IBL Computational Neuroscience Course: Introduction to Statistical Model Fitting

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1. Introduction
   - Of models and likelihoods
   - The psychometric function

2. Model fitting
   - A statistical estimation problem
   - Model fitting via optimization
   - Optimization algorithms
   - Optimization cheat sheets

3. Advanced (Bayesian) topics
   - Bayesian Optimization
   - Bayesian model fitting

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?

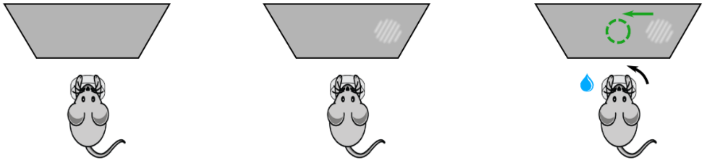
- Quantitative stand-in for a theory
- A *family of probability distributions* over possible datasets:

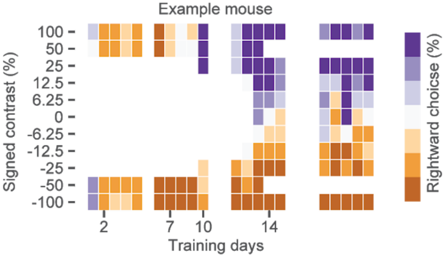
$$p\,(\text{data}|\boldsymbol{\theta})$$

  - data is a dataset with n data points (e.g., trials)
  - $\boldsymbol{\theta}$ is a parameter vector
- **Why?** Description, prediction, and explanation
- Defining $p(\text{data}|\boldsymbol{\theta})$ is the core of model building
  - Wait, what?
- **How?** Think about the data generation process!

We need some data

IBL Task





(IBL et al., *bioRxiv*, 2020)

Hacking time I

Let's have a look at the data

Type of models

- Descriptive
- Mechanistic
- Process
- Normative
- ...

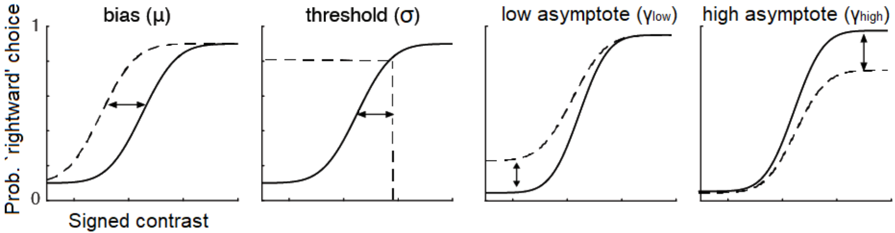
ORIGINAL ARTICLE
Commentary

Appreciating the variety of goals in computational neuroscience

Konrad P. Kording PhD[1] | Gunnar Blohm PhD[2] | Paul Schrater PhD[3] | Kendrick Kay PhD[4]

https://arxiv.org/abs/2002.03211

The psychometric function



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

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

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 $\boldsymbol{\theta}$: $(\mu,\ \sigma,\ \lambda,\ \gamma)$

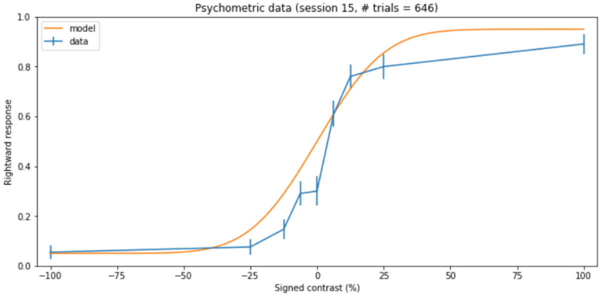
$$p(\text{rightward choice}|s, \boldsymbol{\theta}) = \lambda\gamma + (1 - \lambda) \cdot F(s; \mu, \sigma)$$

Hacking time II

Let's code a psychometric function

Metric for model fitting

We need a quantity to measure *goodness of fit*



- ~~Mean squared error?~~
- The likelihood $p(\text{data}|\boldsymbol{\theta})$

The (log) likelihood

- $p(\text{data}|\boldsymbol{\theta})$ is a *probability density* as you vary data for a fixed $\boldsymbol{\theta}$
- $p(\text{data}|\boldsymbol{\theta})$ is the *likelihood*, a function of $\boldsymbol{\theta}$ for fixed data

