(y|M_i)}{p(y)}. \quad (3)$$

$$\begin{aligned} O_{ij} &:= \underbrace{\frac{p(M_i|y)}{p(M_j|y)}}_{\text{posterior odds}} \\ &= \underbrace{\frac{p(y|M_i)}{p(y|M_j)}}_{\text{BAYES Factor}} \cdot \underbrace{\frac{p(M_i)}{p(M_j)}}_{\text{prior odds}} \quad (4) \\ &= B_{ij} \cdot \frac{p(M_i)}{p(M_j)}. \end{aligned}$$

How do we turn BAYES' theorem into a tool for model comparison?

$\lvert \ln B_{ij} \rvert$	Odds	Strength of evidence
< 1.0	$\lesssim 3:1$	Inconclusive
1.0	$\sim 3:1$	Weak evidence
2.5	$\sim 12:1$	Moderate evidence
5.0	$\sim 150:1$	Strong evidence

Table 1: Empirical scale for evaluating the strength of evidence when comparing two models M_i vs. M_j, adapted from [Trotta 2008]

[Trotta 2008]

Model comparison

Bayesian complexity

$$\mathcal{C}_b = -2 \int \mathrm{d}\boldsymbol{\theta} p(\boldsymbol{\theta}|y, M) \log(\mathcal{L}(\boldsymbol{\theta})) + 2 \log(\mathcal{L}(\tilde{\boldsymbol{\theta}})), \tag{5}$$

$$\mathcal{C}_b = \overline{\chi^2(\boldsymbol{\theta})} - \chi^2(\tilde{\boldsymbol{\theta}}), \tag{6}$$

- describes how many model parameters the data is able to constrain
- is a useful tool for examining models with an increasing number of parameters

[Kunz, Trotta and Parkinson 2006]

Monte-Carlo-Sampling

Benefits of Monte-Carlo-Sampling

$$\langle \boldsymbol{\theta} \rangle \approx \int p(\boldsymbol{\theta}|y)\boldsymbol{\theta} d\boldsymbol{\theta} = \frac{1}{N}\sum_{t=0}^{N-1} \boldsymbol{\theta}^{(t)}, \tag{7}$$

$$\langle f(\boldsymbol{\theta}) \rangle \approx \frac{1}{N}\sum_{t=0}^{N-1} f(\boldsymbol{\theta}^{(t)}). \tag{8}$$

also, *marginal posterior* distributions are obtained trivially by binning values of θ_i ignoring $\theta_{j\neq i}$ [Trotta 2008]

Figure 1: `ArviZ` [*ArviZ: Exploratory analysis of Bayesian models — ArviZ dev documentation* 2021] and `PyMC3` [*PyMC3 Documentation — PyMC3 3.10.0 documentation* 2021]

Monte-Carlo-Sampling

But how exactly do we get samples $\boldsymbol{\theta}^{(t)}$?

Sequential Monte Carlo (SMC)

First let us introduce an auxiliary *temperature parameter* $\beta \in [0, 1]$ and write

$$p(\boldsymbol{\theta}|y)_\beta = \frac{p(y|\boldsymbol{\theta})^\beta \cdot p(\boldsymbol{\theta})}{Z_\beta},$$

with $Z_\beta = \int \mathrm{d}\boldsymbol{\theta} p(y|\boldsymbol{\theta})^\beta \cdot p(\boldsymbol{\theta})$.
Main idea: gradually sample from simple distribution ($\beta = 0$) to complex/true distribution ($\beta = 1$) using Metropolis-Hastings
SMC then allows us to estimate the *marginal likelihood* as

$$\hat{p}(y) = \prod_i \widehat{\frac{Z_{\beta_i}}{Z_{\beta_{i-1}}}}. \tag{9}$$

[Gunawan et al. 2020; *PyMC3 Documentation — Sequential Monte Carlo* 2021]

Savage-Dickey-Density-Ratio (SDDR)

consider model M_j with free parameters ω, ψ and a submodel M_i with one free parameter ψ and fixed $\omega = \omega_\star$. Let us further assume separable priors

$$p(\omega, \psi | M_j) = p(\omega | M_j) p(\psi | M_i).$$

We can then write the Bayes factor as

Savage Dickey-Density-Ratio

$$B_{ij} = B_{ji}^{-1} = \left. \frac{p(\omega | y, M_j)}{p(\omega | M_j)} \right|_{\omega = \omega_\star} \text{(SDDR)}. \tag{10}$$

[Trotta 2007]

Coin Flip

- remember the flipping of a biased coin from the lecture
- we want to verify that the coin is biased by using the Bayes factor
- two models: M_1 – assumes a fair coin, M_2 – assumes biased coin

