The Art of Model Fitting

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What is a model?

What is a model?

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

N. Wiener, *Philosophy of Science* (1945) (with A. Rosenblueth)

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- Defining $p(\text{data}|\boldsymbol{\theta})$ is the core of model building

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

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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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- *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

1. Introduction

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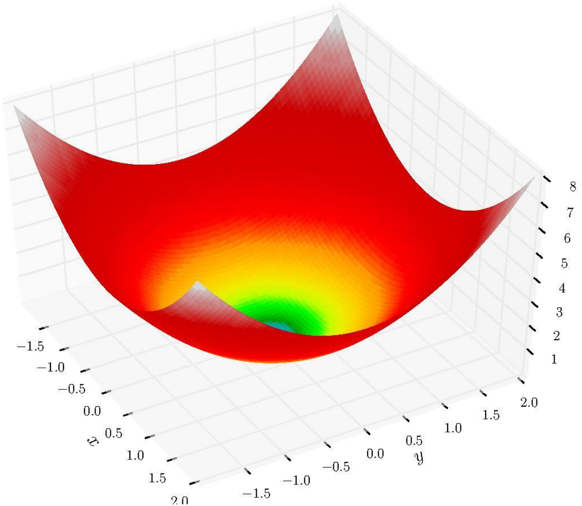
- General case: $f(\boldsymbol{x})$ is a *black box*

How hard can it be?



Source: Wikimedia Commons

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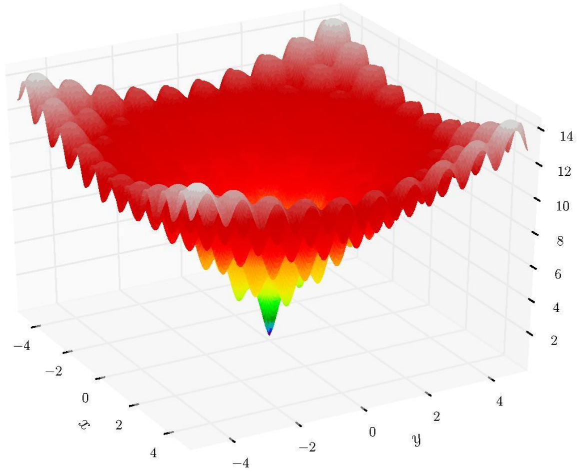

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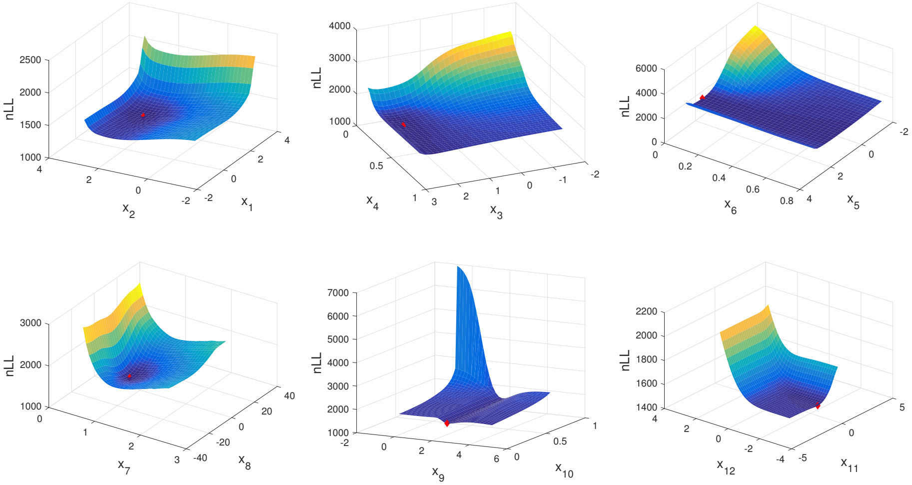

