# Introduction to Optimization for Statistical Model Fitting

Luigi Acerbi

Department of Computer Science
University of Helsinki

INTERNATIONAL BRAIN LABORATORY

BAMB! Summer School – Day 2
September 2022

# What is a model?

# 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

# 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

# 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?**

# What is a mathematical model?

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

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

  - data is a dataset with $n$ data points (e.g., trials)
  - $\boldsymbol{\theta}$ is a parameter vector

- **Why?** Description, prediction, and explanation

# 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

# 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?

# What is a mathematical model?

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

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

  - 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!

# What is a mathematical model?

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

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

  - 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

# Intermission: International Brain Laboratory (IBL)

Neuron
NeuroView

CellPress

## An International Laboratory for Systems and Computational Neuroscience

**The International Brain Laboratory***
*Correspondence: churchland@cshl.edu
https://doi.org/10.1016/j.neuron.2017.12.013

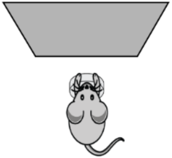
The neural basis of decision-making has been elusive and involves the coordinated activity of multiple brain structures. This NeuroView, by the International Brain Laboratory (IBL), discusses their efforts to develop a standardized mouse decision-making behavior, to make coordinated measurements of neural activity across the mouse brain, and to use theory and analyses to uncover the neural computations that support decision-making.

(IBL, *Neuron*, 2017)

# Intermission: International Brain Laboratory (IBL)

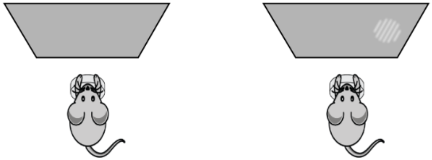

https://www.internationalbrainlab.com

# IBL Task



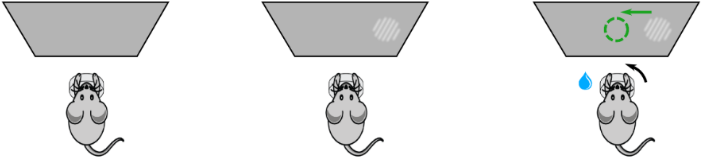
(IBL et al., *eLife*, 2021)

# IBL Task



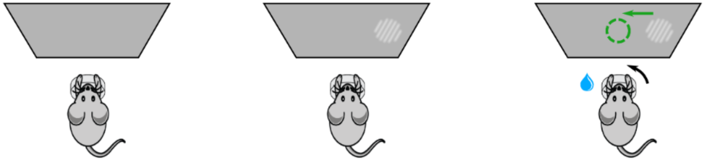
(IBL et al., *eLife*, 2021)

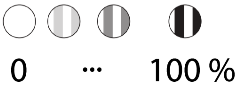
# IBL Task



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

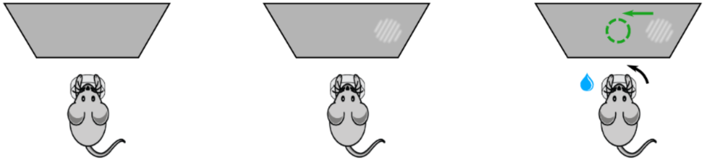
# IBL Task

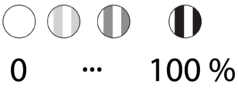


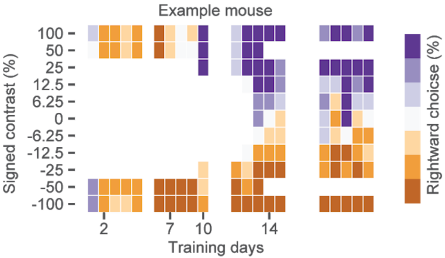



(IBL et al., *eLife*, 2021)