Posterior of the coin flip problem

$$p(\theta|y, M_i) = \frac{p(y|\theta, M_i) \cdot p(\theta|M_i)}{p(y|M_i)} \tag{11}$$

to get $p(y|M_i) = \int_{-\infty}^{+\infty} \mathrm{d}\theta p(y|\theta, M_i)p(\theta|M_i)$ we need to specify a *prior* $p(\theta|M_i)$ and a *likelihood* $p(y|\theta, M_i)$

Coin Flip

Choosing a prior

$$f(\theta;\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$
$$:= \frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}.$$

[*PyMC3 Documentation – Bayes Factors and Marginal Likelihood* 2021]

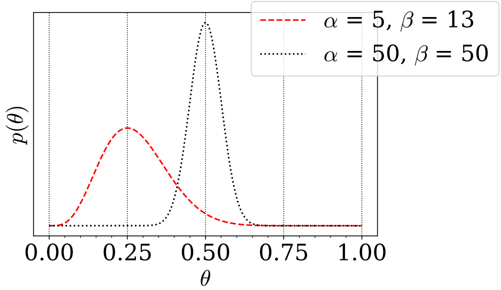

Figure 2: Beta-distribution as *prior* $p(\theta|M_i)$ for the two different models

Coin Flip

Choosing a likelihood

Since we can assume i.i.d. outcomes of the coin flip a natural choice is a *Binomial distribution*. If we observe k heads out of N coin throws ($y = (N, k)$)

$$p(y|\theta, M_i) = \binom{N}{k} \theta^k (1-\theta)^{N-k}.$$

We simulated data for $N = 50$ and the biased coin with $p(H) = 0.25$.

Coin Flip

Finally computing the Bayes factor

$$p(y|M_i) \propto \int_0^1 \mathrm{d}\theta \frac{1}{B(\alpha,\beta)} \cdot \theta^{\alpha+k-1} \cdot (1-\theta)^{N-k+\beta-1} = \frac{B(\alpha+k,\beta+N-k)}{B(\alpha,\beta)}$$

$$\Rightarrow B_{21} = B_{12}^{-1} = \frac{B(\alpha_2+k,\beta_2+N-k)\cdot B(\alpha_1,\beta_1)}{B(\alpha_1+k,\beta_1+N-k)\cdot B(\alpha_2,\beta_2)} = 9.5839$$

Can we reproduce this numerically?

[*PyMC3 Documentation – Bayes Factors and Marginal Likelihood* 2021]

Coin Flip

let us obtain 2000 samples from the posterior distribution using the same *likelihood* and *priors* via the SMC algorithm provided by `PyMC3`

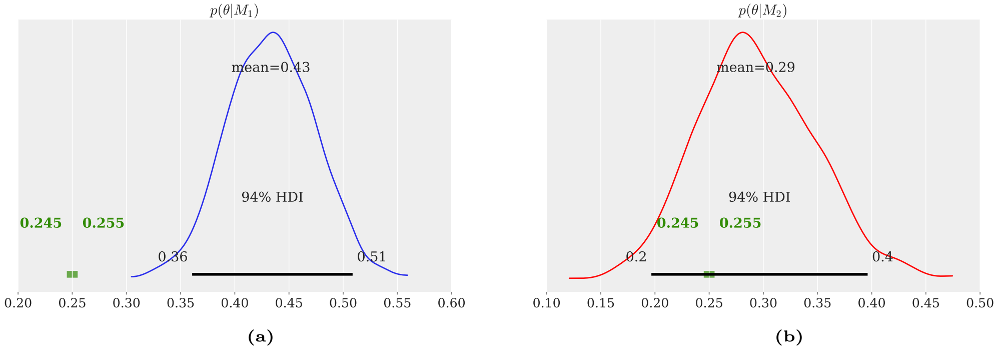

Figure 3: The *marginal posterior* for $\alpha = \beta = 50$ (3a) and $\alpha = 5, \beta = 13$ (3b) of 2000 samples. HDI means highest density interval. The highlighted green intervals denote the expected value.

$$\text{We find } B_{21} = B_{12}^{-1} = 9.5829 \pm 0.4719 \text{ (noice! } \checkmark\text{)}$$

Fitting a polynomial of unknown degree

We wish to determine the true model underlying the generated data depicted in the figure below