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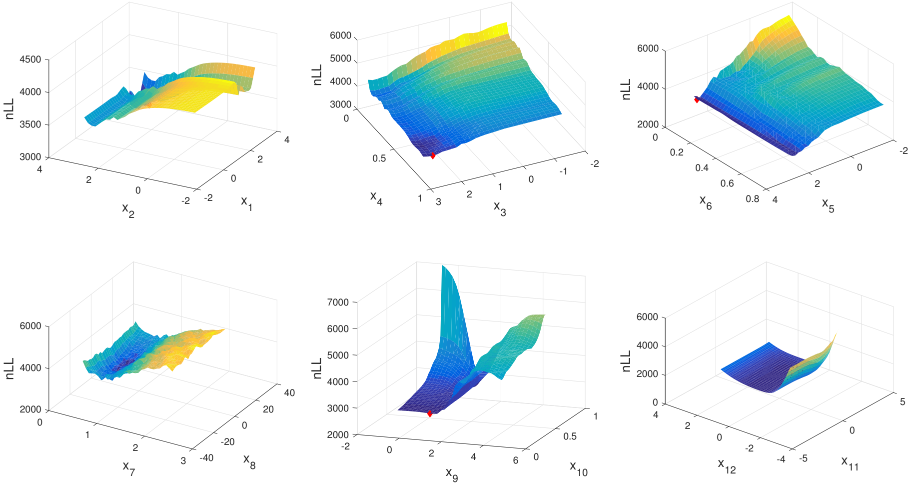

How hard can it be?

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

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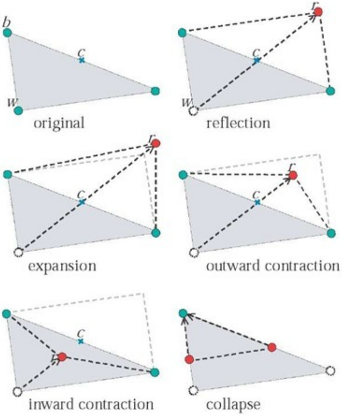
    - If in doubt, start larger
- Consider reparameterizations to achieve
  - Uniformity of effects across parameter range
  - Independence between parameters

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)

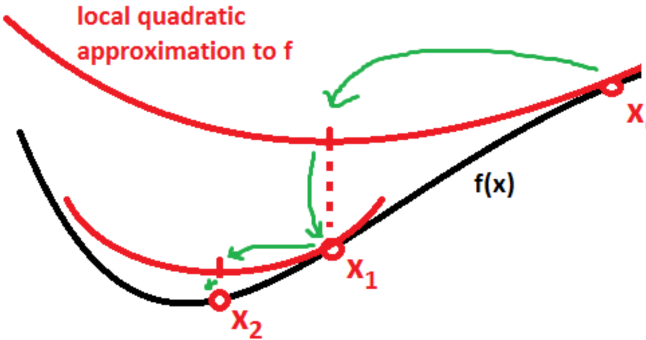
Nelder-Mead (`fminsearch`)

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



Source: Encyclopedia of Artificial Intelligence (2009)

Newton method



Source: StackExchange

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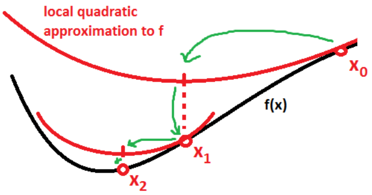

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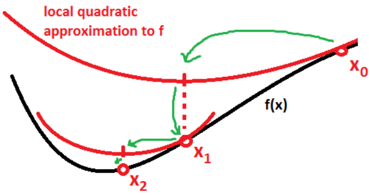
Needs the inverse of the curvature (inverse Hessian)
Very expensive in high dimension

