Introduction to Modeling & Model Fitting for Psychophysics and Neuroscience

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Department of Basic Neuroscience, University of Geneva
International Brain Lab

May, 2019

1. Introduction
   - Of models and likelihoods
2. Model fitting via optimization
   - An introduction to optimization
   - Optimization algorithms
   - Bayesian Optimization and BADS
3. Model selection via point estimates and little more
   - AIC/AICc
   - BIC
   - Cross-validation (CV)
   - Marginal likelihood and Laplace approximation
4. A couple of slides about MCMC

What is a model?

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

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

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  - $p(\text{data}|\boldsymbol{\theta})$ is a *probability density* as you vary data for a fixed $\boldsymbol{\theta}$
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  - Think about the data generation process!

Example: Psychometric function

Task: heading direction 'discrimination' task

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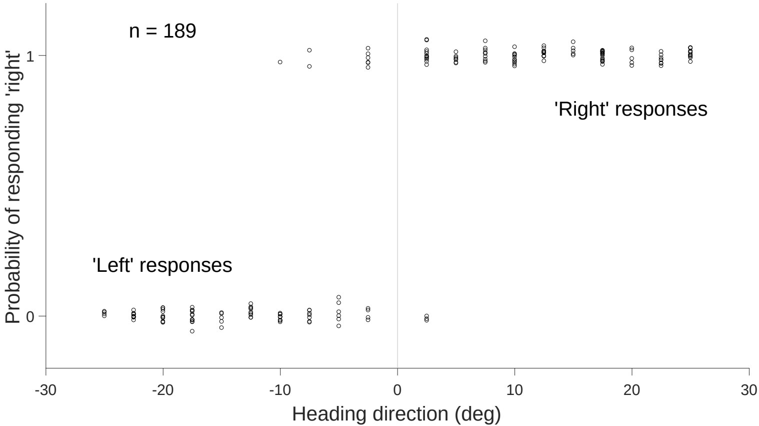

(data from Acerbi et al., *PLoS Comput Biol*, 2018)

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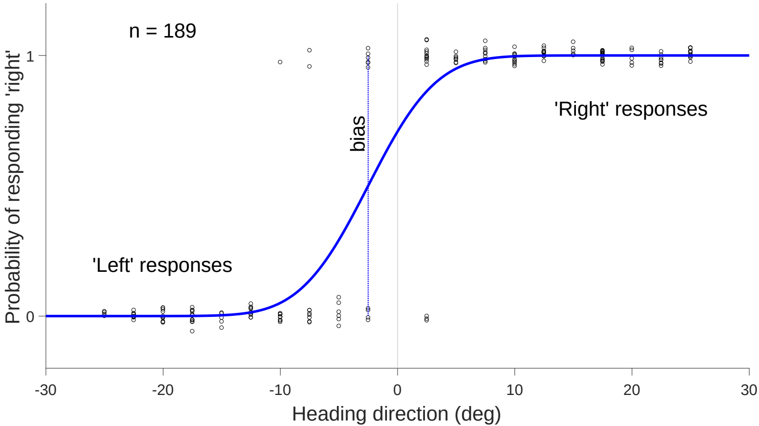

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\begin{aligned}
\log p\left(\text{data}|\boldsymbol{\theta}\right) &= \log p(\boldsymbol{y}^{(1)}, \ldots, \boldsymbol{y}^{(n)}|\boldsymbol{\theta}) \\
&= \log \prod_{i=1}^{n} p_i\left(\boldsymbol{y}^{(i)}|\boldsymbol{\theta}\right) \\
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- Write function that takes data and $\boldsymbol{\theta}$ as input arguments and returns $\log p(\text{data}|\boldsymbol{\theta})$

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- For $n \to \infty$ converges to MLE (if $p(\hat{\boldsymbol{\theta}}_{\text{ML}}) \neq 0$)
- *Full posterior*: informative about parameter uncertainty and trade-offs
- *Maximum-a-posteriori (MAP)*: $\hat{\boldsymbol{\theta}}_{\text{MAP}} = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\text{data})$

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Approximate/full Bayesian posterior

- Things are a tad more complicated...
- Standard approach: Markov-Chain Monte Carlo (MCMC) sampling

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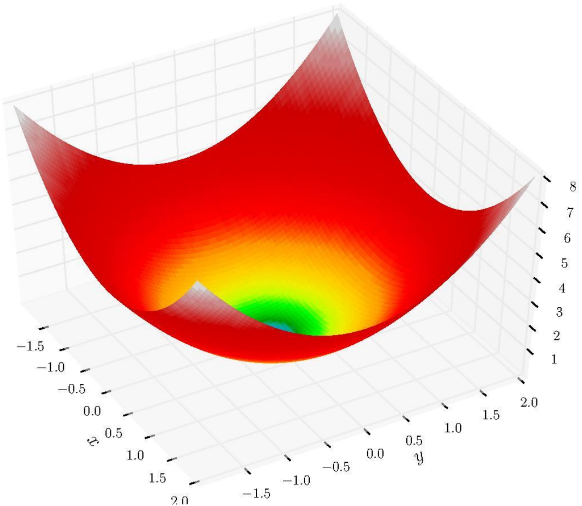
- General case: $f(\boldsymbol{x})$ is a *black box*

How hard can it be?



