

Bayesian model fitting made easy with Variational Bayesian Monte Carlo

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1 A recap of statistical modelling

- Of models and likelihoods
- The psychometric function

2 Bayesian model fitting

- Refresher of Bayesian inference
- Bayesian inference for model fitting

3 Computing the posterior distribution

- Computing the posterior “by hand”
- Choosing the prior
- Inference algorithms

4 Making use of a Bayesian posterior

The group @ University of Helsinki



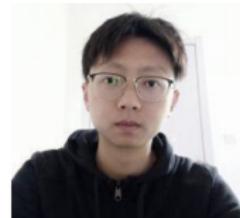
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Postdoc
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PhD student



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PhD student
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Research Assistant

What this is all about

By the end of this tutorial, we will:

Perform Bayesian inference on a real dataset and model from neuroscience

- Recap the basics of **statistical modelling**
- Review the **psychometric model** used in cognitive & neuroscience
- Explain the **Bayesian approach** to model fitting
- Briefly introduce **variational inference** algorithms
- Set up and run **(Py)VBMC** on a real dataset

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What is a model?



The best material model of a cat is another, or preferably the same, cat.

Wiener, *Philosophy of Science* (1945) (with Rosenblueth)

What is a mathematical model?

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- A *family of probability distributions* over possible datasets:

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We need some data

Data from International Brain Laboratory (IBL)



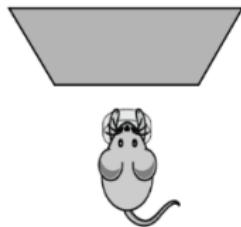
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International Brain Laboratory

Experimental & theoretical neuroscientists collaborating to understand
brainwide circuits for complex behavior

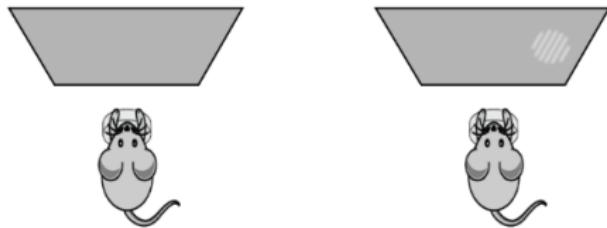
<https://www.internationalbrainlab.com>

IBL Task



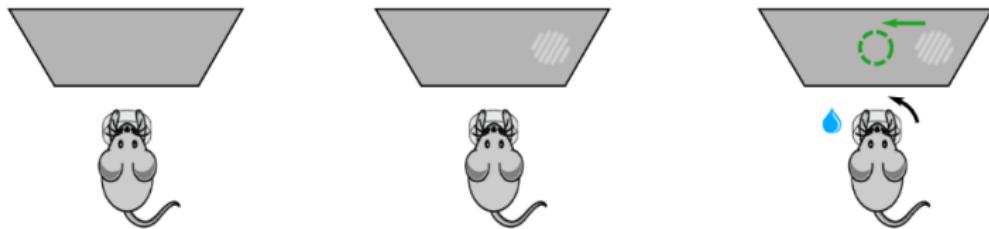
(IBL et al., *eLife*, 2021)

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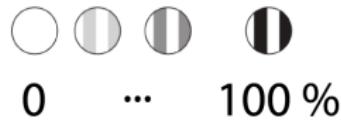
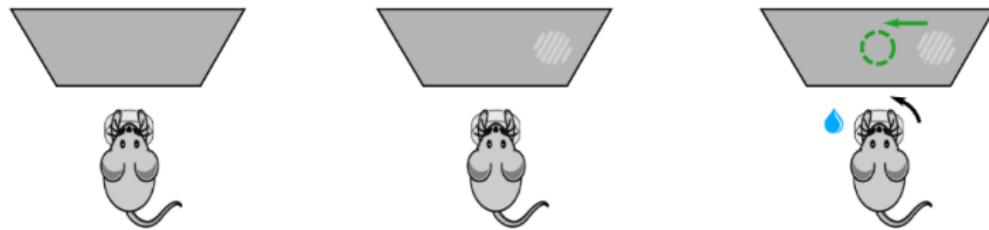
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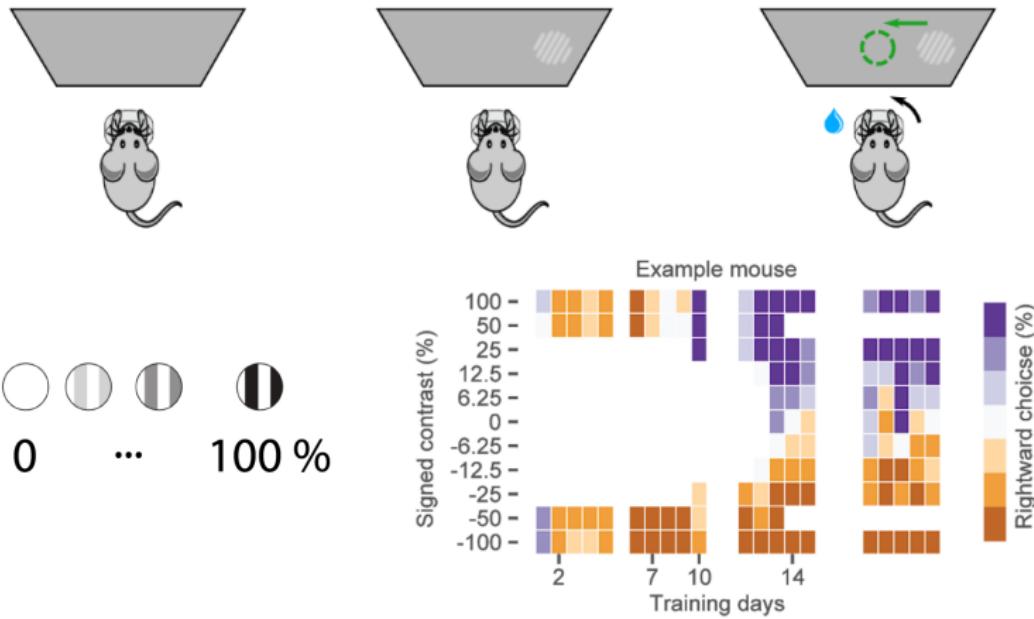
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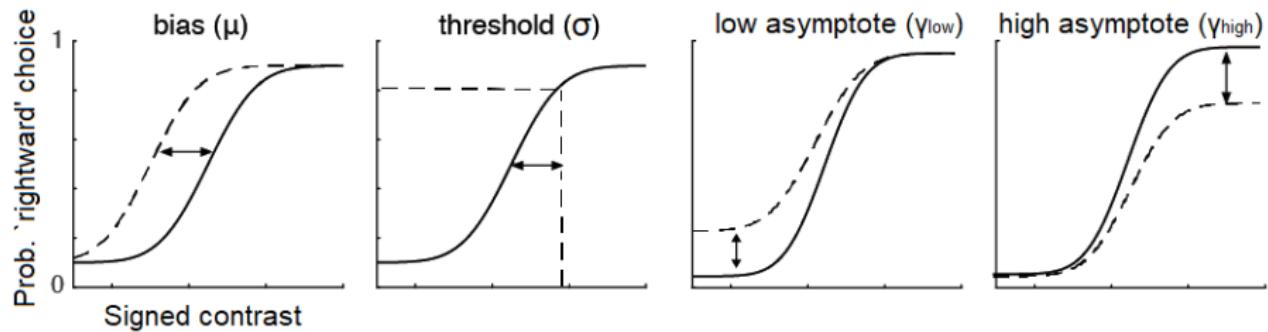


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Hacking time I

Let's have a look at the data

The psychometric function



- Data: (signed contrast, choice) for each trial
- Parameters θ : $(\mu, \sigma, \gamma_{\text{low}}, \gamma^{\text{high}})$

$$p(\text{rightward choice} | s, \theta) = \gamma_{\text{low}} + (1 - \gamma_{\text{low}} - \gamma^{\text{high}}) \cdot F(s; \mu, \sigma)$$

The psychometric function (alt version)