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

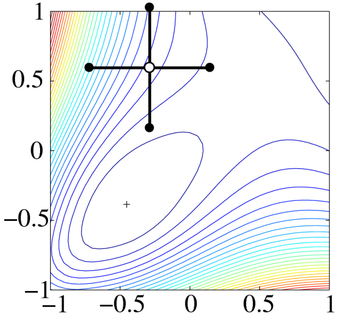


Source: StackExchange

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

Direct search (`patternsearch`)

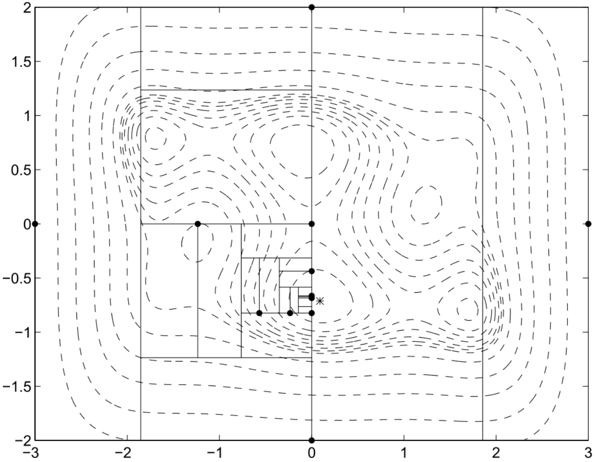
R. Hooke and T.A. Jeeves, "Direct search" solution of numerical and statistical problems (1961)



Source: Wikimedia Commons

Multilevel Coordinate Search (`mcs`)

[*] W. Huyer and A. Neumaier, Global Optimization by Multilevel Coordinate Search (1999)



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Genetic Algorithms (ga)

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

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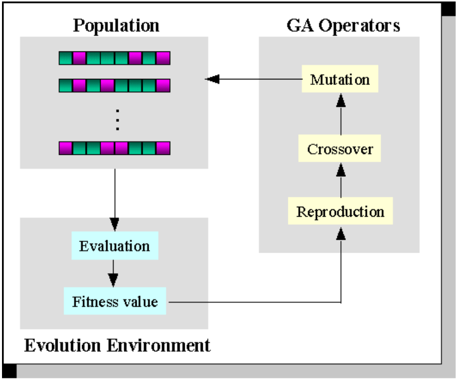
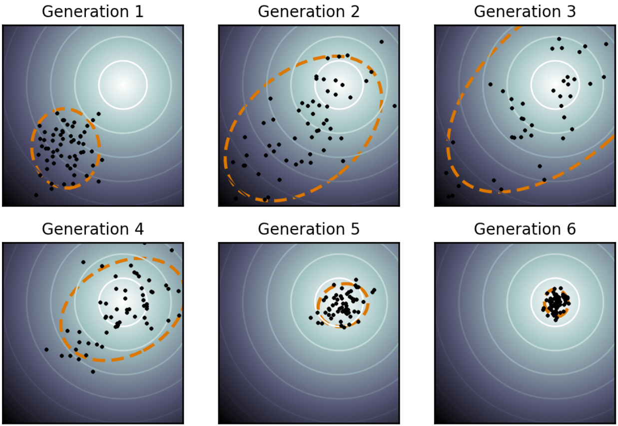


Source: An Educational GA Learning Tool (IEEE)

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)



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5. `goto 2`

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- Performance depends on quality of global approximation

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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

L. Acerbi & W.J. Ma, NIPS (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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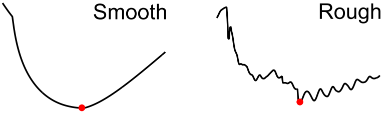
- Check your landscape



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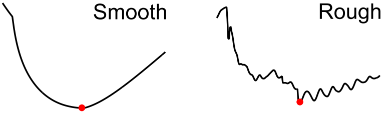

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  - If you can compute the gradient, do it!

