Introduction to Bayesian Inference for Statistical Model Fitting (DRAFT)

Luigi Acerbi

Department of Computer Science University of Helsinki Finnish Center for Artificial Intelligence FCAI



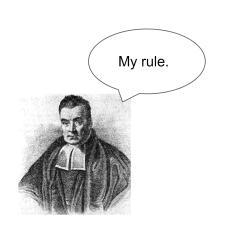




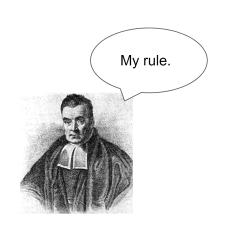
BAMB! Summer School – Day 2 September 2022

- Introduction and motivation
 - Bayes rule
 - Bayesian inference for model fitting
- Computing the posterior distribution
 - Computing the posterior "by hand"
 - Inference algorithms
 - The prior
- Making use of a Bayesian posterior
 - Visualizing the posterior
 - Posterior prediction

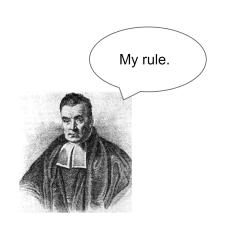
- Introduction and motivation
 - Bayes rule
 - Bayesian inference for model fitting
- 2 Computing the posterior distribution
 - Computing the posterior "by hand"
 - Inference algorithms
 - The prior
- Making use of a Bayesian posterior
 - Visualizing the posterior
 - Posterior prediction



$$p(oldsymbol{ heta}|\mathsf{data}) = rac{p(\mathsf{data}|oldsymbol{ heta})p(oldsymbol{ heta})}{p(\mathsf{data})}$$

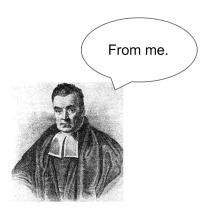


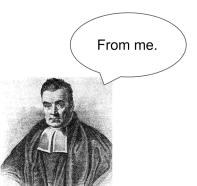
$$\underbrace{p(\theta|\mathsf{data})}_{\mathsf{posterior}} = \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\mathsf{data})}}_{\substack{\mathsf{evidence}}} \underbrace{\frac{p(\mathsf{data})}{p(\mathsf{data})}}_{\substack{\mathsf{evidence}}}$$

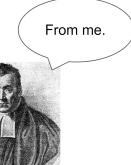


$$\underbrace{p(\theta|\mathsf{data})}_{p(\mathsf{data})} = \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\mathsf{data})} \underbrace{p(\theta)}_{evidence}}_{p(\mathsf{data})}$$

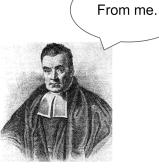
$$p(\mathsf{data}) = \int p(\mathsf{data}|oldsymbol{ heta})p(oldsymbol{ heta})doldsymbol{ heta}$$





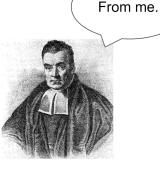


Really, just basic rules of probability:



$$p(\theta, \mathsf{data}) = p(\mathsf{data}|\theta)p(\theta)$$





What's new in Bayesian inference for model fitting?

The output of Bayesian inference is a probability distribution (posterior) over model parameters:

$$p(\theta|\mathsf{data})$$

Before, we only had a single best point estimate θ_{\star} .

What's new in Bayesian inference for model fitting?

The output of Bayesian inference is a probability distribution (posterior) over model parameters:

$$p(\theta|\mathsf{data})$$

Before, we only had a single best point estimate θ_{\star} .