- Default decision process $F(s; \mu, \sigma)$
- Lapses with probability $\lambda \in [0, 1]$ (*lapse rate*)
- If lapse, respond 'rightward' with probability $\gamma \in [0, 1]$ (*lapse bias*)
- Parameters θ : $(\mu, \sigma, \lambda, \gamma)$

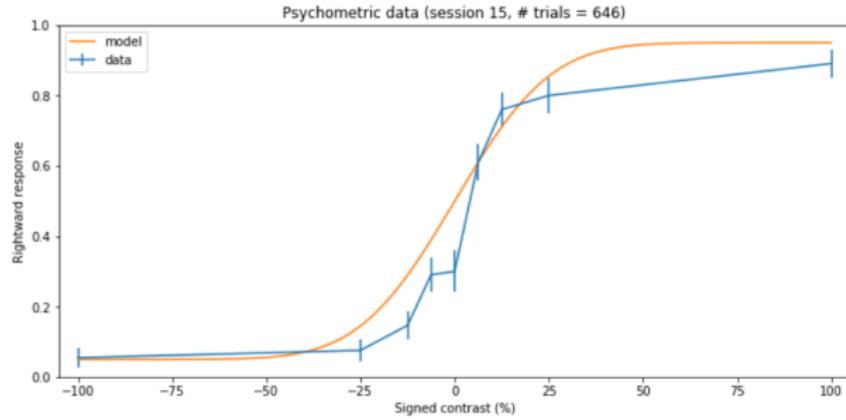
$$p(\text{rightward choice}|s, \theta) = \lambda\gamma + (1 - \lambda) \cdot F(s; \mu, \sigma)$$

Hacking time II

Let's have a look at the psychometric function

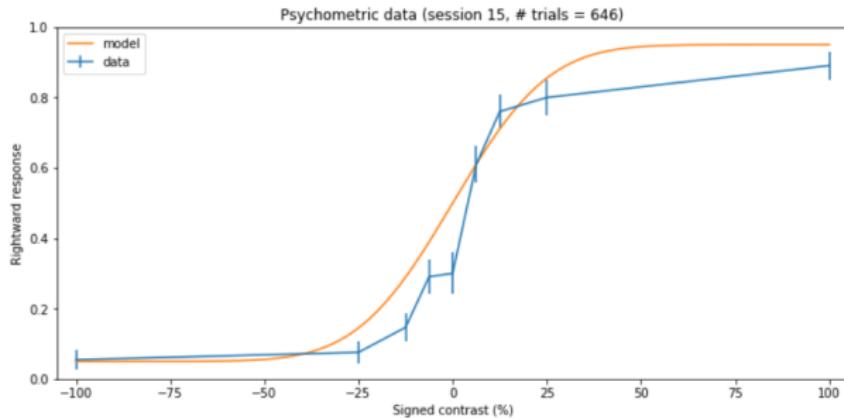
Metric for model fitting

We need a quantity to measure *goodness of fit*



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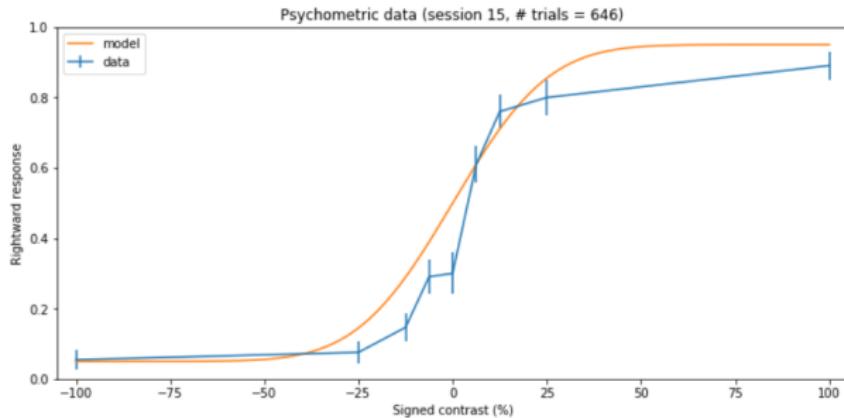
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- Mean squared error?

Metric for model fitting

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- Mean squared error?
- The likelihood $p(\text{data}|\theta) \equiv L(\theta; \text{data})$

Likelihood vs. probability distribution

$p(\text{data}|\theta)$ has two interpretations

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- ➊ $p(\text{data}|\theta)$ is a *probability distribution* as you vary **data** for a fixed θ

Likelihood vs. probability distribution

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- ① $p(\text{data}|\theta)$ is a *probability distribution* as you vary **data** for a fixed θ
- ② $p(\text{data}|\theta) \equiv L(\theta; \text{data})$ is the *likelihood*, a function of θ for fixed data

The (log) likelihood

- For numerical reasons we work with $\log p(\text{data}|\theta) \equiv LL(\theta; \text{data})$

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$$\begin{aligned}\log p(\text{data}|\boldsymbol{\theta}) &= \log \prod_{i=1}^n p_i \left(\mathbf{y}^{(i)} | \mathbf{s}^{(i)}, \boldsymbol{\theta} \right) \\ &= \sum_{i=1}^n \log p_i \left(\mathbf{y}^{(i)} | \mathbf{s}^{(i)}, \boldsymbol{\theta} \right)\end{aligned}$$

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- Model building: Write function with
 - ▶ Input: θ and data
 - ▶ Output: $\log p(\text{data}|\theta)$

Hacking time III

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My rule.

$$p(\theta|\text{data}) = \frac{p(\text{data}|\theta)p(\theta)}{p(\text{data})}$$

What is Bayesian inference?



$$\overbrace{p(\theta|data)}^{\text{posterior}} = \frac{\underbrace{p(data|\theta)}_{\text{likelihood}} \underbrace{p(\theta)}_{\text{prior}}}{\underbrace{p(data)}_{\text{evidence}}}$$

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Bayesian probability

- We are treating both data and θ as **random variables**.
- Probability as **degree of belief**.

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

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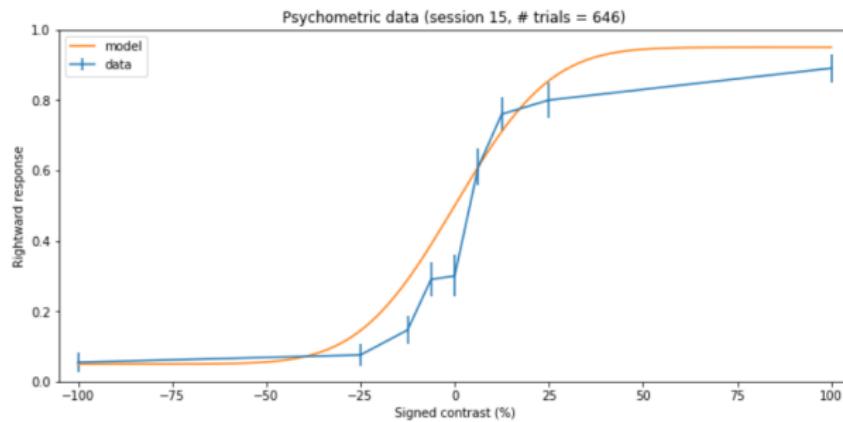
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Data and model

- Same data from before (IBL mouse behavioral data)
- Same model as before (psychometric function model)



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- We assume a **uniform-box prior $p(\sigma)$** for $\sigma \in [1, 100]$

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- The normalization is $Z = \int p(\text{data} | \mu_*, \sigma, \lambda_*, \gamma_*) p(\sigma) d\sigma$

Hacking time IV

Let's do Bayesian inference by hand!