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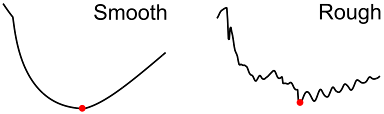

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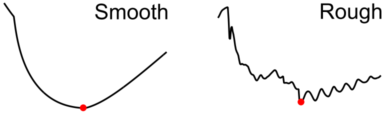

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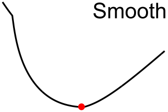

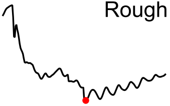

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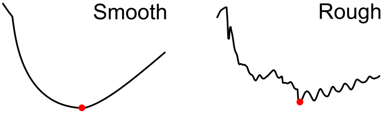

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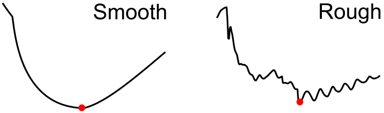

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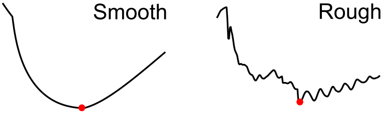

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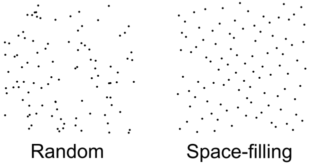

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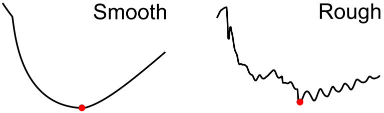

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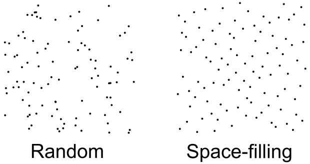

- If you can afford many fcn evals... consider MCMC instead of optimization!

The problem

- Several models $\mathcal{M}_1, \ldots, \mathcal{M}_M$
- For each $\mathcal{M}_m$ we know $\log p(\text{data}|\hat{\boldsymbol{\theta}}_{\text{ML}}, \mathcal{M}_m)$
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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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$$\text{AIC} = \log p(\text{data}|\hat{\theta}_{\text{ML}}, \mathcal{M}_m) - k$$

Akaike information criterion (AIC)

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

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?

Akaike information criterion (AIC), part two

Why penalty is k?

(Do you really want to know?)

Akaike information criterion (AIC), part two

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- 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

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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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- Use MCMC

Another slide about MCMC

Another slide about MCMC

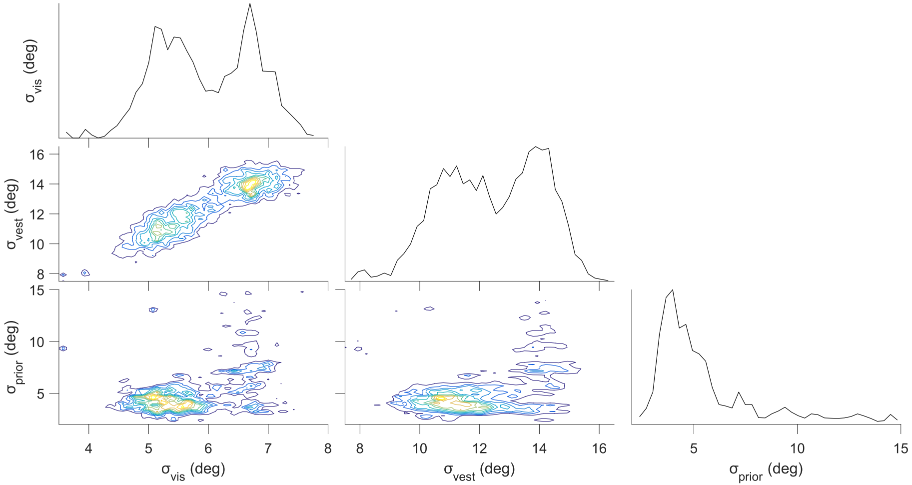

Figure made with `cornerplot.m`, by Will T. Adler

Another slide about MCMC

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  - Deeper understanding of your model
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Use *slice sampling* (Neal, 2003)

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

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