Questions:

- How do we compute $p(\theta|\text{data})$?
- ② What do we do once we have $p(\theta|\text{data})$?
- Why should we bother?

$$\underbrace{p(\theta|\mathsf{data})}_{\mathsf{posterior}} = \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\mathsf{data})}}_{\mathsf{evidence}} \underbrace{p(\mathsf{data})}_{\mathsf{posterior}} p(\mathsf{data}) = \int p(\mathsf{data}|\theta)p(\theta)d\theta$$

$$\underbrace{p(\theta|\mathsf{data})}_{\substack{\mathsf{p}(\mathsf{data}|\theta)\\\mathsf{evidence}}} \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\theta)}}_{\substack{\mathsf{p}(\mathsf{data})\\\mathsf{evidence}}} p(\mathsf{data}) = \int p(\mathsf{data}|\theta)p(\theta)d\theta$$

- Uncertainty quantification
- Optimal experiment design
- Robustness
- Interpretability

$$\underbrace{p(\theta|\mathsf{data})}_{\mathsf{posterior}} = \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\mathsf{data})}}_{\mathsf{posterior}} \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\theta)}}_{\mathsf{posterior}} \underbrace{\frac{$$

$$p(\mathsf{data}) = \int p(\mathsf{data}|oldsymbol{ heta})p(oldsymbol{ heta})doldsymbol{ heta}$$

- Uncertainty quantification
- Optimal experiment design
- Robustness
- Interpretability

- Hyperparameter tuning
- Model selection

$$\underbrace{p(\theta|\mathsf{data})}_{\mathsf{posterior}} = \underbrace{\frac{p(\mathsf{data}|\theta)}{p(\mathsf{data})}}_{\mathsf{evidence}} \underbrace{\frac{p(\mathsf{data})}{p(\mathsf{data})}}_{\mathsf{evidence}}$$

$$p(\mathsf{data}) = \int p(\mathsf{data}|oldsymbol{ heta})p(oldsymbol{ heta})doldsymbol{ heta}$$

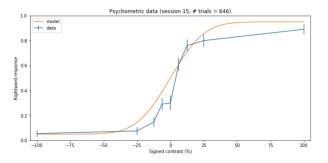
- Uncertainty quantification
- Optimal experiment design
- Robustness
- Interpretability
- Better predictions

- Hyperparameter tuning
- Model selection

- Introduction and motivation
 - Bayes rule
 - Bayesian inference for model fitting
- Computing the posterior distribution
 - Computing the posterior "by hand"
 - Inference algorithms
 - The prior
- Making use of a Bayesian posterior
 - Visualizing the posterior
 - Posterior prediction

Data and model

- Same data from before (IBL mouse behavioral data)
- Same model as before (psychometric function model)
 - Parameters $\theta = (\mu, \sigma, \lambda, \gamma)$



Let's just apply Bayes rule!

- We consider a 1-D posterior (one free parameter, σ)
- We fix μ, λ, γ to some values $\mu_{\star}, \lambda_{\star}, \gamma_{\star}$
- We assume a uniform prior $p(\sigma)$ for $\sigma \in [1, 100]$
- We compute

$$p(\sigma|\mu_{\star}, \lambda_{\star}, \gamma_{\star}, \mathsf{data}) = \frac{p(\mathsf{data}|\mu_{\star}, \sigma, \lambda_{\star}, \gamma_{\star})p(\sigma)}{Z}$$

• The normalization is $Z=\int p({\sf data}|\mu_\star,\sigma,\lambda_\star,\gamma_\star)p(\sigma)d\sigma$

Let's do this!

Bayesian inference solved?

- ullet Not really a grid only works in low dimension $(D\sim 1-4)$
- ullet Curse of dimensionality: N points per dimension $\Rightarrow N^D$ points
- We need inference algorithms!

Inference algorithms

- A general-purpose inference algorithm
 - ▶ takes as input an inference problem (likelihood, prior,...)
 - returns an approximate posterior
- Abstractly, similar to optimization...
 - take as input an optimization problem (target function)
 - return the optimum
- ...in practice, way more complex algorithms
 - Inference is harder

Main families of inference algorithms

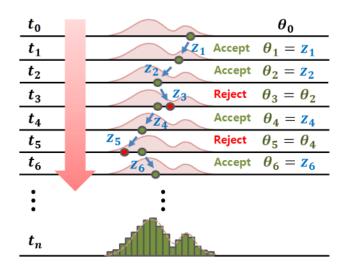
- Markov Chain Monte Carlo (MCMC)
- Variational inference