Source: Wikimedia Commons

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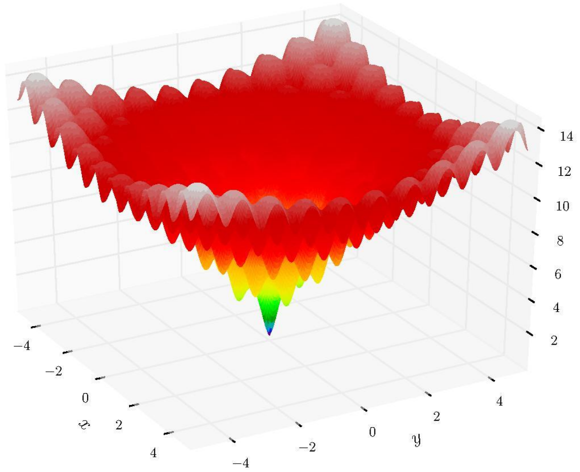

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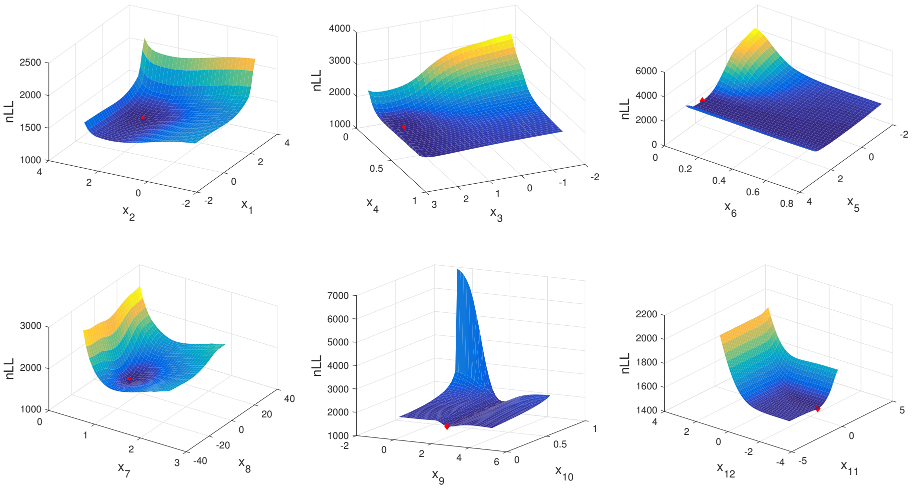

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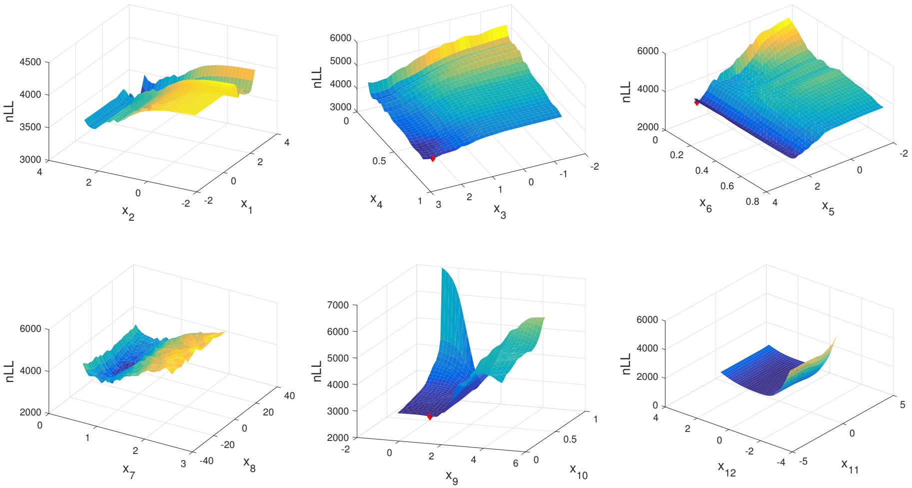

How hard can it be?

neval	x_1	x_2	$f(\mathbf{x})$
1	-0.500	2.500	508.500
2	-0.525	2.500	497.110
3	-0.500	2.625	566.313
4	-0.525	2.375	443.063
5	-0.537	2.250	386.953
6	-0.563	2.250	376.320
7	-0.594	2.125	316.702
8	-0.606	1.875	229.824
9	-0.647	1.563	133.598
10	-0.703	1.438	91.847
11	-0.786	1.031	20.292
12	-0.839	0.469	8.918
13	-0.962	-0.359	168.785
14	-0.978	-0.063	107.796
15	-0.895	0.344	24.553
16	-0.730	1.156	41.905
17	-0.854	0.547	6.760
18	-0.907	-0.016	73.917
19	-0.816	0.770	4.366
20	-0.831	0.848	5.818
21	-0.793	1.070	22.655
22	-0.839	0.678	3.448
23	-0.824	0.600	3.955
24	-0.846	0.508	7.766
25	-0.824	0.704	3.391
26	-0.839	0.782	4.004
27	-0.828	0.645	3.497
28	-0.835	0.737	3.523
29	?	?	?

Optimization can be hard

1. Optimizer does not see the landscape!
2. Multiple local minima or saddle points ('non-convex')
3. Expensive function evaluation
4. Noisy function evaluation
5. Rough landscape (numerical approximations, etc.)