Preparing for inference

- *Domain* of parameter vector $\boldsymbol{\theta} = (\theta_1, \theta_2, \dots, \theta_D) \in \Theta$

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- Consider reparameterizations to achieve
 - ▶ Uniformity of effects across parameter range
 - ▶ Independence between parameters
 - ▶ Parameterization matters

Choose your prior

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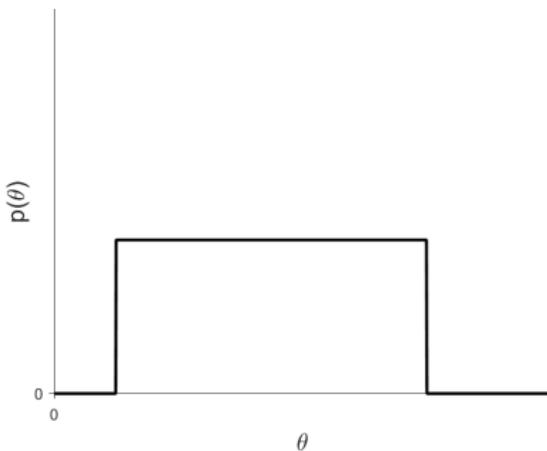
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 - ▶ Choose the prior $p(\theta_d)$ for each parameter
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- Remember that the prior is a probability distribution $\int p(\theta)d\theta = 1$
- Okay, but how do I pick a prior for each parameter?

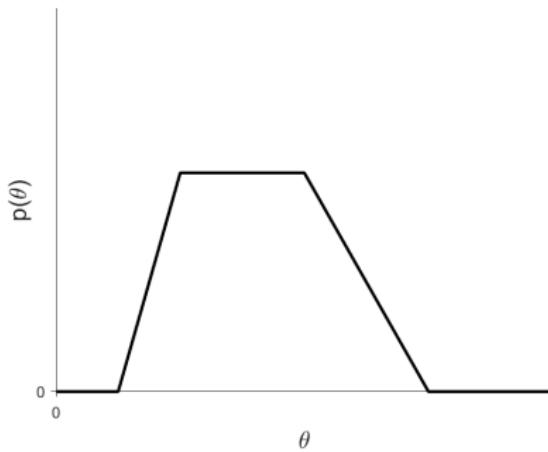
Example priors: uniform box

- Bounded parameter
- Uniform in the range (lower/upper bound), zero outside
- **Pros:** Easy to define and to justify (if wide bounds)
- **Cons:** Non-informative



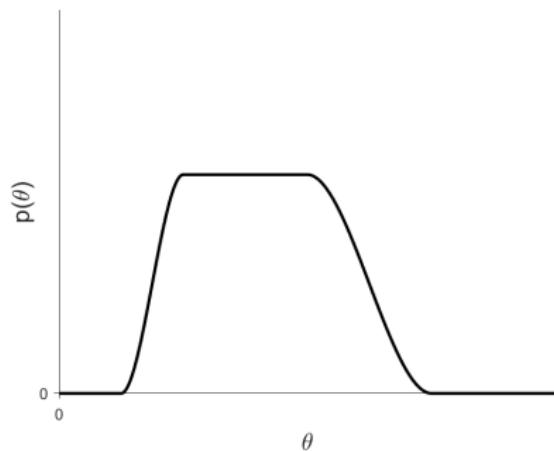
Example priors: tent/trapezoidal

- Bounded parameter
- Uniform in a range, then falls off, zero outside the bounds
- Can use 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/trapezoidal

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



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- Gamma distributions
- Half-truncated Gaussians or t distributions

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Hot take:

- I generally recommend **bounded** parameters
- Half-bounded / unbounded parameters \Rightarrow numerical issues

Hacking time V

Let's have a look at the priors.

Bayesian inference done?

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- Not really – a grid only works in low dimension ($D \sim 1 - 4$)
- 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**

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 - ▶ 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!**
 - ▶ Need to compute a full distribution instead of a single point

Main families of general-purpose inference algorithms

- ① Markov Chain Monte Carlo (MCMC)
- ② Variational inference

(there are others)

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- Various rules for drawing $\theta_{n+1} | \theta_n$ depending on the algorithm
 - ▶ These will generally depend on $p(\theta_n, \text{data})$, $p(\theta_{n+1}, \text{data})$

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 - ▶ These will generally depend on $p(\theta_n, \text{data})$, $p(\theta_{n+1}, \text{data})$
- **Output:** A set of samples $\theta_0, \dots, \theta_N$

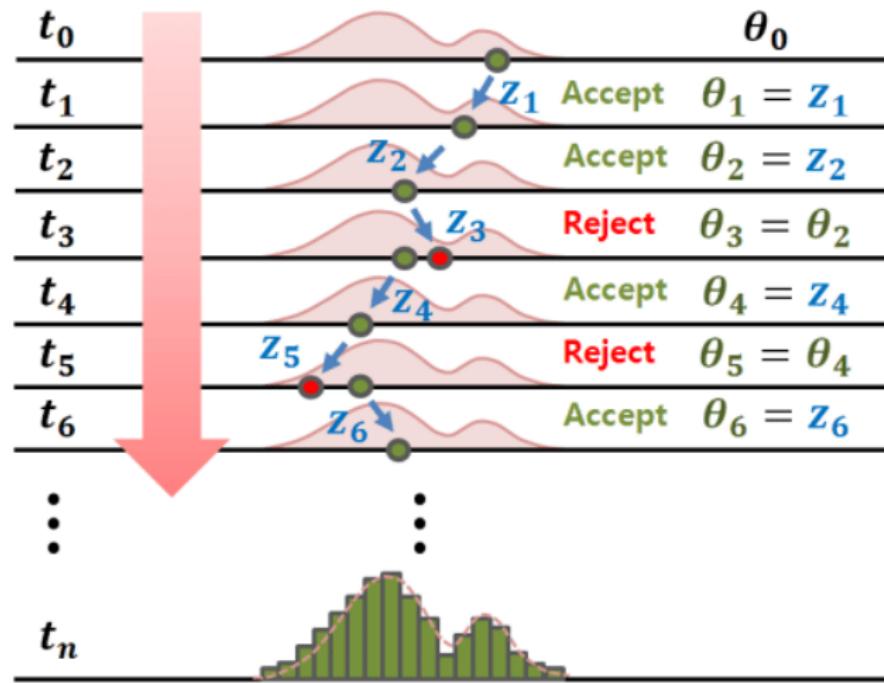
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 - ▶ In practice, lot of tweaking to ensure **convergence** of the Markov chain
 - ▶ State-of-the-art MCMC methods are (to a degree) **self-tuning**
 - ▶ Still a lot of tweaking involved

Example MCMC algorithm: Metropolis-Hastings



Source: Jin et al. (2019)

Variational inference

- Approximate $p(\theta|\text{data})$ with $q_\phi(\theta)$

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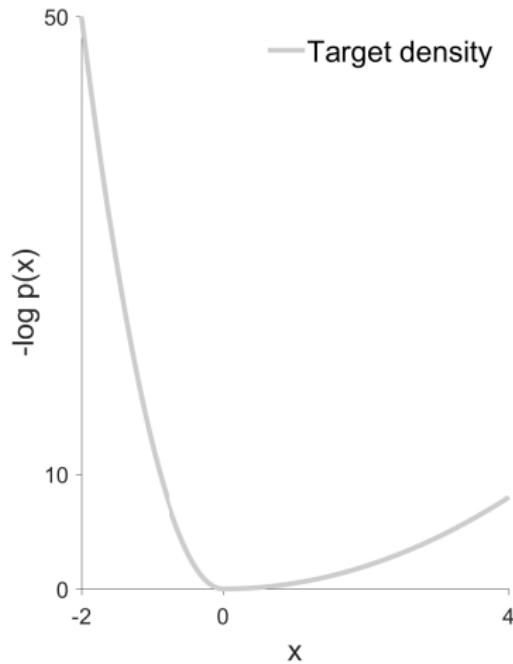
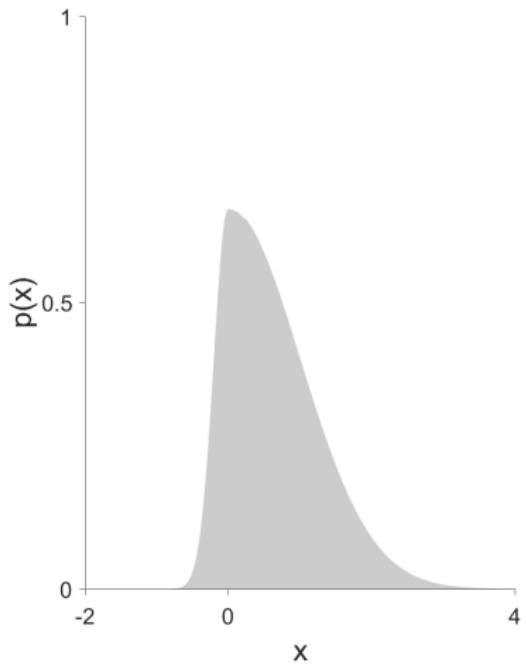
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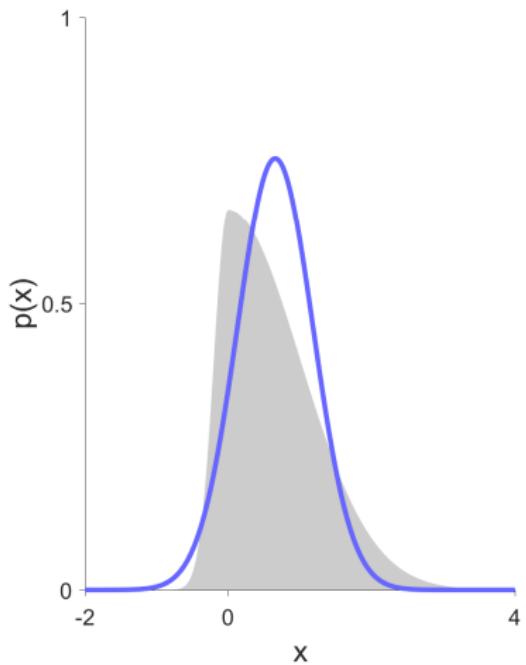
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VI casts Bayesian inference into optimization + integration