(there are others)

Markov Chain Monte Carlo (MCMC)

- ullet Generates a random sequence $oldsymbol{ heta}_0, oldsymbol{ heta}_1, \dots$ (a Markov chain)
- ullet Various rules for drawing $heta_{n+1}| heta_n$ depending on the algorithm
 - ▶ These will generally depend on $p(\theta_n, \text{data})$, $p(\theta_{n+1}, \text{data})$
- **Output:** A set of samples $\theta_0, \dots, \theta_N$
- If all goes well, $\theta_0, \dots, \theta_N \sim p(\theta|\mathsf{data})$
 - ▶ In practice, lot of tweaking to ensure convergence of the Markov chain
 - ► State-of-the-art MCMC methods are (to a degree) self-tuning
 - Still a lot of tweaking involved

Example MCMC algorithm: Metropolis-Hastings



Source: Jin et al. (2019)

ullet Approximate $p(oldsymbol{ heta}|\mathsf{data})$ with $q_\phi(oldsymbol{ heta})$

- ullet Approximate $p(heta| ext{data})$ with $q_{\phi}(heta)$
- ullet Minimize Kullback-Leibler divergence between q and p

- ullet Approximate $p(heta|\mathsf{data})$ with $q_{\phi}(heta)$
- Minimize Kullback-Leibler divergence between q and p

Obtains

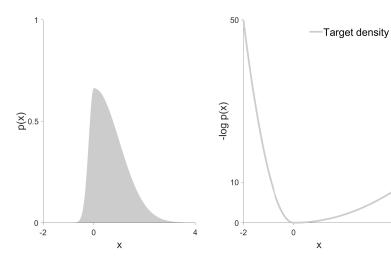
- ullet An approximate posterior $q_\phi(heta)$
- ullet A lower bound to the log marginal likelihood, ELBO (ϕ)

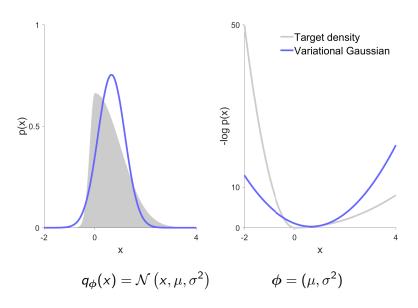
- ullet Approximate $p(heta|\mathsf{data})$ with $q_{\phi}(heta)$
- Minimize Kullback-Leibler divergence between q and p

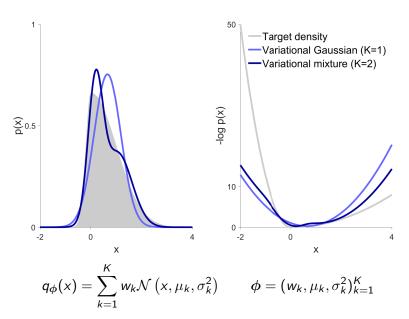
Obtains

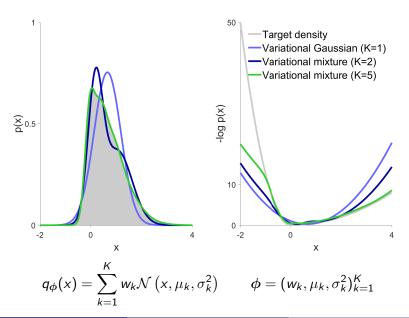
- ullet An approximate posterior $q_\phi(heta)$
- ullet A lower bound to the log marginal likelihood, ELBO (ϕ)

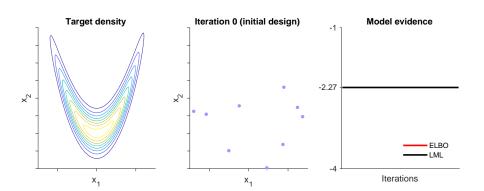
 ${\sf VI}$ casts Bayesian inference into optimization + integration