Preparing for optimization

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

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

Which algorithm to use?

Deterministic		MATLAB Toolbox
Nelder-Mead	`fminsearch`	—
Quasi-Newton methods	`fminunc`,`fmincon`	Optimization
Direct search	`patternsearch`	Global Optimization
Multi-level Coordinate Search	`mcs`	— (free)
Stochastic		
Simulated Annealing	`simulannealbnd`	Global Optimization
Genetic Algorithm	`ga`	Global Optimization
Particle Swarm	`particleswarm`	Global Optimization
CMA-ES	`cmaes`	— (free)
Bayesian Optimization	`bayesopt`	Stats & ML
Bayesian Adaptive Direct Search	`bads`	— (free)

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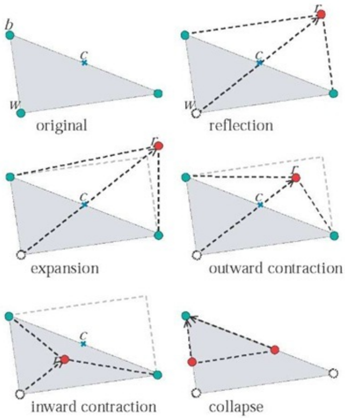
Nelder-Mead (`fminsearch`)

J. A. Nelder & R. Mead, A simplex method for function minimization (1965)



Source: Encyclopedia of Artificial Intelligence (2009)

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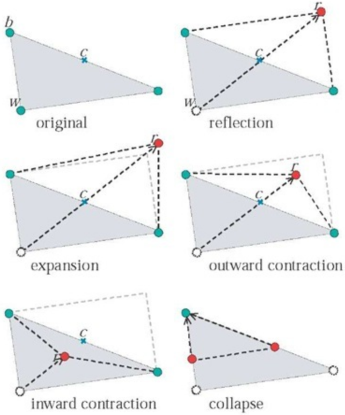

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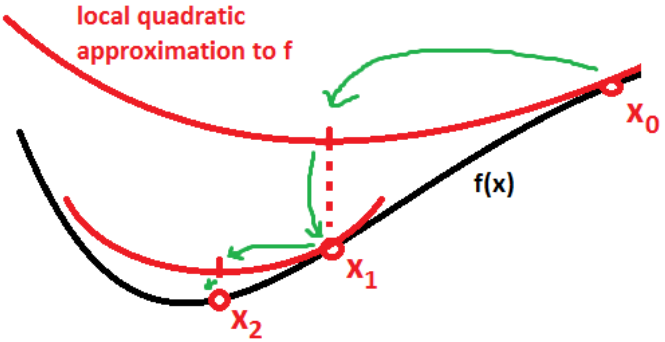
Bounded optimization: `fminsearchbnd` (John d'Errico)

Newton method



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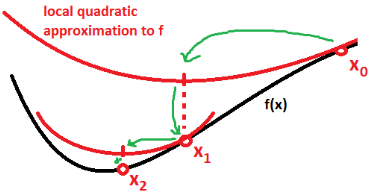

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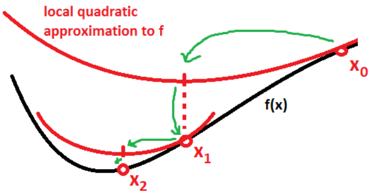
Needs the inverse of the curvature (inverse Hessian)
Very expensive in high dimension

Quasi-Newton methods (`fminunc`,`fmincon`)

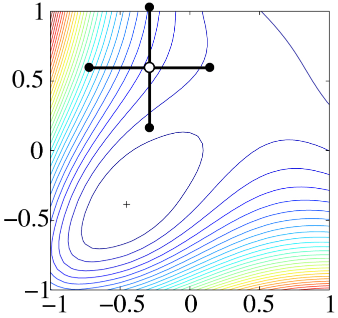


Source: StackExchange

Approximate Hessian (DFP) or inverse Hessian (BFGS) via gradient
Very fast and efficient on smooth problems

Direct search (`patternsearch`)

R. Hooke and T.A. Jeeves, "Direct search" solution of numerical and statistical problems (1961)



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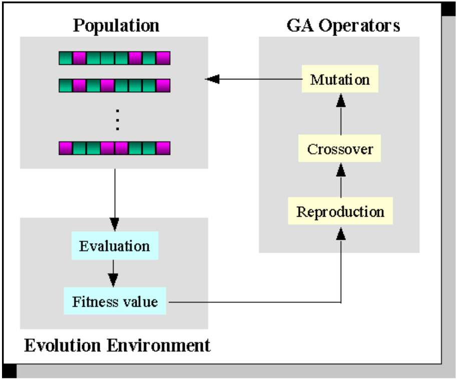
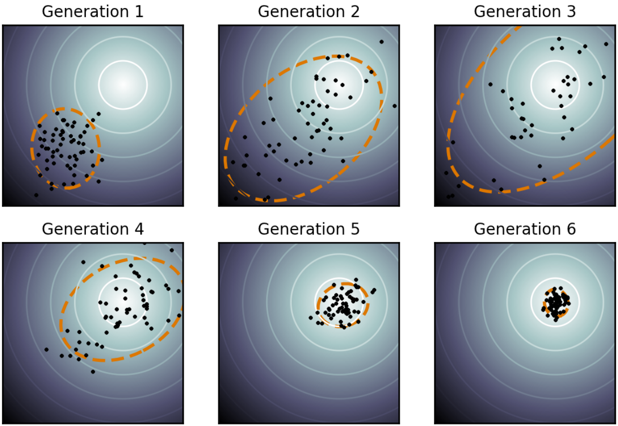