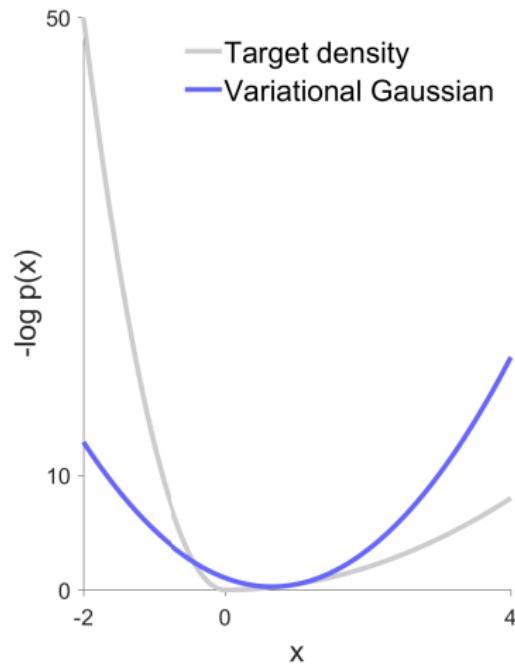
Variational inference: example



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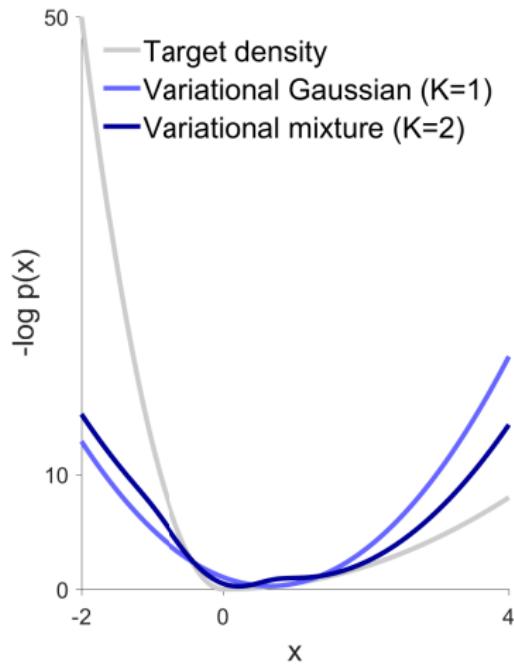
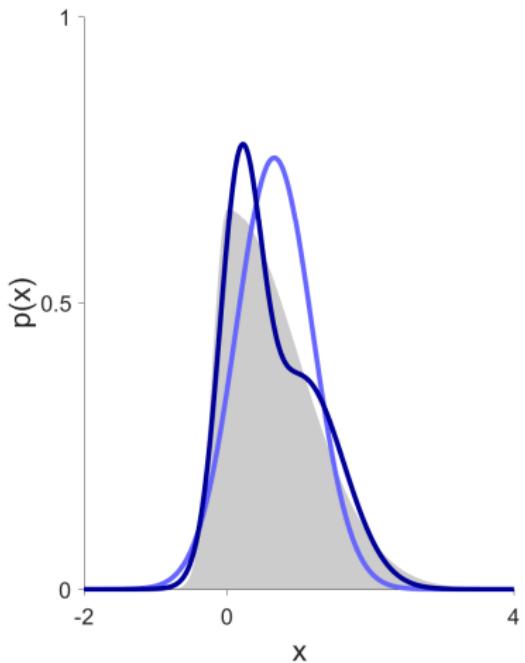


$$q_\phi(x) = \mathcal{N}(x, \mu, \sigma^2)$$



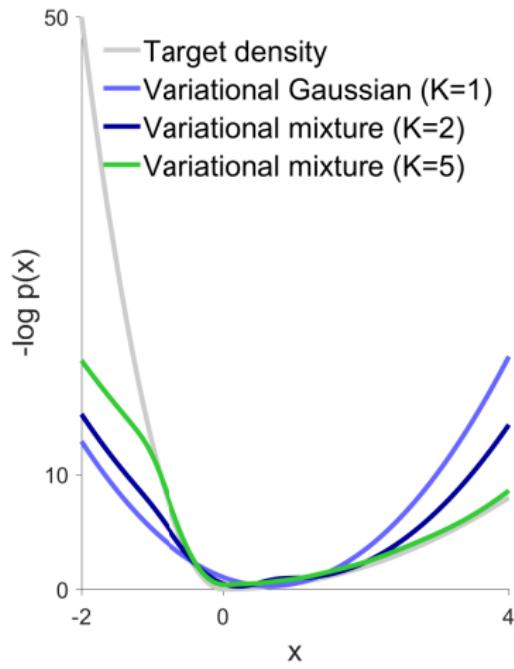
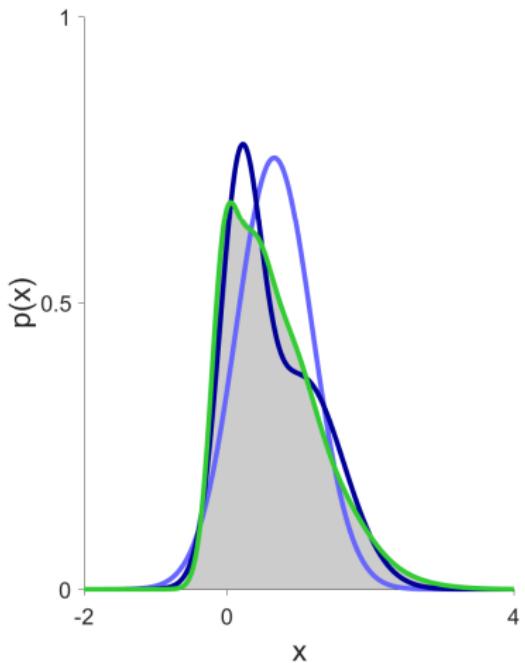
$$\phi = (\mu, \sigma^2)$$