- For numerical reasons we work with $\log p(\text{data}|\boldsymbol{\theta})$
- Using the rules of probability and logarithms:

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

- Simplest case: $\log p\left(\text{data}|\boldsymbol{\theta}\right) = \sum_{i=1}^{n} \log p_i \left(\boldsymbol{r}^{(i)} | \boldsymbol{s}^{(i)}, \boldsymbol{\theta} \right)$
- Model building: Write function with
  - Input: $\boldsymbol{\theta}$ and data
  - Output: $\log p(\text{data}|\boldsymbol{\theta})$

Hacking time III

Let's code up a log-likelihood function

Model fitting

Model fitting $\sim$ *statistical estimation* problem

1. Maximum likelihood estimation (MLE)

- Find maximum of $p(\text{data}|\boldsymbol{\theta})$

$$\hat{\boldsymbol{\theta}}_{\text{ML}} = \arg\max_{\boldsymbol{\theta}} p(\text{data}|\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \log p(\text{data}|\boldsymbol{\theta})$$

2. Bayesian posterior

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

- 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)*: $\hat{\boldsymbol{\theta}}_{\text{MAP}} = \arg\max_{\boldsymbol{\theta}} p(\boldsymbol{\theta}|\text{data})$

How to do model fitting?

Maximum likelihood estimation (MLE), Maximum-a-posteriori (MAP)

- Model fitting $\sim$ *optimization problem*

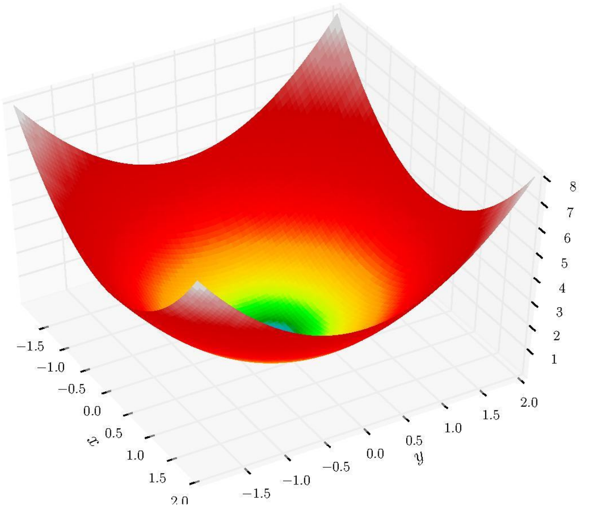
Bayesian posterior

- How do we represent/approximate an arbitrary posterior distribution?
  1. Use a known (easier) distribution (*variational inference*)
  2. Use a bunch of discrete samples (*Markov-Chain Monte Carlo*)

Model fitting via optimization

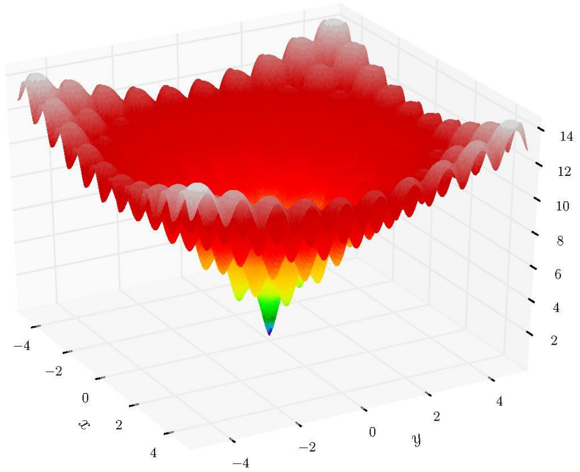
- Find single $\boldsymbol{\theta}$ that best describes the data
- (For this section we switch notation from $\boldsymbol{\theta}$ to $\boldsymbol{x}$)
- Given $\tilde{f}(\boldsymbol{x}) \equiv \begin{cases} \log p(\text{data}|\boldsymbol{x}) & \text{maximum likelihood} \\ \log p(\text{data}|\boldsymbol{x}) + \log p(\boldsymbol{x}) & \text{maximum-a-posteriori} \end{cases}$
- By convention, we *minimize* $f(x) \equiv -\tilde{f}(\boldsymbol{x})$
- $\Longrightarrow$ Find $\boldsymbol{x}_{opt} \approx \arg\min_{\boldsymbol{x}} f(\boldsymbol{x})$ as fast as possible
- General case: $f(\boldsymbol{x})$ is a *black box*
  - Sometimes we can compute the gradient

How hard can it be?