Source: An Educational GA Learning Tool (IEEE)

Cov. Matrix Adaptation - Evolution Strategies (cmaes)

[*] N. Hansen, S. D. Müller, P. Koumoutsakos, Reducing the time complexity of the derandomized evolution strategy with covariance matrix adaptation (CMA-ES), (2003)



Source: Wikipedia

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5. `goto 2`

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- Scales badly with n, computation time $\sim O(n^3)$
- Performance depends on quality of global approximation

Bayesian Adaptive Direct Search (`bads`)

- Combines Mesh-Adaptive Direct Search (MADS) with Bayesian Optimization (BO)

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Algorithm

1. Take as input f, `x0`, `LB`, `UB`, `PLB`, `PUB`
2. Evaluate f on an initial design and $x \leftarrow \arg\min_i f(x_i)$
3. Until convergence or `MaxFunEvals` do
    - Poll Step: Evaluate up to $2D$ points around x, update x
    - (Train Step: Train GP on neighborhood of x)
    - Search Step: Perform multiple iterations of BO in neighborhood of x

Acerbi & Ma, NeurIPS (2017)

Bayesian Adaptive Direct Search (`bads`)

- Good for moderately costly ($\gtrsim 0.1$ s) or noisy functions
- Scales okay with n (uses only local neighborhood)
- Local approximation deals with nonstationarity
- Explicit support for noise

Optimization: The take-home slide

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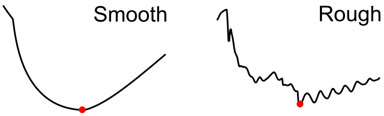

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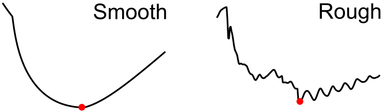

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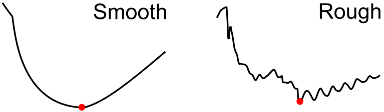

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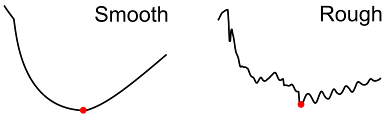

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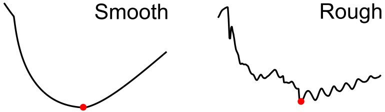

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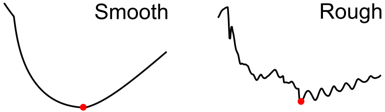

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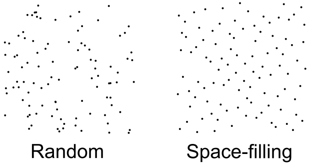

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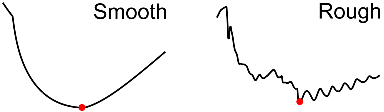

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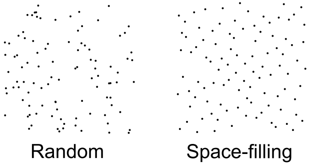

- If you can afford many fcn evals... consider MCMC instead of optimization!

1 Introduction

- Of models and likelihoods

2 Model fitting via optimization

- An introduction to optimization
- Optimization algorithms
- Bayesian Optimization and BADS

3 Model selection via point estimates and little more

- AIC/AICc
- BIC
- Cross-validation (CV)
- Marginal likelihood and Laplace approximation

4 A couple of slides about MCMC

The problem

- Several models $\mathcal{M}_1, \ldots, \mathcal{M}_M$
- For each $\mathcal{M}_m$ we know $\log p(\text{data}|\hat{\boldsymbol{\theta}}_{\text{ML}}, \mathcal{M}_m)$
- Find the *best* model

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Typical form of model comparison metric

$$MCM(\text{data}, \mathcal{M}_m) \propto \overbrace{\log p(\text{data}|\hat{\boldsymbol{\theta}}_{\text{ML}}, \mathcal{M}_m)}^{\text{Goodness of fit}} - \overbrace{f\left(\text{data}, \mathcal{M}_m\right)}^{\text{Model complexity}}$$

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Notation:

- k number of parameters
- n number of trials

Akaike information criterion (AIC)

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$$\mathrm{AIC} = \log p(\mathrm{data}|\hat{\theta}_{\mathrm{ML}}, \mathcal{M}_m) - k$$

Akaike information criterion (AIC)

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$$\mathrm{AIC} = -2 \log p(\mathrm{data}|\hat{\theta}_{\mathrm{ML}}, \mathcal{M}_m) + 2k$$

Akaike information criterion (AIC)

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- **Goal:** Find best predictive model
  - Does not assume $\mathcal{M}_{\text{true}}$ is in the model set
  - Find closest statistical approximation (lowest KL-divergence from $\mathcal{M}_{\text{true}}$)

Akaike information criterion (AIC), part two

Why penalty is k?