Variational inference: example



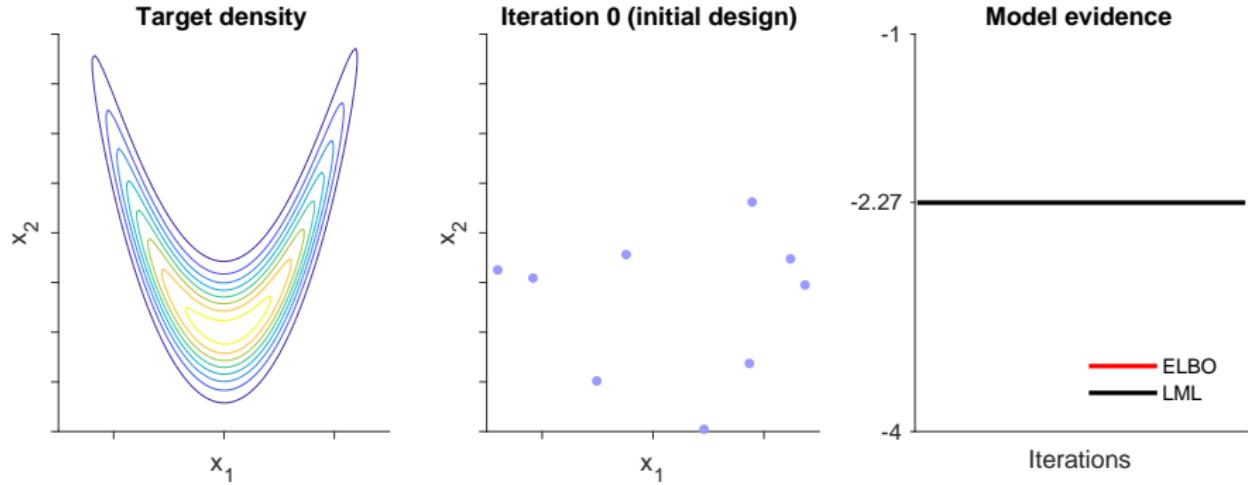
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Variational inference: example



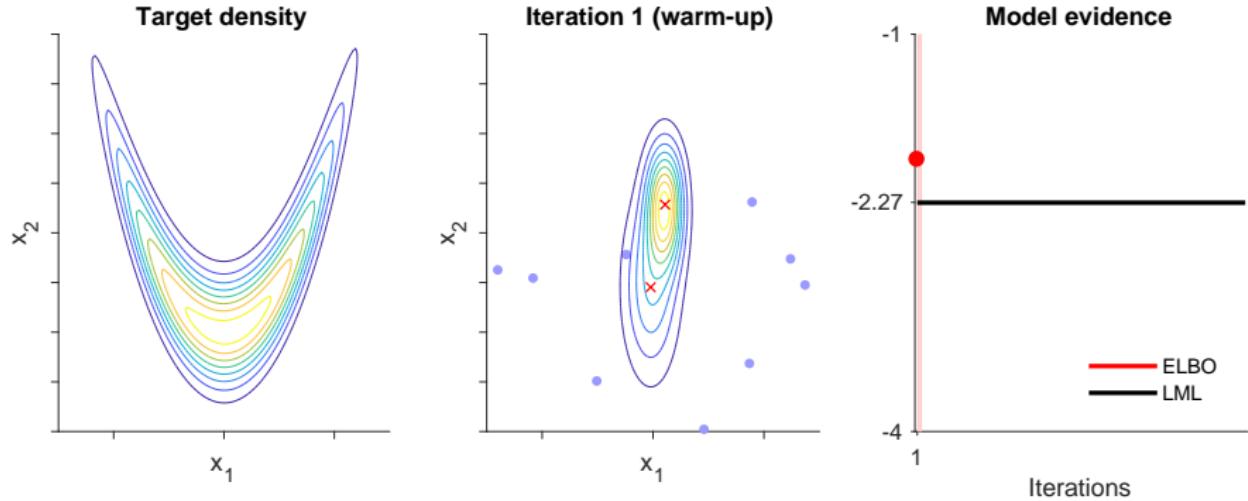
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Variational Bayesian Monte Carlo (VBMCMC)



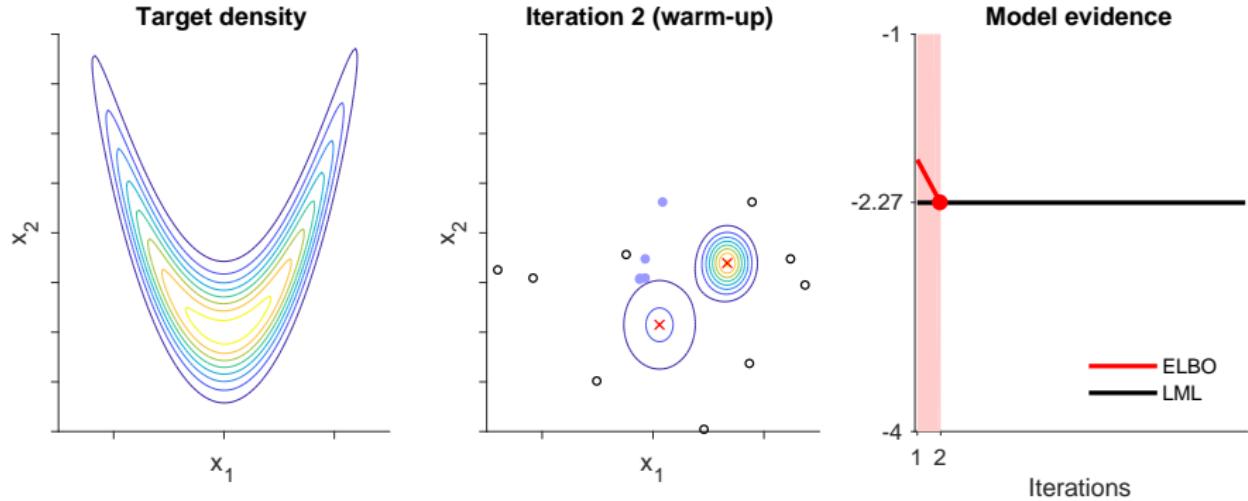
Acerbi, *NeurIPS* (2018; 2020)