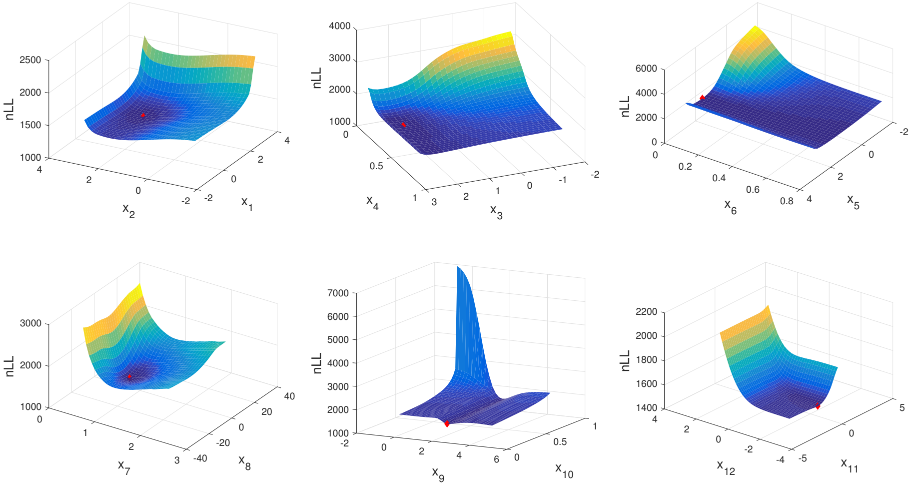
Source: Wikimedia Commons

How hard can it be?

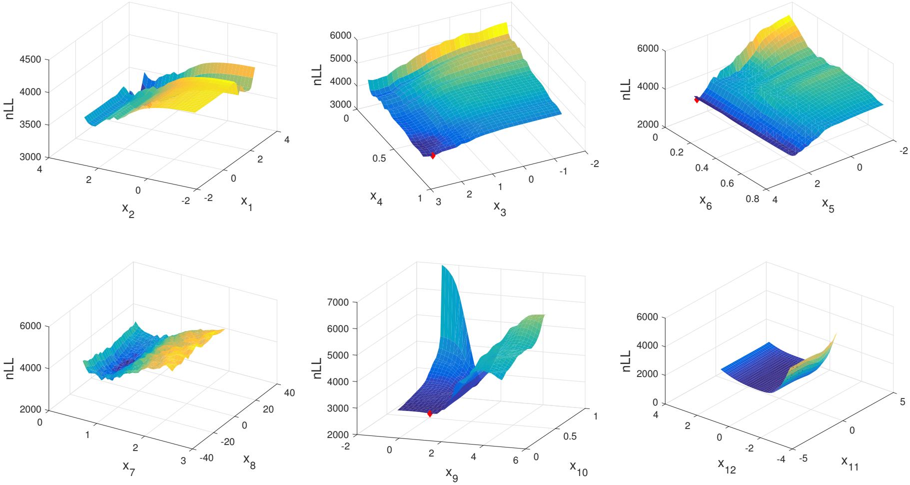


Source: Wikimedia Commons

How hard can it be?



How hard can it be?



How hard can it be?

neval	x_1	x_2	$f(\boldsymbol{x})$
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.)

Optimization algorithms

Gradient-based methods

- Stochastic gradient descent (e.g., ADAM)
- Quasi-Newton methods (e.g., BFGS aka `fminunc`/`fmincon`)

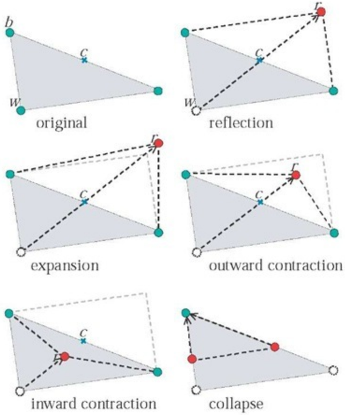
Gradient-free methods

- Nelder-Mead (`fminsearch`)
- Pattern/direct search (`patternsearch`)
- Simulated annealing
- Genetic algorithms
- CMA-ES
- Bayesian optimization
- Bayesian Adaptive Direct Search (BADS; Acerbi & Ma, *NeurIPS* 2017)