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Why penalty is k?

(Do you really want to know?)

Akaike information criterion (AIC), part two

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$$\mathcal{M}_m \text{ that maximizes } \left\langle \log p(y|\hat{\theta}_{\text{ML}}, \mathcal{M}_m) \right\rangle_{y \sim p_{\text{true}}}$$

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- Bias correction per trial $\approx \frac{1}{n} k$
- Assumptions:
  - CLT (large n), log likelihood $\sim$ quadratic near MLE
  - p close to p_{true}
  - model identifiable (bijective mapping $\boldsymbol{\theta} \longleftrightarrow p(y|\boldsymbol{\theta})$)

Corrected Akaike information criterion (AICc)

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- Correction derived for linear models
  - Still, better than AIC for small sample size

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- *Consistent:* for $n \to \infty$ selects $\mathcal{M}_{\text{true}}$ if $\mathcal{M}_{\text{true}}$ in model set

Cross-validation

- **Goal:** Find best predictive model

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  - AIC tends to LOO
- Essentially no assumptions (but caveats)
- Computationally expensive

Marginal likelihood

Can we be more Bayesian?

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(Not really, with only point estimates)

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  - Can be good or terrible, depending on posterior and on the basis

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  - Leave-one-out CV can be computed easily in some cases

One slide about MCMC

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- Use MCMC

Another slide about MCMC

Another slide about MCMC

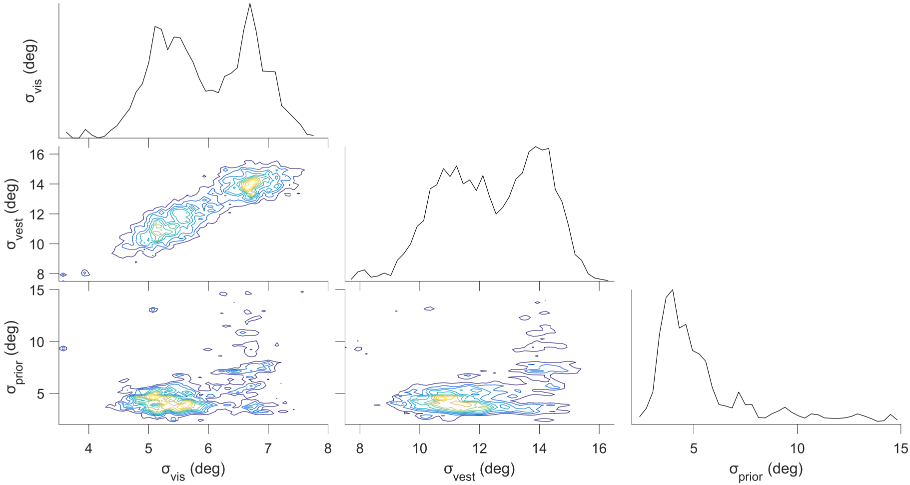

Figure made with `cornerplot.m`, by Will T. Adler

Another slide about MCMC

- Check for parameter uncertainty, trade-offs, identifiability
  - Deeper understanding of your model
  - Robustness of claims (Acerbi, Ma, Vijayakumar, 2014)

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Use *slice sampling* (Neal, 2003)

Variational Bayesian Monte Carlo

Alternative to MCMC (for low-D, moderately costly problems)

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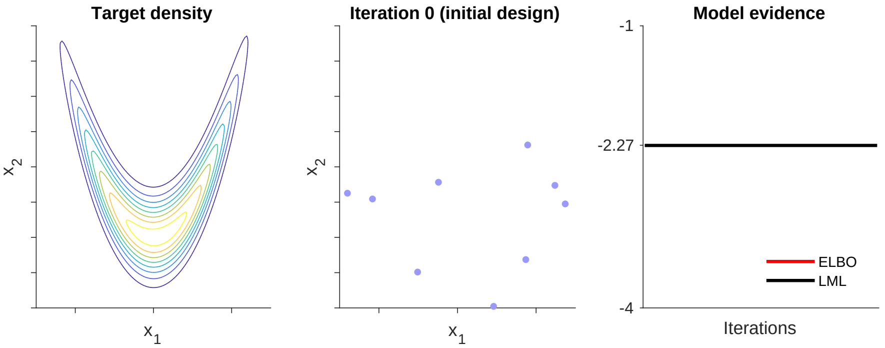

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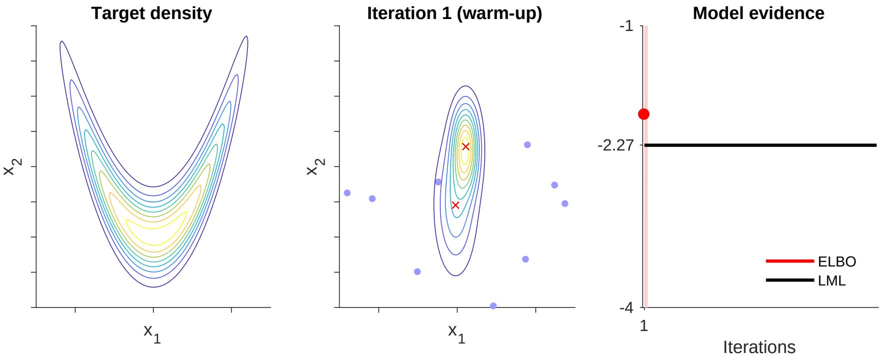