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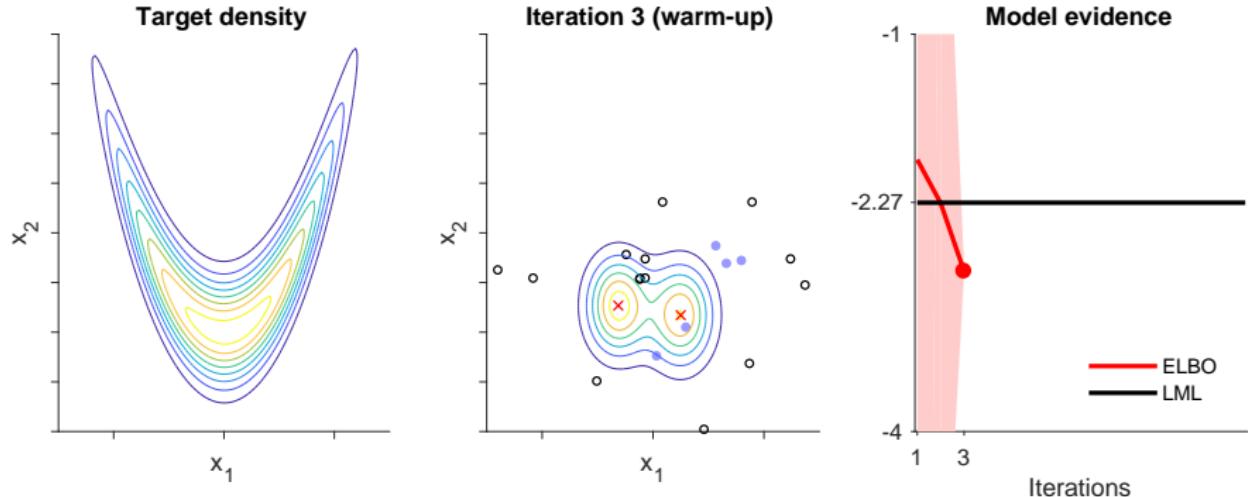
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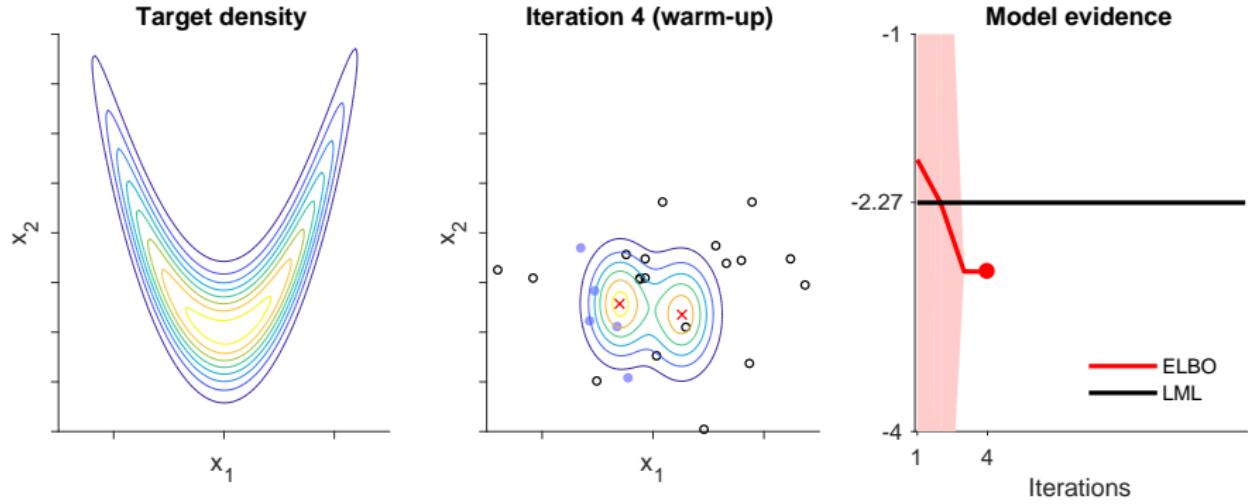
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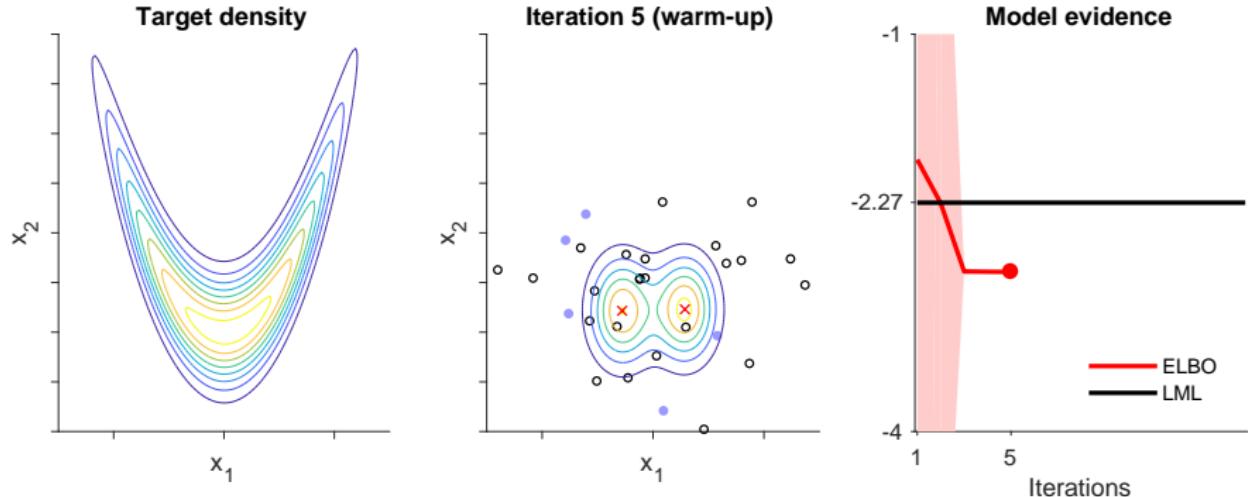
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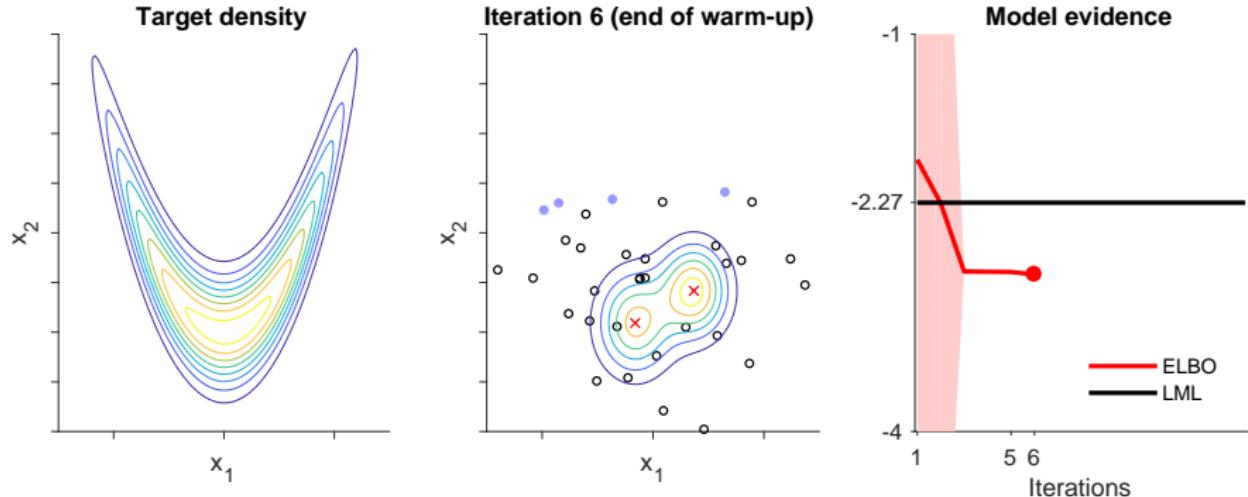
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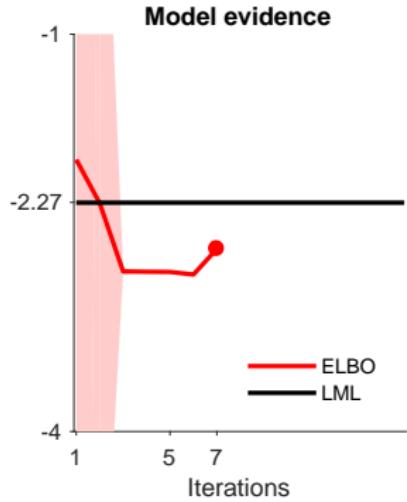
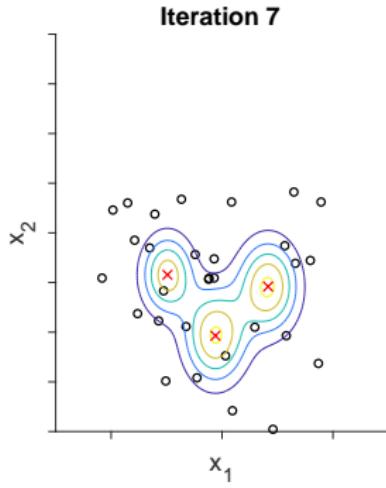
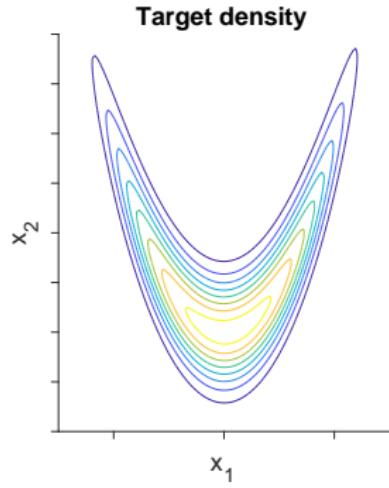
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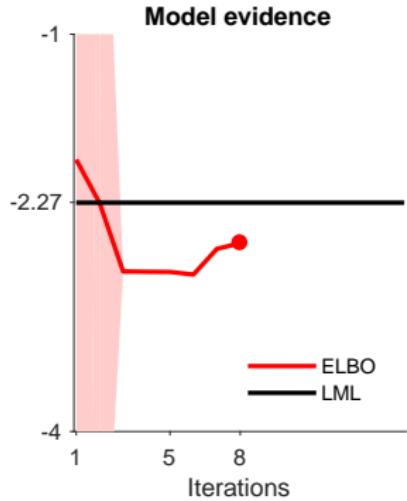
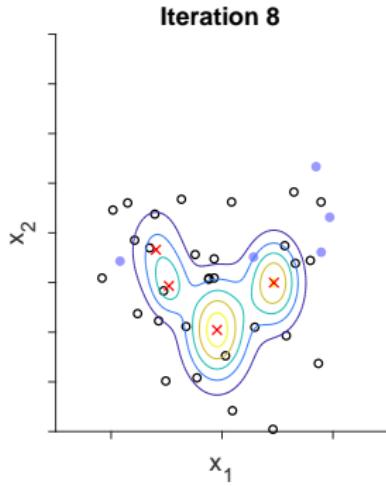
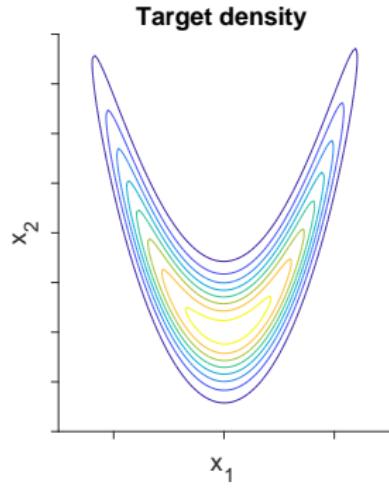
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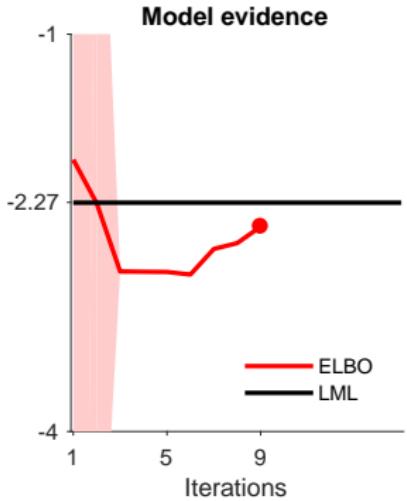
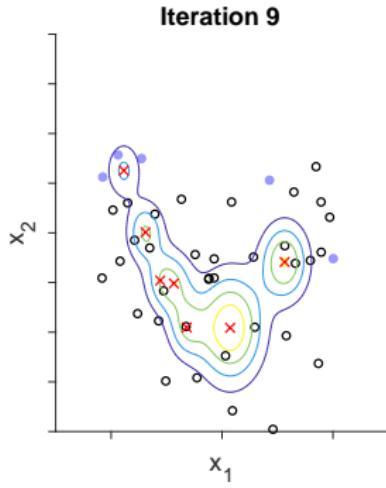
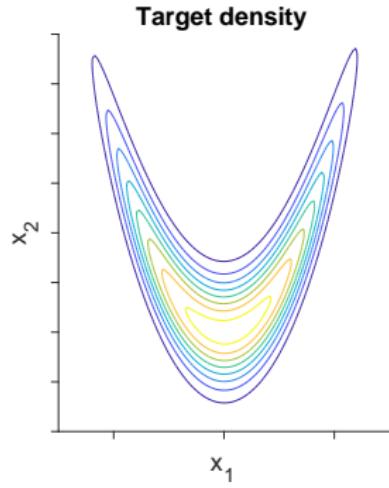