Demos: `https://github.com/lacerbi/optimviz`

Nelder-Mead (`fminsearch`)

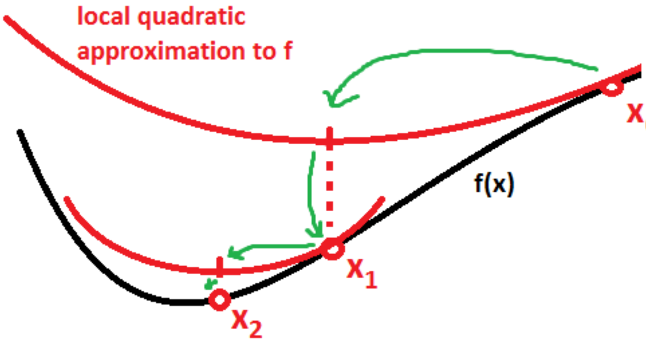
J. A. Nelder & R. Mead, A simplex method for function minimization (1965)



Source: Encyclopedia of Artificial Intelligence (2009)

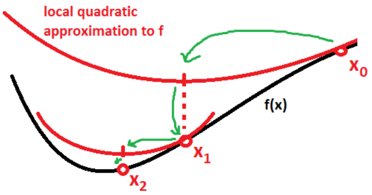
Bounded optimization: `fminsearchbnd` (John d'Errico)

Newton method



Source: StackExchange

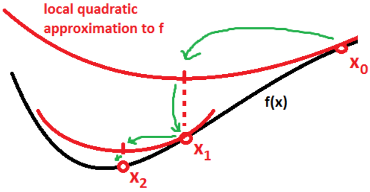
Newton method



Source: StackExchange

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

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

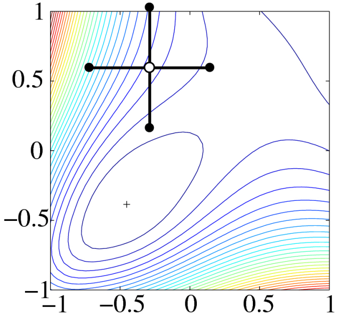


Source: StackExchange

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)

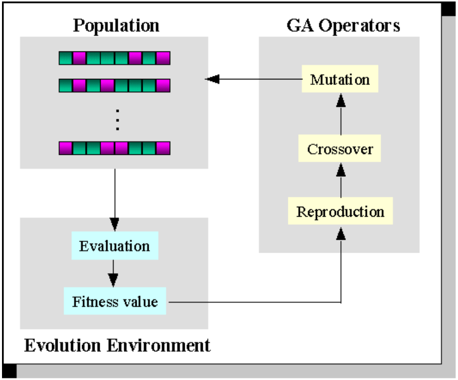


Source: Wikimedia Commons

Genetic Algorithms (ga)

J.H. Holland, Adaptation in Natural and Artificial Systems (1975)

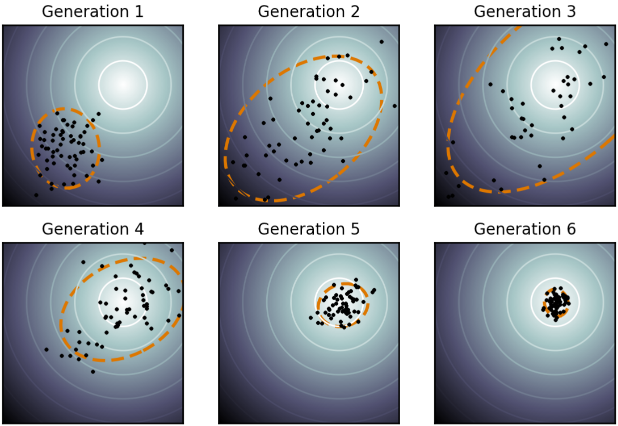
- Evolutionary algorithm
- Population based



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

Hacking time IV

Let's optimize the log-likelihood for the psychometric model

Local vs. global optimization

Local ⟷ Global

Local			Global
BFGS (`fmincon`)	Nelder-Mead (`fminsearch`)	BADS	Bayesian Optimization
	`patternsearch`	CMA-ES	MCS
	SGD	Genetic algorithms	
		Simulated annealing	

Optimization cheat sheet, page 1

Rule zero

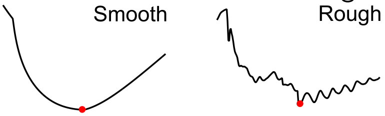
Understand your problem $\Longrightarrow$ often a *gray* box