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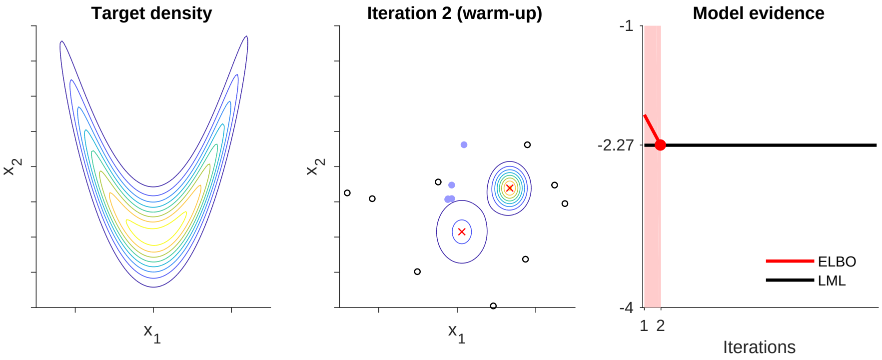

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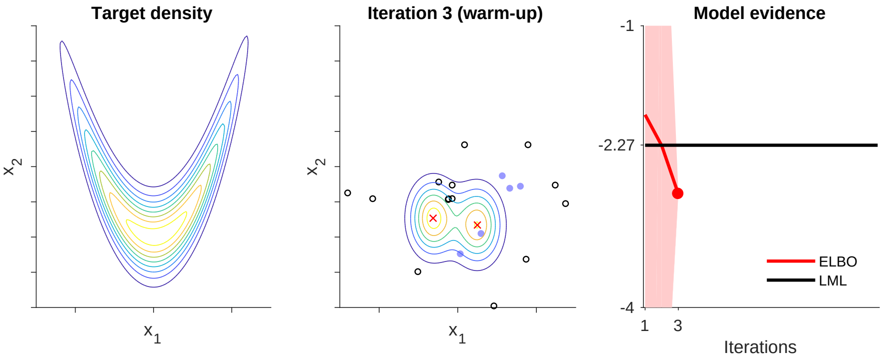

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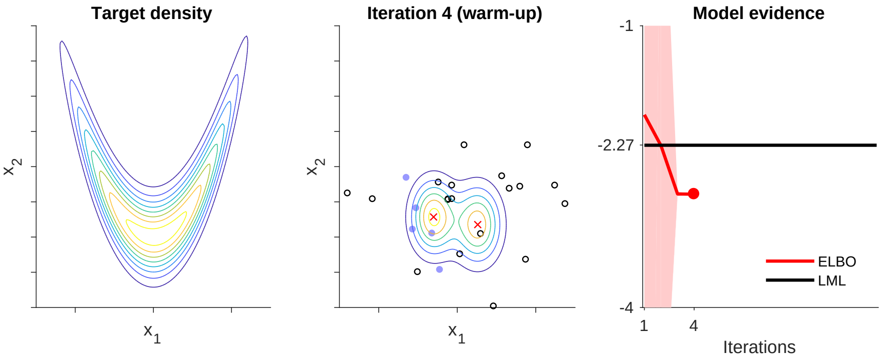

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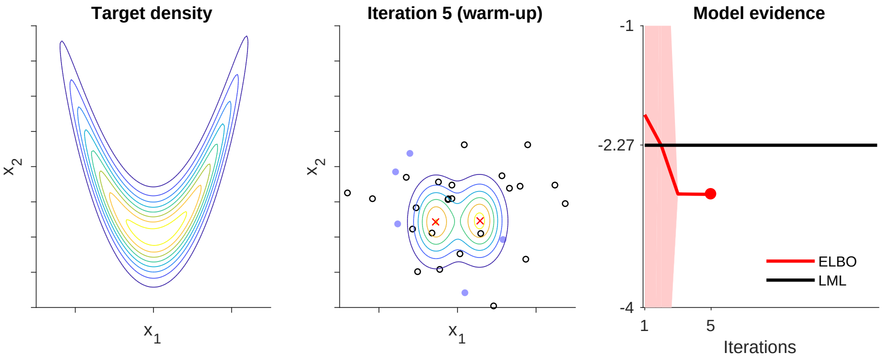

Acerbi, NeurIPS (2018)

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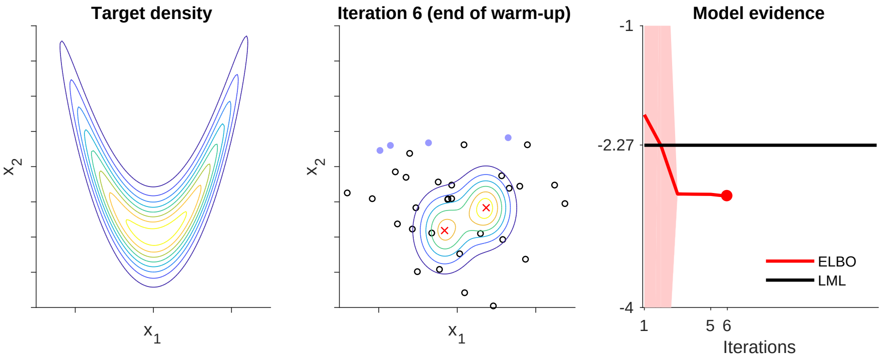