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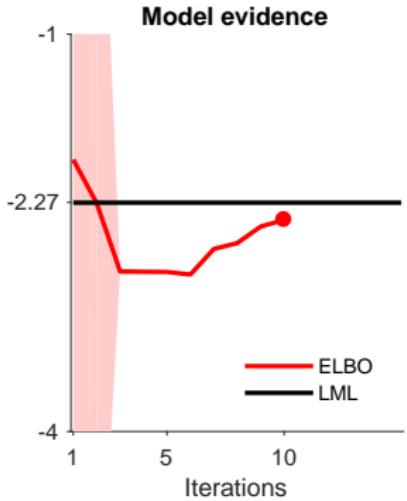
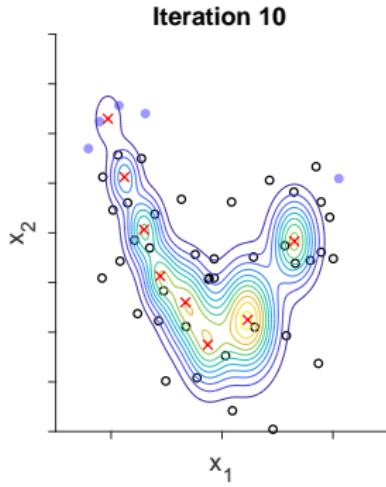
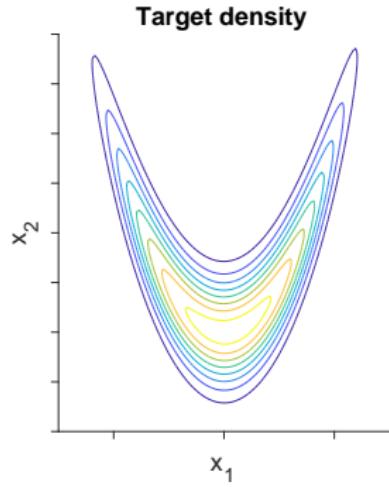
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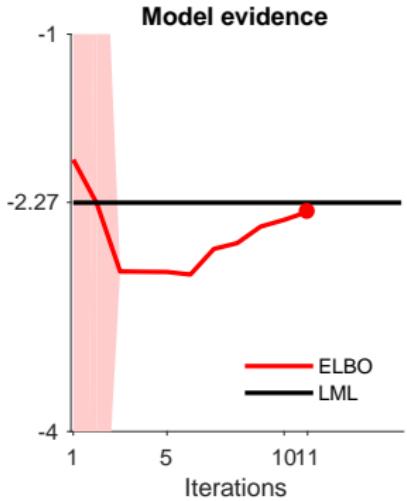
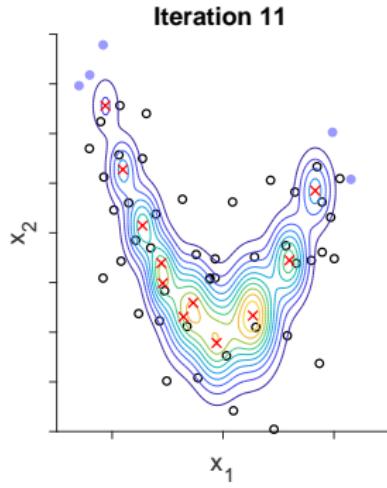
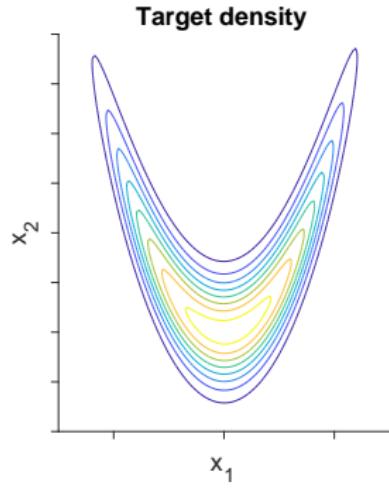
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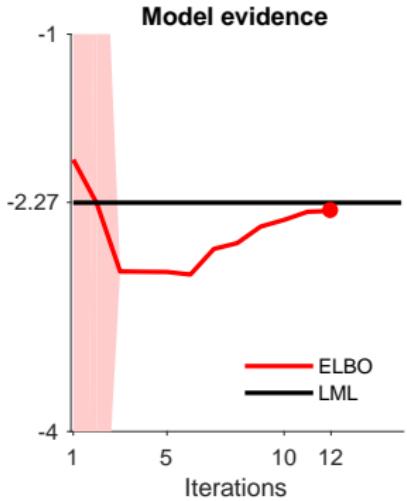
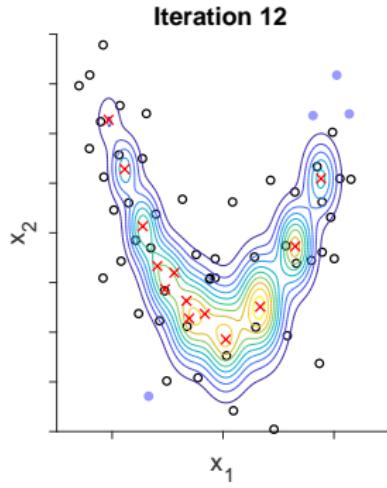
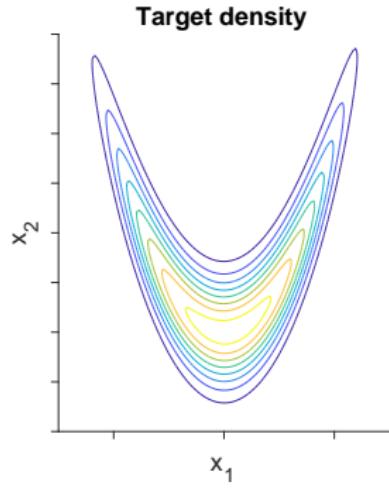
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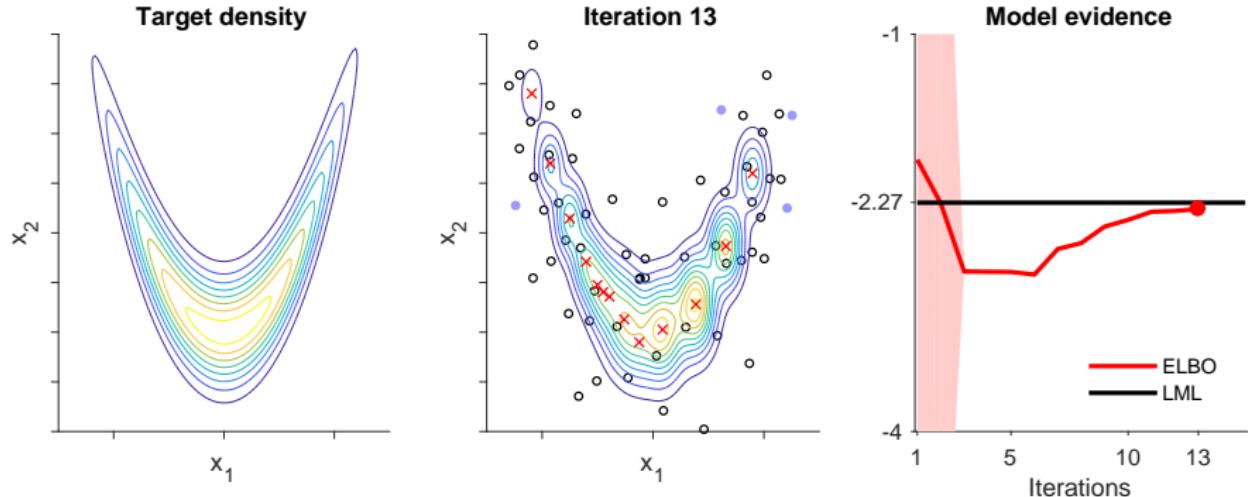
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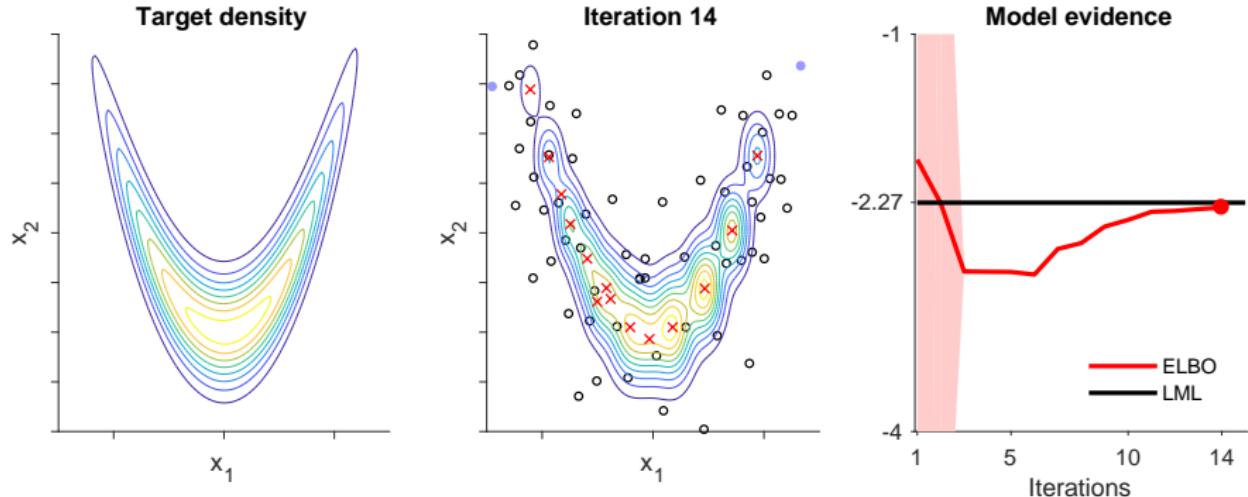
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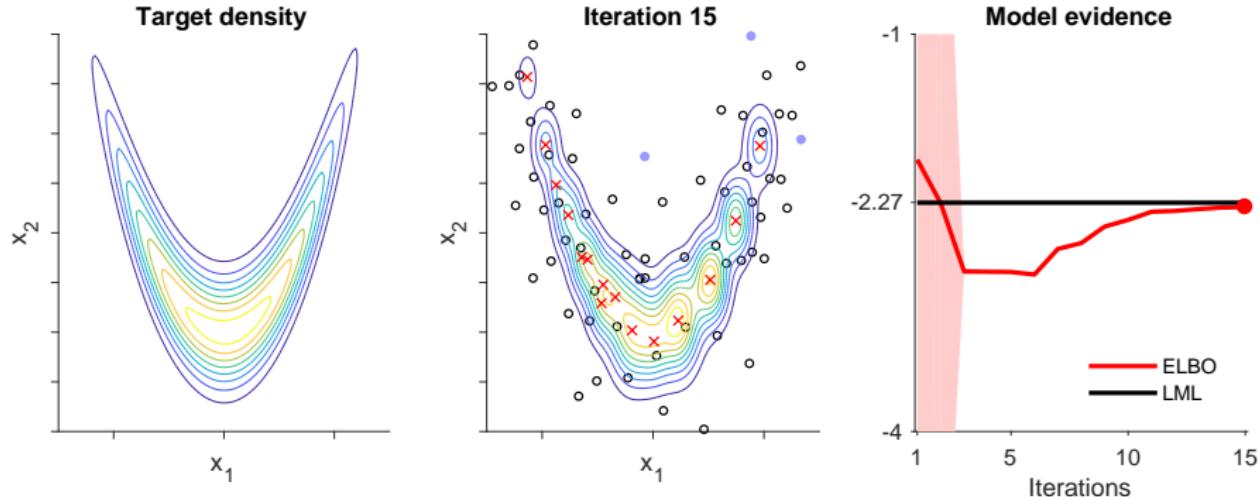
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Hacking time VI

