Bayesian inference and Bayesian model selection

Klaas Enno Stephan







Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich Lecture as part of "Methods & Models for fMRI data analysis", University of Zurich & ETH Zurich, 27 November 2018

With slides from and many thanks to: Kay Brodersen, Will Penny, Sudhir Shankar Raman

Why should I know about Bayesian inference?

Because Bayesian principles are fundamental for

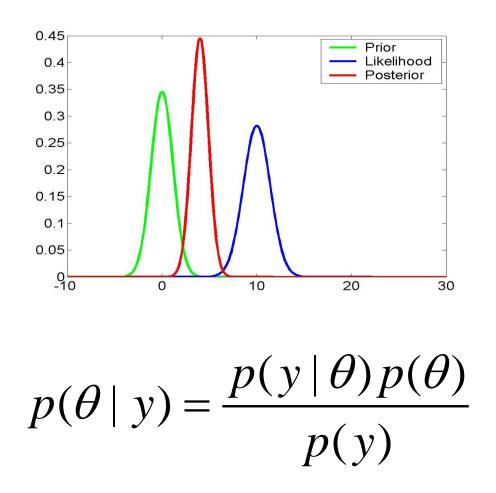
- statistical inference in general
- system identification
- translational neuromodeling ("computational assays")
 - computational psychiatry
 - computational neurology
 - computational psychosomatics
- contemporary theories of brain function (the "Bayesian brain")
 - predictive coding
 - free energy principle
 - active inference

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Bayes' theorem



posterior = likelihood • prior / evidence

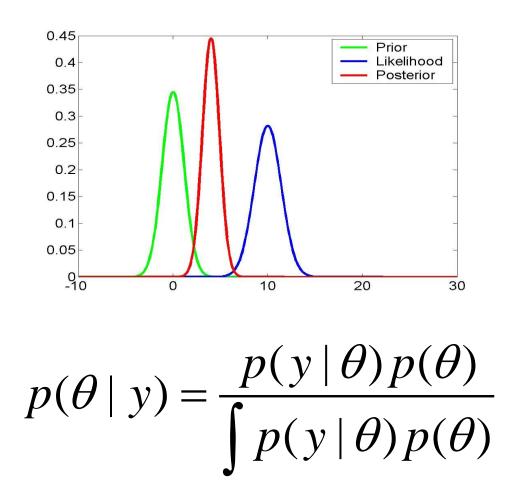


The Reverend Thomas Bayes (1702-1761)

"... the theorem expresses how a ... degree of belief should rationally change to account for availability of related evidence."

Wikipedia

Bayes' theorem



posterior = likelihood • prior / evidence

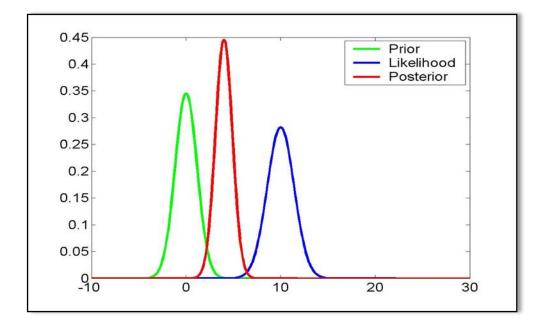


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Wikipedia

Bayesian inference: an animation



The evidence term

continuous
$$\theta$$

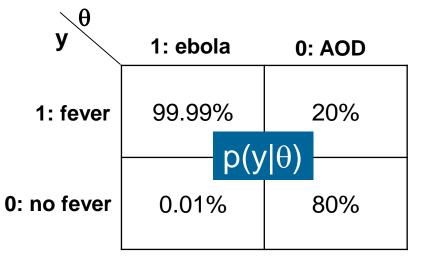
$$p(\theta \mid y) = \frac{p(y \mid \theta) p(\theta)}{\int p(y \mid \theta) p(\theta)}$$

discrete θ

$$p(\theta \mid y) = \frac{p(y \mid \theta) p(\theta)}{\sum_{\theta \in \Theta} p(y \mid \theta) p(\theta)}$$

Bayesian inference: An example (with fictitious probabilities)

- symptom:
 y=1: fever
 y=0: no fever
- disease: θ=1: Ebola
 θ=0: any other disease (AOD)



• A priori:

$$p(Ebola) = 10^{-6}$$

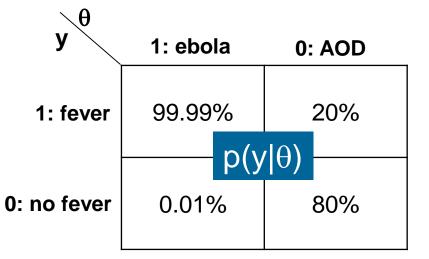
 $p(AOD) = (1-10^{-6})$

• A patient presents with fever. What is the probability that he/she has ebola?

$$p(\theta = 1 \mid y = 1) = \frac{p(y = 1 \mid \theta = 1) p(\theta = 1)}{\sum_{j \in \{0,1\}} p(y = 1 \mid \theta = j) p(\theta = j)}$$

Bayesian inference: An example (with fictitious probabilities)