# IBL Task






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

# Hacking time I

Let's have a look at the data

# Type of models

# Type of models

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

# Type of models

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

NB
DT

**ORIGINAL ARTICLE**

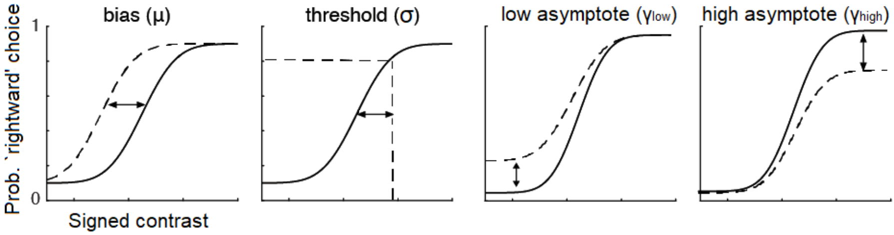
**Commentary**

**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]**

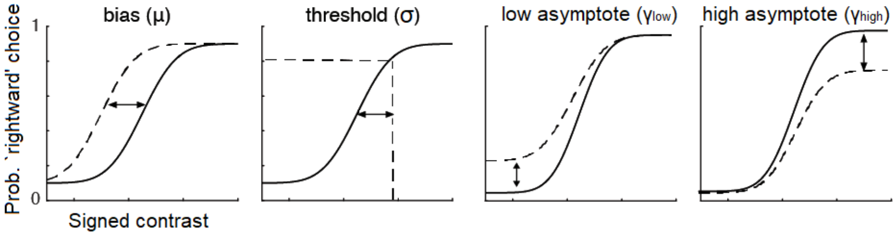
(Körding et al., *NBDT*, 2020)

# The psychometric function




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

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

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

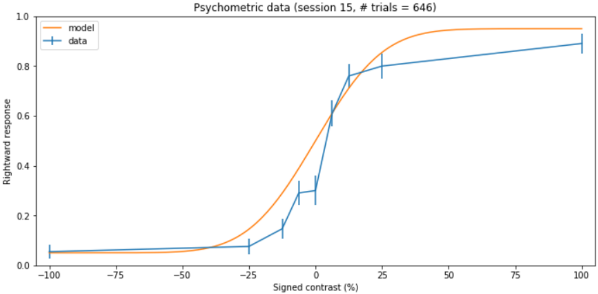
$$p(\text{rightward choice}|s, \boldsymbol{\theta}) = \lambda\gamma + (1 - \lambda) \cdot F(s; \mu, \sigma)$$

# Hacking time II

Let's code a psychometric function

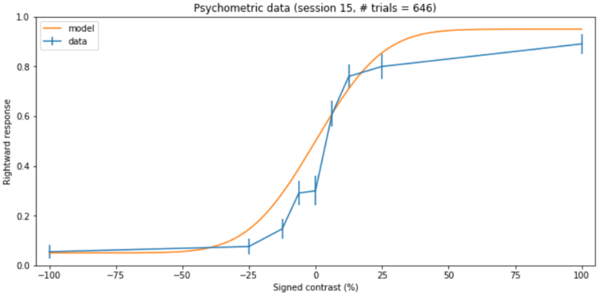
# Metric for model fitting

We need a quantity to measure *goodness of fit*



# Metric for model fitting

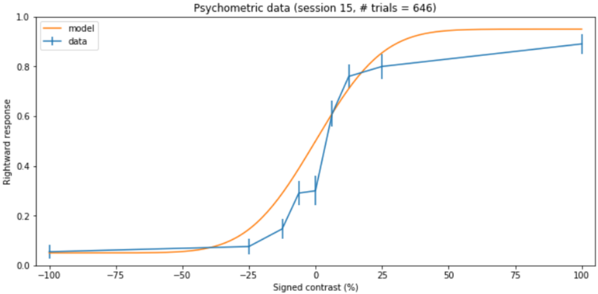
We need a quantity to measure *goodness of fit*




- Mean squared error?

# 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

# The (log) likelihood

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

# The (log) likelihood

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

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

# The (log) likelihood

- 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: $\log p\left(\text{data}|\boldsymbol{\theta}\right) = \sum_{i=1}^{n} \log p_i \left(\boldsymbol{r}^{(i)} | \boldsymbol{s}^{(i)}, \boldsymbol{\theta}\right)$

# The (log) likelihood

- 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

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

2. Model fitting
   - A statistical estimation problem
   - Model fitting via point estimation

3. Intro to optimization
   - The problem
   - Optimization algorithms
   - Optimization cheat sheets

# Model fitting

Model fitting $\sim$ *statistical estimation* problem

# Model fitting

Model fitting $\sim$ *statistical estimation* problem

*1. Maximum likelihood estimation* (MLE)