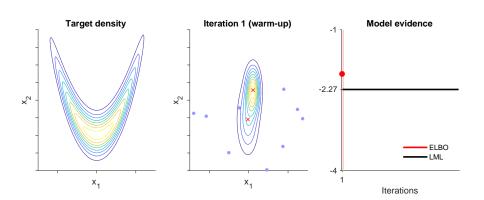




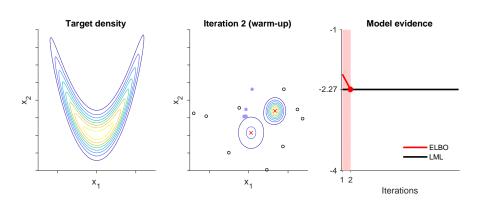




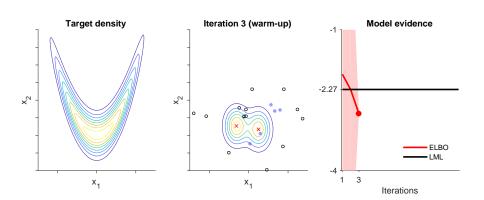
Acerbi, NeurIPS (2018; 2020)



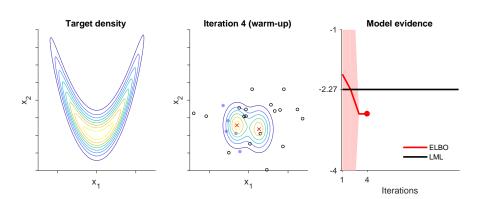
Acerbi, NeurIPS (2018; 2020)



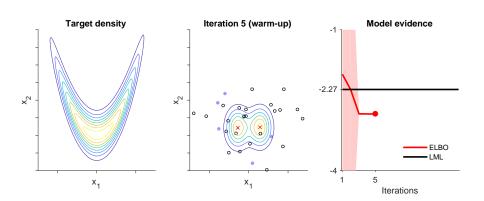
Acerbi, NeurIPS (2018; 2020)



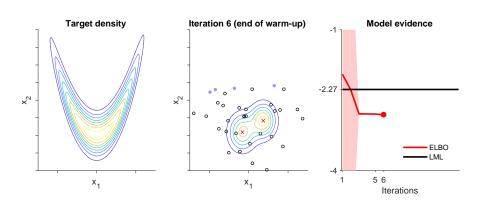
Acerbi, NeurIPS (2018; 2020)



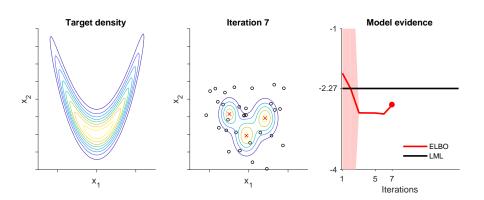
Acerbi, NeurIPS (2018; 2020)



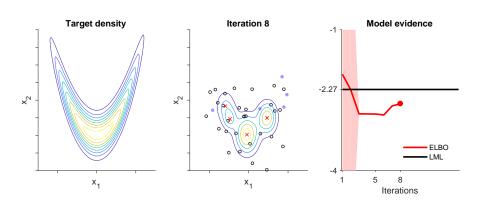
Acerbi, NeurIPS (2018; 2020)



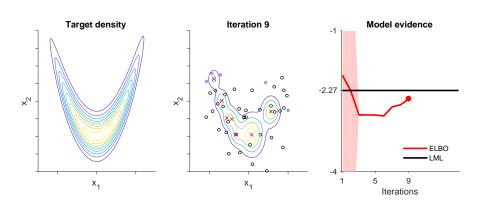
Acerbi, NeurIPS (2018; 2020)



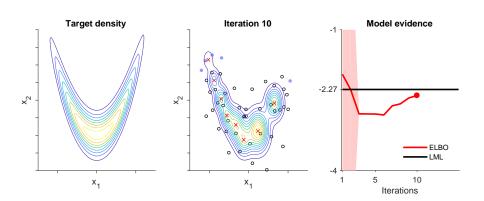
Acerbi, NeurIPS (2018; 2020)