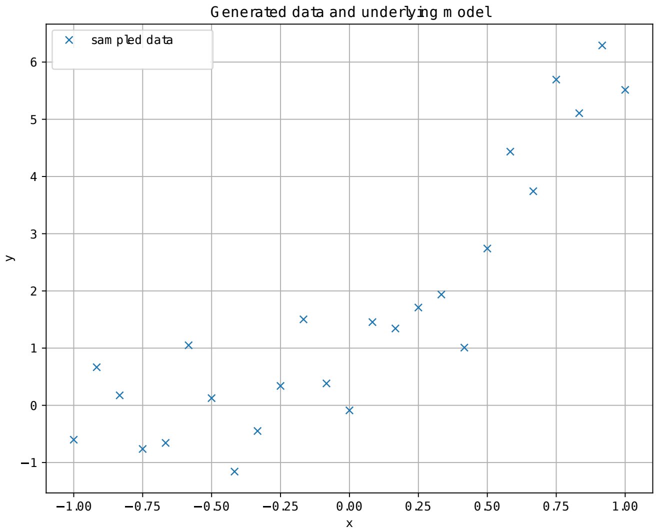

Figure 4: $N = 25$ datapoints distributed with a gaussian noise of $\sigma = 0.7$. Linear? Quadratic? Cubic?

Fitting a polynomial of unknown degree

we want to find the correct model by using

- BAYES factor
- SDDR (as sanity check)
- BAYESIAN complexity

We will tackle this problem numerically by sampling from the *posterior* $\rightarrow$ we need to assign *priors* and *likelihoods* again

Fitting a polynomial of unknown degree

a suitable choice for *prior* and *likelihood* are normal distributions, since the noise is Gaussian [Sivia and Skilling 2006].

Choosing a prior

The *priors* for the fit-parameters a, b and c are each described by a normal distribution with $\mu_{\text{prior}} = 0$ and $\sigma_{\text{prior}} = 2$

Choosing a likelihood

$$p(y|\boldsymbol{\theta}, M_i) = \prod_{k=1}^{N} \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(f(y_k;\boldsymbol{\theta}) - y_k)^2}{2\sigma^2}\right].$$

where $f(y_k;\boldsymbol{\theta})$ is the fit function $f_i(x) = \sum_{\alpha=0}^{i} a_\alpha x^\alpha$, with $i = 1, 2, 3$

Fitting a polynomial of unknown degree

Now lets generate 2000 samples following the *posterior*

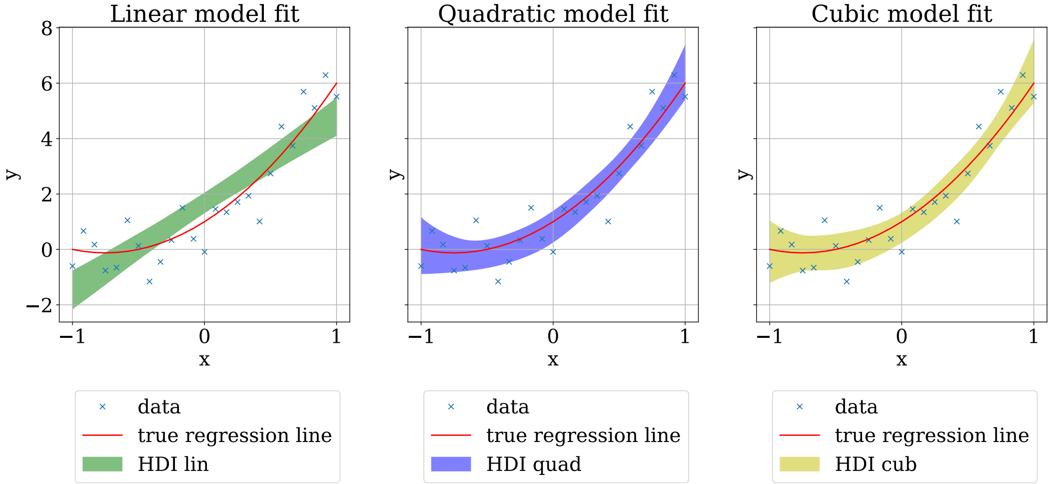

Figure 5: Result of parameter estimation with SMC. The data was generated with $\sigma = 0.7$

Fitting a polynomial of unknown degree

Comparison M_1 vs. M_2	$\ln(B_{12}(\sigma = 0.7))$
square vs. linear	8.5507 ± 0.053
cubic vs. linear	7.6225 ± 0.094
square vs. cubic	0.9371 ± 0.1093

Table 2: Results of Bayes factor via SMC

Comparison M_1 vs. M_2	$\ln(B_{12}(\sigma = 0.7))$
square vs. linear	$> 2.4301 \pm 0.27613$
square vs. cubic	0.8091 ± 0.0265
cubic vs. linear	$> 0.3329 \pm 0.1292$

Table 3: Results of Bayes factor via SDDR.