Acerbi, NeurIPS (2018)

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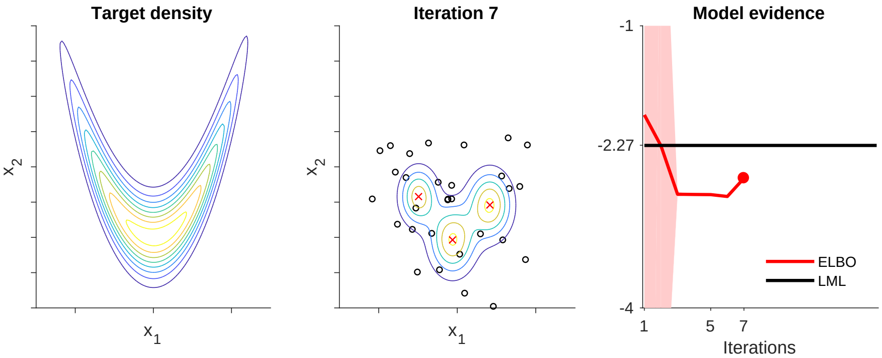

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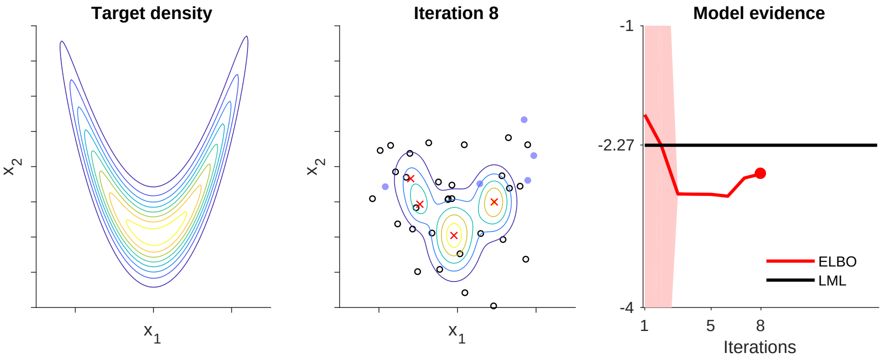

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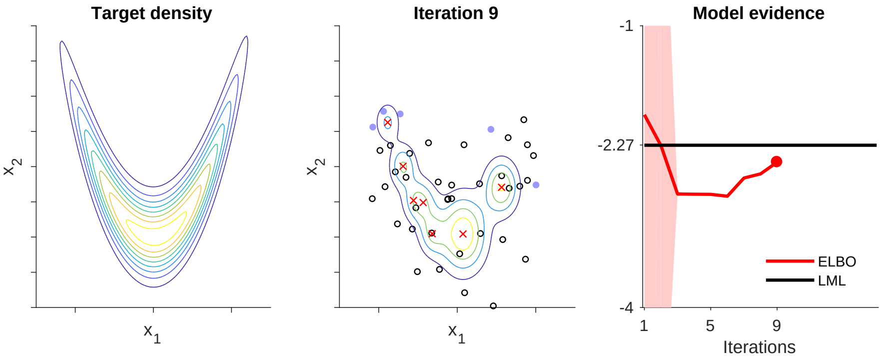

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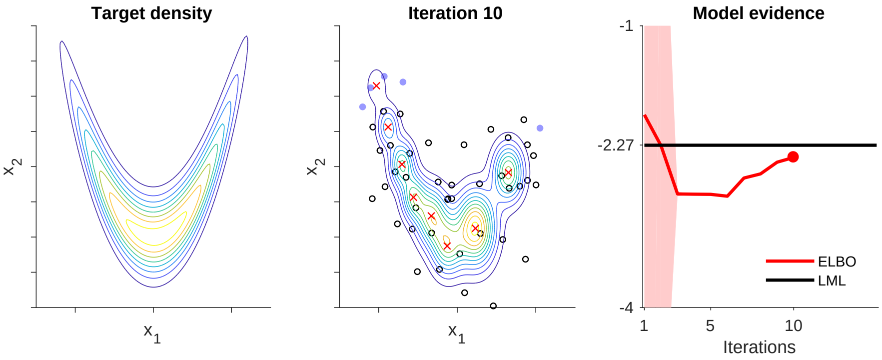

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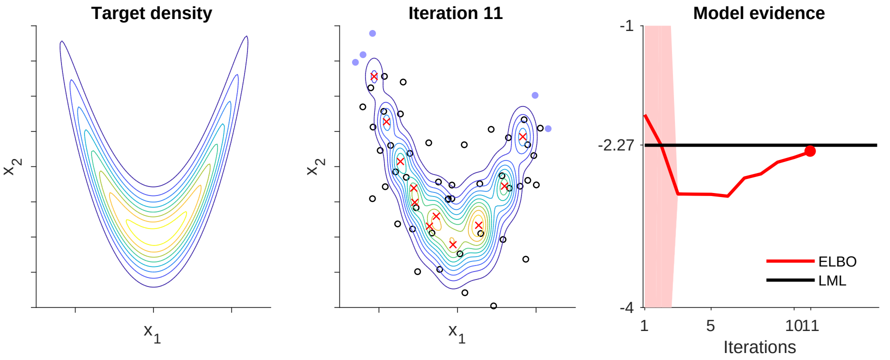