Let's set up and run a Bayesian inference algorithm

1 A recap of statistical modelling

- Of models and likelihoods
- The psychometric function

2 Bayesian model fitting

- Refresher of Bayesian inference
- Bayesian inference for model fitting

3 Computing the posterior distribution

- Computing the posterior “by hand”
- Choosing the prior
- Inference algorithms

4 Making use of a Bayesian posterior

OK so we have a posterior what now

OK so we have a posterior what now

- Visualize the posterior distribution
- Represent uncertainty (e.g., credible intervals)
- Make posterior predictions (“Bayesian fit”) and compare to data

Hacking time VII

Let's use this posterior

What we learnt

By the end of this tutorial, we will:

Perform Bayesian inference on a real dataset and model from neuroscience

- Recap the basics of **statistical modelling**
- Review the **psychometric model** used in cognitive & neuroscience
- Explain the **Bayesian approach** to model fitting
- Briefly introduce **variational inference** algorithms
- Set up and run **(Py)VBMC** on a real dataset

This was a lot

This was a lot

You deserve another cat picture



This was a lot

You deserve another cat picture



- Bayesian model fitting could fill an entire year
- This tutorial is just the first steps on the Bayesian way

Final slide

Contacts:

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- Twitter: @AcerbiLuigi

Acknowledgments:

- The PyVBFMC development team
- FCAI

Code:

- VBFMC (MATLAB): github.com/lacerbi/vbmc
- PyVBFMC: github.com/acerbilab/pyvbmc



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Questions?