# Model fitting

Model fitting $\sim$ *statistical estimation* problem

*1. Maximum likelihood estimation* (MLE)

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

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

# 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

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

# 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 $p(\hat{\boldsymbol{\theta}}_{\text{ML}}) \neq 0$)

# 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

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

# Two ways of model fitting

# Two ways of model fitting

### "Point estimation"

- Maximum likelihood estimation (MLE), Maximum-a-posteriori (MAP)
- Model fitting $\sim$ *optimization problem*
- Returns a single 'best' parameter vector $\hat{\boldsymbol{\theta}}$ ($\hat{\boldsymbol{\theta}}_{ML}$ or $\hat{\boldsymbol{\theta}}_{MAP}$)

# Two ways of model fitting

## "Point estimation"

- Maximum likelihood estimation (MLE), Maximum-a-posteriori (MAP)
- Model fitting $\sim$ *optimization problem*
- Returns a single 'best' parameter vector $\hat{\boldsymbol{\theta}}$ ($\hat{\boldsymbol{\theta}}_{ML}$ or $\hat{\boldsymbol{\theta}}_{MAP}$)

## Bayesian posterior estimation

- True Bayesian way
- Returns a *distribution* (the posterior distribution $p(\boldsymbol{\theta}|\text{data})$)
- In practice, it returns an *approximation* of the posterior
    1. In parametric form $q(\boldsymbol{\theta})$ (e.g., *variational inference*)

# Two ways of model fitting

## "Point estimation"

- Maximum likelihood estimation (MLE), Maximum-a-posteriori (MAP)
- Model fitting $\sim$ *optimization problem*
- Returns a single 'best' parameter vector $\hat{\boldsymbol{\theta}}$ ($\hat{\boldsymbol{\theta}}_{ML}$ or $\hat{\boldsymbol{\theta}}_{MAP}$)

## Bayesian posterior estimation

- True Bayesian way
- Returns a *distribution* (the posterior distribution $p(\boldsymbol{\theta}|\text{data})$)
- In practice, it returns an *approximation* of the posterior
  1. In parametric form $q(\boldsymbol{\theta})$ (e.g., *variational inference*)
  2. As a bunch of discrete samples (e.g., *Markov-Chain Monte Carlo*)

# Model fitting via point estimation

- Find single $\boldsymbol{\theta}$ that best describes the data

# Model fitting via point estimation

- Find single $\boldsymbol{\theta}$ that best describes the data
- (For this section we switch notation from $\boldsymbol{\theta}$ to $\boldsymbol{x}$)

# Model fitting via point estimation

- Find single $\boldsymbol{\theta}$ that best describes the data
- (For this section we switch notation from $\boldsymbol{\theta}$ to $\boldsymbol{x}$)
- Given $\tilde{f}(\boldsymbol{x}) \equiv \begin{cases} \log p(\text{data}|\boldsymbol{x}) & \text{maximum likelihood} \\ \log p(\text{data}|\boldsymbol{x}) + \log p(\boldsymbol{x}) & \text{maximum-a-posteriori} \end{cases}$

# Model fitting via point estimation

- 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* $f(x) \equiv -\tilde{f}(\boldsymbol{x})$

# Model fitting via point estimation

- 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

# Model fitting via point estimation

- 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

# Model fitting via point estimation

- 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

## Solution

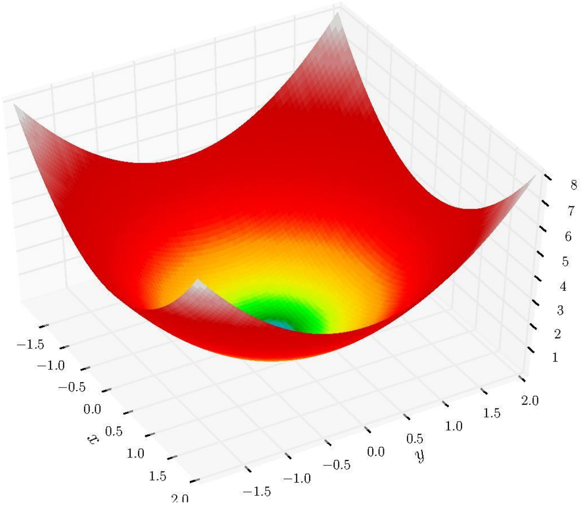
Feed $f(\boldsymbol{x})$ to an optimization algorithm