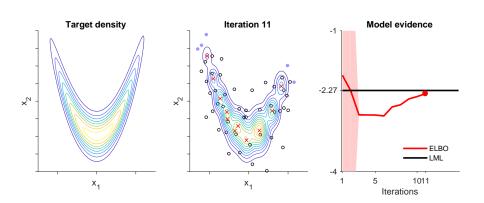
Acerbi, NeurIPS (2018; 2020)



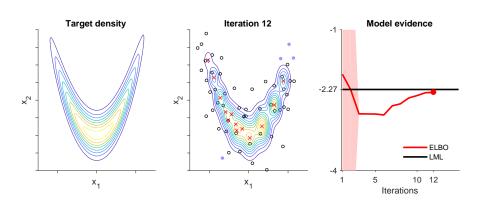
Acerbi, NeurIPS (2018; 2020)



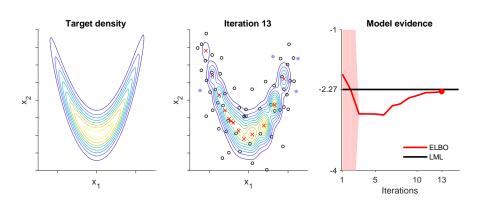
Acerbi, NeurIPS (2018; 2020)



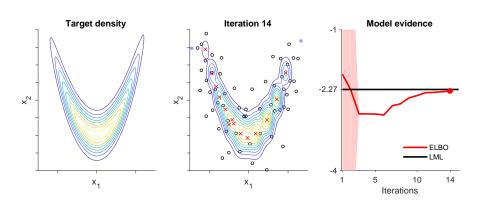
Acerbi, NeurIPS (2018; 2020)



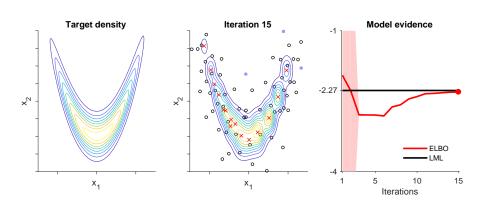
Acerbi, NeurIPS (2018; 2020)



Acerbi, NeurIPS (2018; 2020)



Acerbi, NeurIPS (2018; 2020)



Acerbi, NeurIPS (2018; 2020)

Pick your prior

- ullet In Bayesian inference you need a prior over parameters, p(heta)
- Common choice: independent priors $p(\theta) = \prod_{d=1}^{D} p(\theta_d)$
 - ▶ Choose the prior $p(\theta_d)$ for each parameter
 - ▶ Independent prior does not mean that the posterior is independent!
- Remember that the prior is a probability distribution $\int p(\theta)d\theta=1$
- Okay, but how do I pick a prior for each parameter?

Example priors: uniform box

- Bounded parameter
- Uniform in the full range
- Pros: Easy to define and to justify
- Cons: Non-informative

Example priors: tent

- Bounded parameter
- Uniform in a range, then falls off
- Uses the hard/plausible bounds defined previously
- Pros: Still easy to define, "weakly" informative
- Cons: Need some thought to define the plausible range

Example priors: smoothed tent

- Bounded parameter
- Just like tent prior but with smooth edges
- Pros: Better numerical properties than tent prior
- Cons: More complex to implement (can use provided functions)

OK so we have a posterior what now

. . .

Predictions

. . .

Final slide

- Contact me at luigi.acerbi@helsinki.fi
- Optimization demos: github.com/lacerbi/optimviz

MATLAB toolboxes:

BADS available at github.com/lacerbi/bads

Final slide

- Contact me at luigi.acerbi@helsinki.fi
- Optimization demos: github.com/lacerbi/optimviz

MATLAB toolboxes:

BADS available at github.com/lacerbi/bads

Thanks!

(Time for questions?)