Input variables:

- Dimensionality: low ($D \lesssim 10$) or high ($D \gg 20$)
- Bounds: Think of *hard* and *plausible* bounds
- Parameterization: Not all parameterizations are created equal

Target function:

- Convexity: convex or non-convex
- Smoothness: smooth or rough



- Deterministic or stochastic
  - If stochastic $\Longrightarrow$ minimize $\mathbb{E}\left[f(\boldsymbol{x})\right]$
- Computational cost:
  cheap ($\ll 0.01$ s), moderate (0.01-1 s), or expensive ($\gg 1$ s)

Optimization cheat sheet, page 2

Fundamental theorem

'No Free Lunch' theorem $\Longrightarrow$ no single best optimizer for all problems
(But not all methods are created equal!)

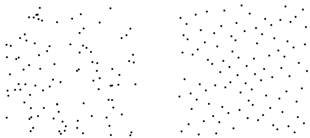
- Is your problem smooth?
  - If you have the gradient $\Longrightarrow$ BFGS
  - If low-D and cheap $\Longrightarrow$ BFGS with finite differences
  - If low-D and (moderately) costly $\Longrightarrow$ BADS
- Is your problem rough or noisy?
  - First, try and make it smooth and deterministic!
  - If gradient is available and high-D $\Longrightarrow$ SGD (e.g., ADAM)
  - If high-D and cheap $\Longrightarrow$ CMA-ES
  - If low-D and (moderately) costly $\Longrightarrow$ BADS
- Is your problem high-D, costly, and you do not have the gradient?
  - Give up and pray

Optimization cheat sheet, page 3

The golden rule

No optimizer can guarantee to find the global optimum
$\Longrightarrow$ Always perform multiple distinct optimization runs ('restarts')

- How to choose starting points?
  - Draw from prior distribution
  - Draw from a 'plausible' box
  - Sieve method
  - Use space-filling designs (quasi-random sequences)



- How many restarts?
  - As many as you need
  - Informally, check that 'most' points converge to the same solution
  - *Bootstrap* approach (Acerbi, Dokka et al., *PLoS Comp Biol* 2018)

Bayesian Optimization

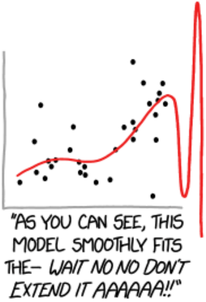
1. Start with a prior over functions (Gaussian process)
2. Find $\tilde{\boldsymbol{x}}$ that maximizes *acquisition function* (exploration/exploitation)
3. Evaluate $f(\tilde{\boldsymbol{x}})$
4. Compute posterior over functions (Gaussian process)
5. `goto 2`

J. Mockus, *Journal of Global Optimization* (1994)

Review paper: Frazier (2018) `https://arxiv.org/abs/1807.02811`

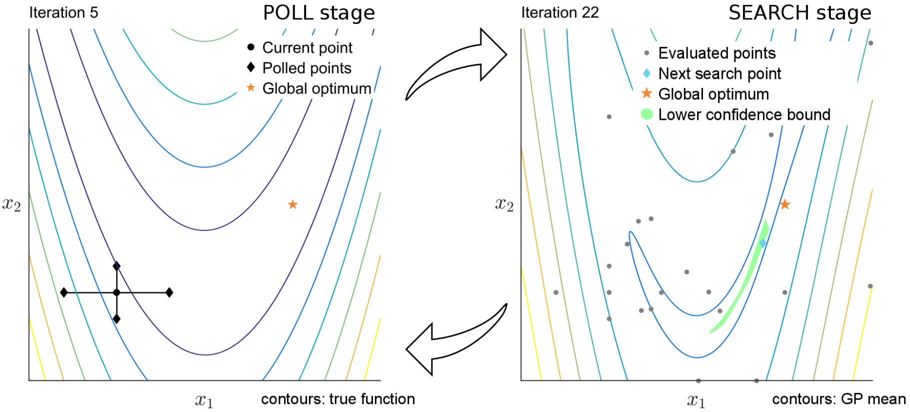
Why don't we use Bayesian optimization *all the time*?