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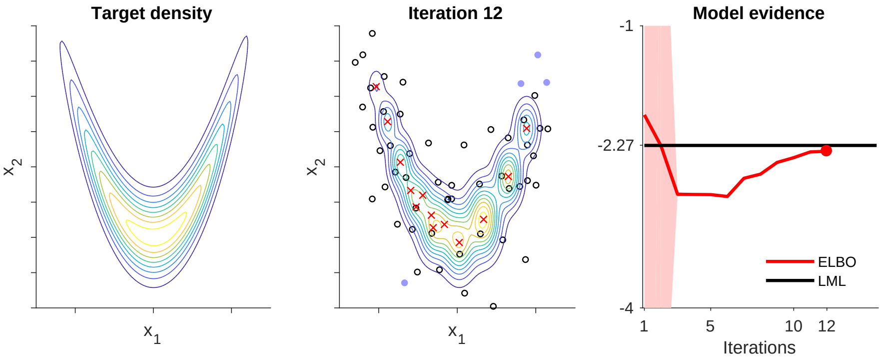

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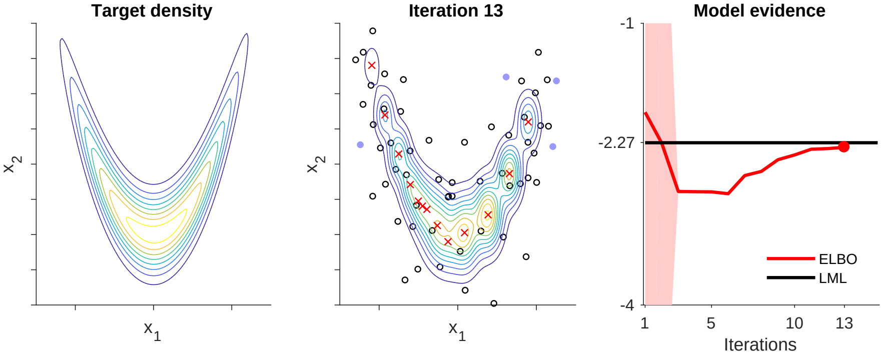

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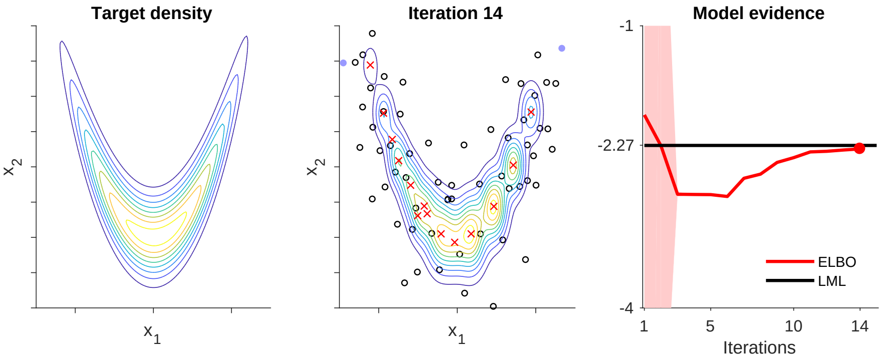

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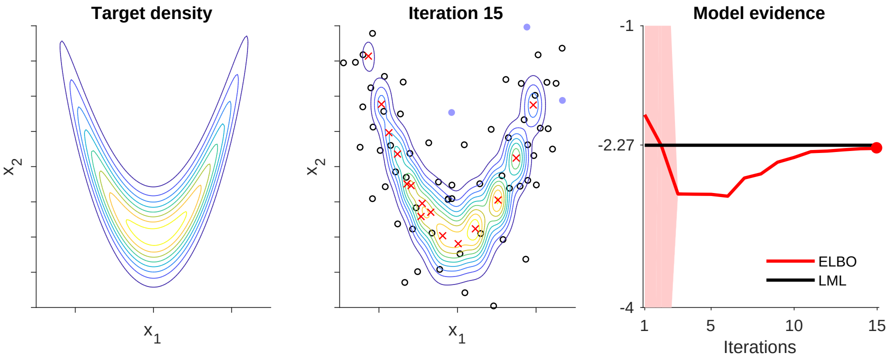

Acerbi, NeurIPS (2018)

Applied example

OPEN ACCESS PEER-REVIEWED

RESEARCH ARTICLE

Bayesian comparison of explicit and implicit causal inference strategies in multisensory heading perception

Luigi Acerbi, Kalpana Dokka, Dora E. Angelaki, Wei Ji Ma

Published: July 27, 2018 • https://doi.org/10.1371/journal.pcbi.1006110

Final slide

- Contact me at luigi.acerbi@gmail.com
- Optimization demos: github.com/lacerbi/optimviz
- BADS available at github.com/lacerbi/bads
- VBMC available at github.com/lacerbi/vbmc
- Tutorial: github.com/lacerbi/workshop-bristol-2019

Final slide

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Thanks!

(Time for questions?)