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

2. Model fitting
   - A statistical estimation problem
   - Model fitting via point estimation

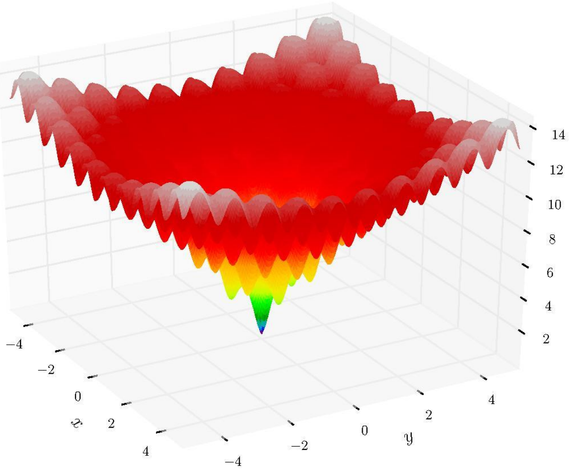
3. Intro to optimization
   - The problem
   - Optimization algorithms
   - Optimization cheat sheets

# How hard can it be?



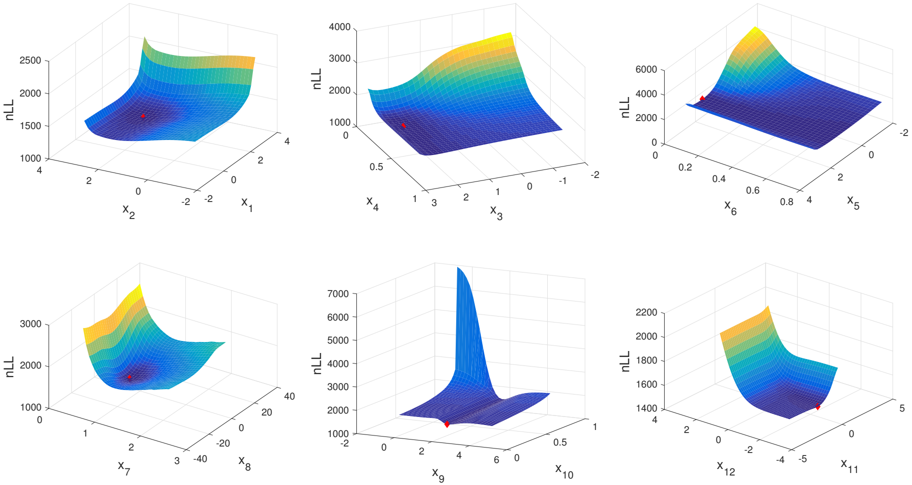

Source: Wikimedia Commons

# How hard can it be?

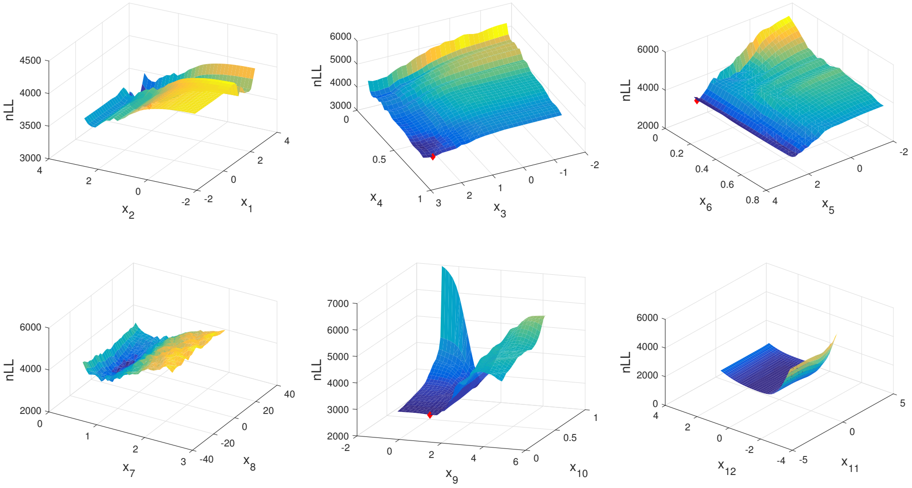



Source: Wikimedia Commons

# 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!

# Optimization can be hard

1. Optimizer does not see the landscape!
2. Multiple local minima or saddle points ('non-convex')

# Optimization can be hard

1. Optimizer does not see the landscape!
2. Multiple local minima or saddle points ('non-convex')
3. Expensive function evaluation