- Matrix inversion is $O(n^3)$
- Model mismatch



from `xkcd.com/2048`

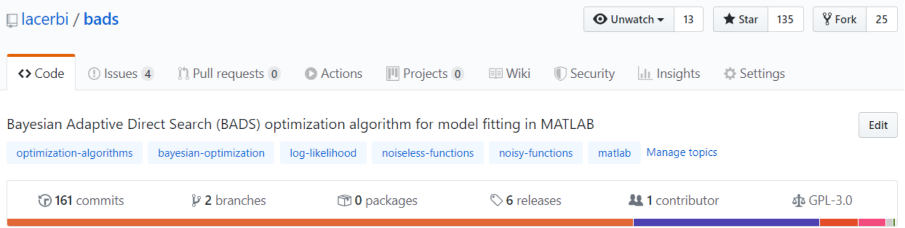
Bayesian Adaptive Direct Search (bads)



Acerbi & Ma, *NeurIPS* (2017)

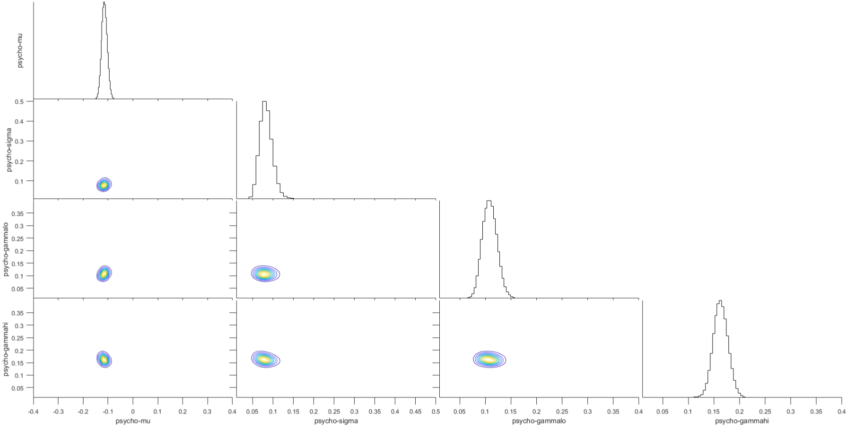
BADS summary

- 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
- Outperforms other algorithms (Acerbi & Ma, 2017)



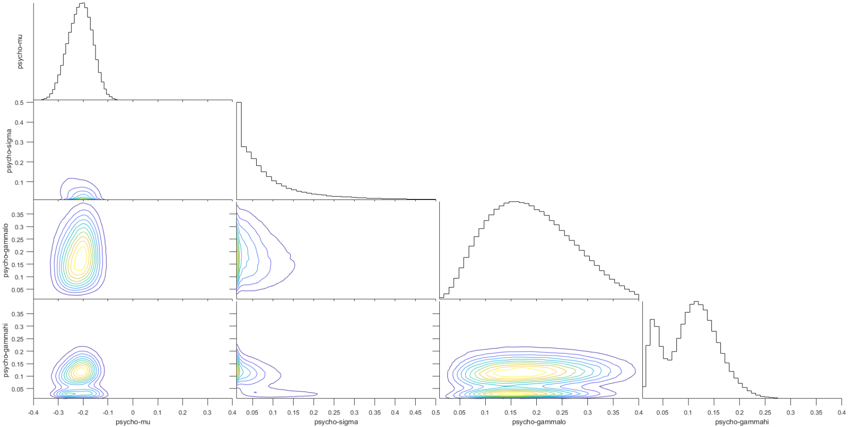
https://github.com/lacerbi/bads

Bayesian posteriors



$n = 1353$ trials

Bayesian posteriors



$n = 90$ trials

Benefits of Bayesian posteriors

- Check for parameter uncertainty, trade-offs, identifiability
  - Deeper understanding of your model
  - Robustness of claims (Acerbi, Ma, Vijayakumar, *NeurIPS* 2014)
- Less overfitting
- Use posterior samples to compute model comparison metrics
  - DIC, WAIC, LOO-CV
- Fully taking into account uncertainty is just *better*

How do I get Bayesian posteriors?

- Markov Chain Monte Carlo (MCMC; e.g. slice sampling, NUTS)
- Variational inference

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@internationalbrainlab.org
- Python tutorial: github.com/lacerbi/ibl-2020-tutorial
- Optimization demos: github.com/lacerbi/optimviz

MATLAB toolboxes:

- BADS available at github.com/lacerbi/bads
- VBMC available at github.com/lacerbi/vbmc

Thanks!

(Time for questions?)