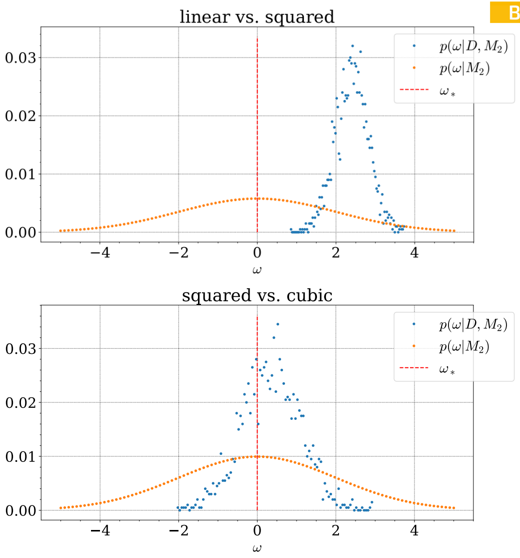

Figure 6: Computation of the SDDR ($\sigma = 0.7$)

Fitting a polynomial of unknown degree

What about the complexity?

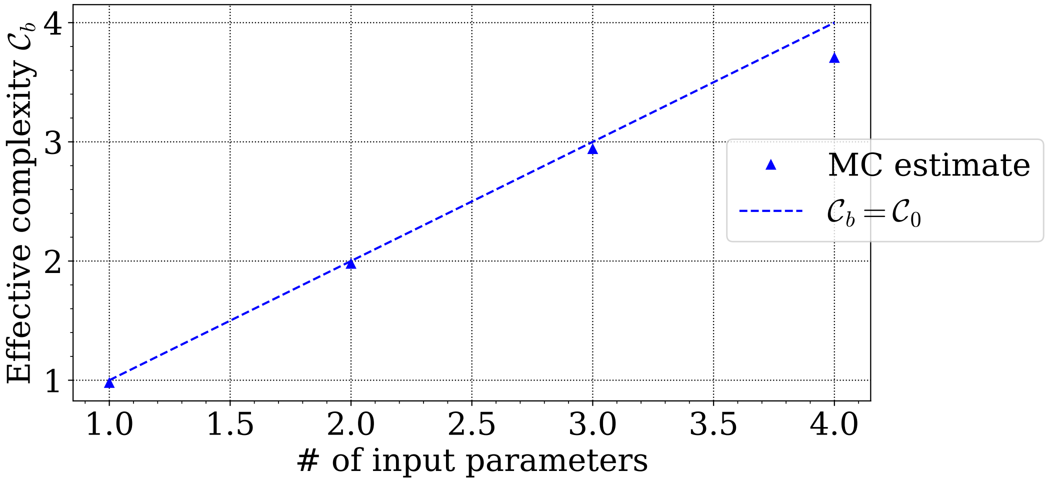

Figure 7: Numerical computation of the complexity $\mathcal{C}_b$, 3 parameters are supported.

Fitting a polynomial of unknown degree

And the true regression line is...

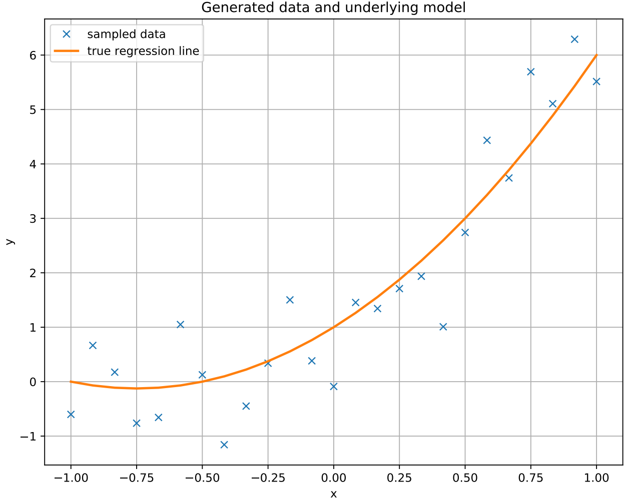

Figure 8: True regression line

$$
\begin{aligned}
f(x;\boldsymbol{\theta}) &= a \cdot x^2 + b \cdot x + c \\
&= 2 \cdot x^2 + 3 \cdot x + 1.
\end{aligned}
$$

(again, nice! ✓)

Summary

Theory and methods

- BAYESIAN statistics provides the BAYES factor and BAYESIAN complexity as measures of *model comparison*
- Monte-Carlo-techniques can be used to compute both quantities

Examples

- We can say with weak to moderate confidence that the coin is biased
- We can say with weak to moderate evidence that the quadratic model is favoured over the others
- The BAYESIAN complexity diverges for $\dim \boldsymbol{\theta} > 3$

Outlook

- Highly scalable
- physics, actually

GitHub.com

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