# 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)

# Optimization algorithms

Gradient-based methods

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

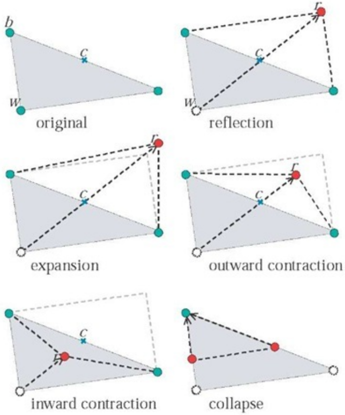
Gradient-free methods

- 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`)

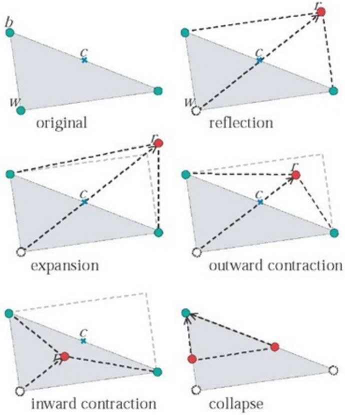
J. A. Nelder & R. Mead, A simplex method for function minimization (1965)




Source: Encyclopedia of Artificial Intelligence (2009)

# Nelder-Mead (`fminsearch`)

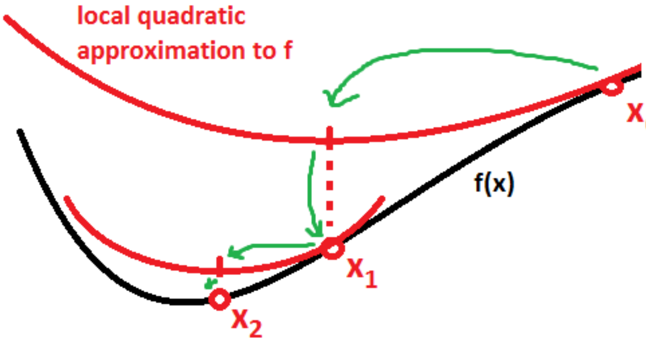
J. A. Nelder & R. Mead, A simplex method for function minimization (1965)




Source: Encyclopedia of Artificial Intelligence (2009)

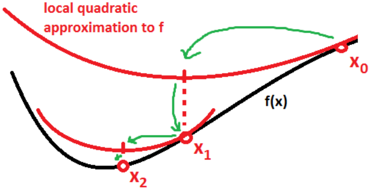
Bounded optimization: `fminsearchbnd` (John d'Errico)

# Newton method




Source: StackExchange

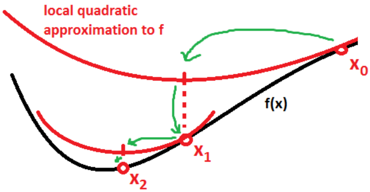
# Newton method




Source: StackExchange

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

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

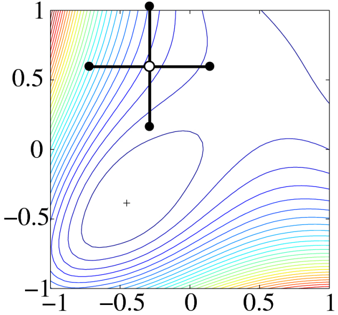



Source: StackExchange

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)

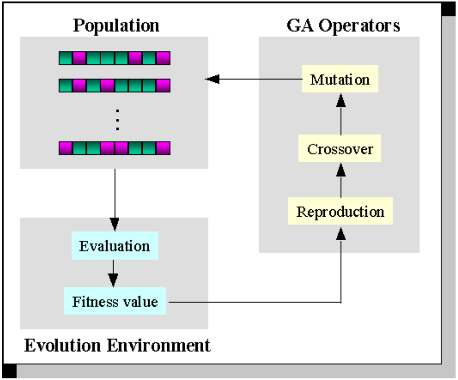
J.H. Holland, Adaptation in Natural and Artificial Systems (1975)

- Evolutionary algorithm
- Population based

# Genetic Algorithms (ga)

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

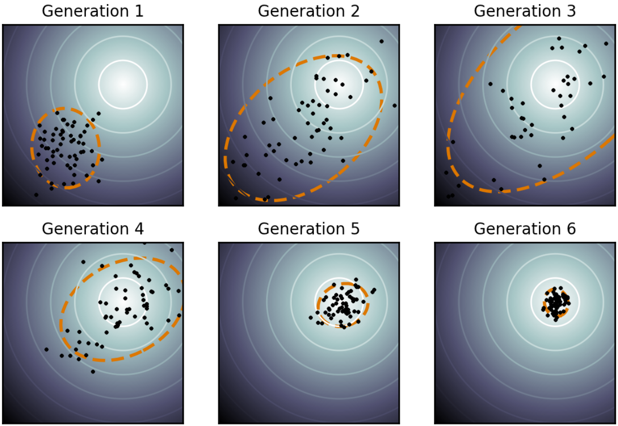
- Evolutionary algorithm
- Population based




Source: An Educational GA Learning Tool (IEEE)

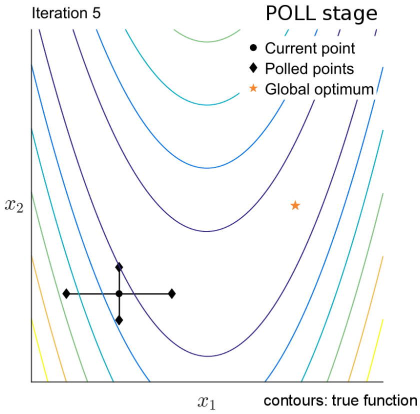
# Cov. Matrix Adaptation - Evolution Strategies (cmaes)

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



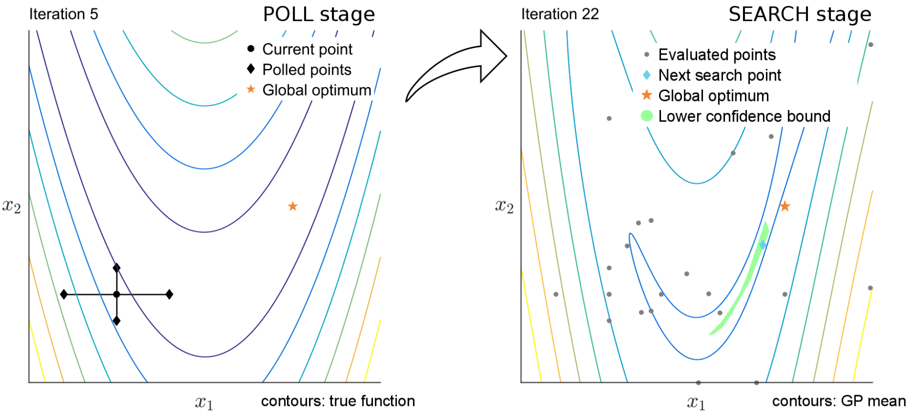

Source: Wikipedia

# Bayesian Adaptive Direct Search (bads)



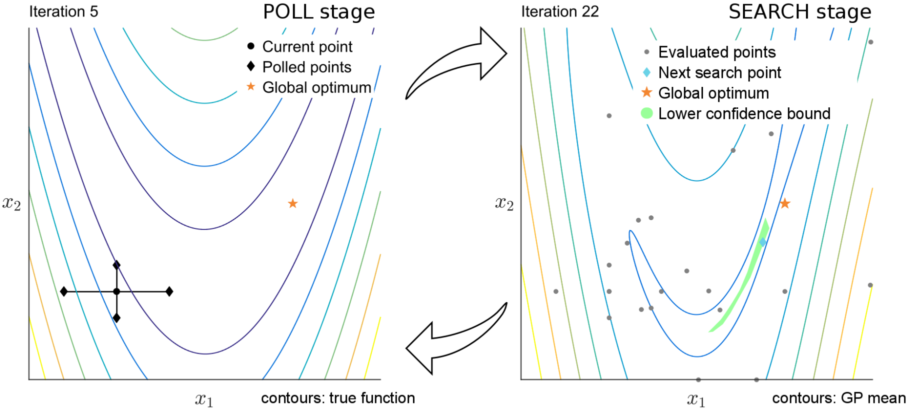

Acerbi & Ma, *NeurIPS* (2017)

# Bayesian Adaptive Direct Search (bads)




Acerbi & Ma, *NeurIPS* (2017)

# Bayesian Adaptive Direct Search (bads)




Acerbi & Ma, *NeurIPS* (2017)

# Local vs. global optimization

Local ↔ Global

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

# Hacking time IV

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

# Optimization cheat sheet, page 1

## Rule zero

# Optimization cheat sheet, page 1

## Rule zero

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

# Optimization cheat sheet, page 1

## Rule zero

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

**Input variables:**

- Dimensionality: low ($D \lesssim 10$) or high ($D \gg 20$)

# 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

# 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

# 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

# Optimization cheat sheet, page 1

## Rule zero

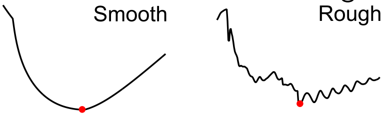
Understand your problem $\Longrightarrow$ often a *gray* box

**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



# Optimization cheat sheet, page 1

## Rule zero

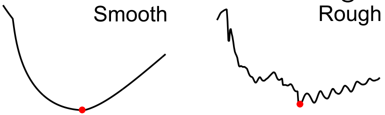
Understand your problem $\Longrightarrow$ often a *gray* box

**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

# Optimization cheat sheet, page 1

**Rule zero**

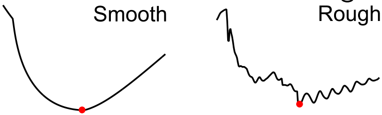
Understand your problem $\Longrightarrow$ often a *gray* box

**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 $\mathbb{E}[f(\boldsymbol{x})]$

# Optimization cheat sheet, page 1

## Rule zero

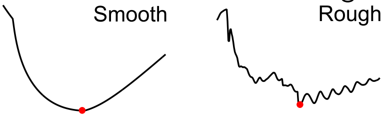
Understand your problem $\Longrightarrow$ often a *gray* box

**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 $\mathbb{E}[f(\boldsymbol{x})]$
- Computational cost:
  cheap ($\ll 0.01$ s), moderate (0.01-1 s), or expensive ($\gg 1$ s)

# Optimization cheat sheet, page 2

## Fundamental theorem

# Optimization cheat sheet, page 2

## Fundamental theorem

'No Free Lunch' theorem $\Longrightarrow$ no single best optimizer for all problems

# 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!)

# 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?

# 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

# 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

# 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

# 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?

# 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!

# 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)

# 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

# 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

# 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?

# 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

# Optimization cheat sheet, page 3

## The golden rule

No optimizer can guarantee to find the global optimum

# 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')

# 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?

# 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

# Optimization cheat sheet, page 3

## The golden rule

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

- How to choose starting points?
  - Draw from prior distribution
  - Draw from a 'plausible' box

# 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')

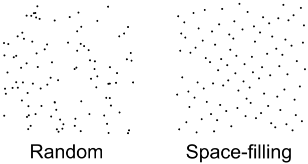
- How to choose starting points?
  - Draw from prior distribution
  - Draw from a 'plausible' box
  - Sieve method

# 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)

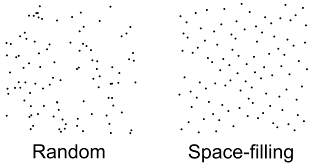


# Optimization cheat sheet, page 3

## 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)



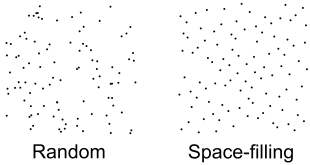

- How many restarts?

# 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)



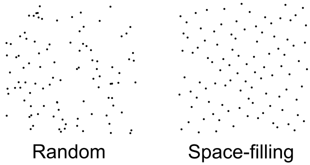

- How many restarts?
  - As many as you need

# 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)



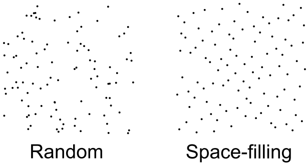

- How many restarts?
  - As many as you need
  - Informally, check that 'most' points converge to the same solution

# 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)

# 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?)