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• A priori:

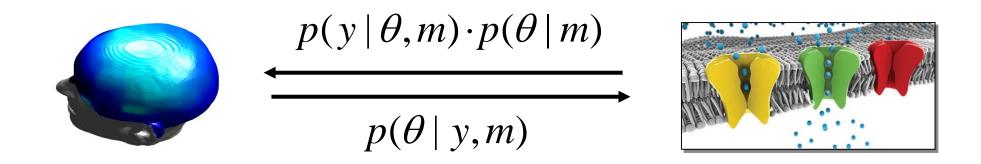
$$p(Ebola) = 10^{-6}$$

 $p(AOD) = (1-10^{-6})$

• A patient presents with fever. What is the probability that he/she has ebola?

$$p(\theta = 1 \mid y = 1) = \frac{0.999 \cdot 10^{-6}}{0.999 \cdot 10^{-6} + 0.2 \cdot (1 - 10^{-6})} = 4.995 \cdot 10^{-6}$$

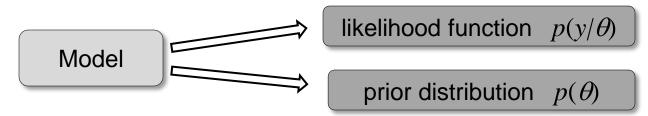
Generative models



- 1. specify the joint probability over data (observations) and parameters
- 2. enforce mechanistic thinking: how could the data have been caused?
- 3. generate synthetic data (observations) by sampling from the prior can model explain certain phenomena at all?
- 4. inference about parameters $\rightarrow p(\theta|y)$
- 5. model evidence p(y|m): index of model quality

Bayesian inference in practice

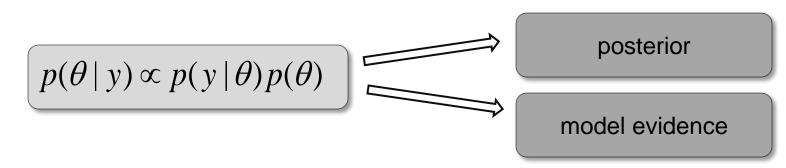
⇒ Formulation of a **generative model**



⇒ Observation of data

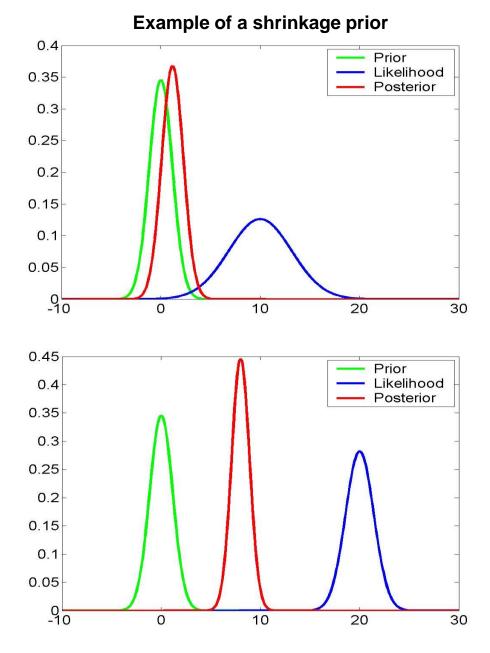


⇒ **Model inversion** – updating one's beliefs

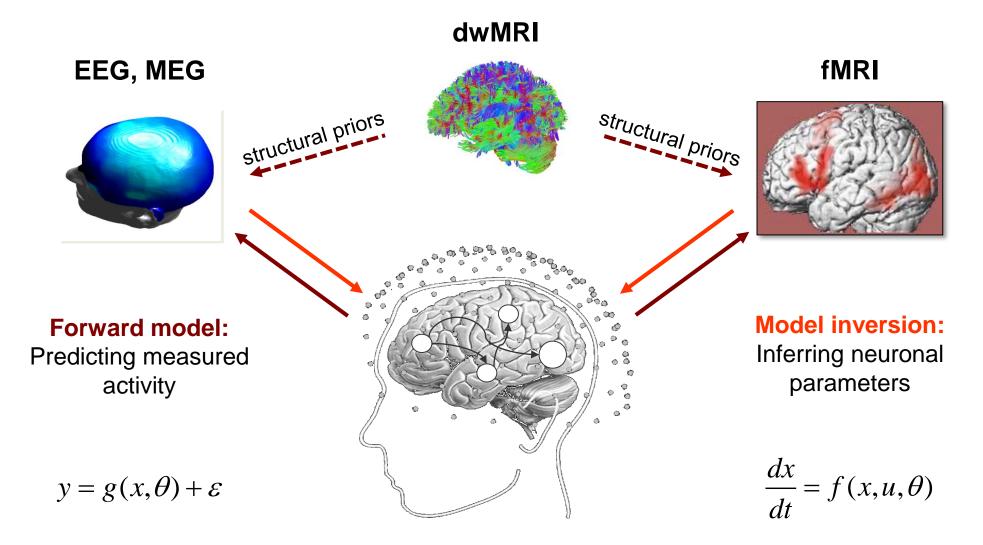


Priors

- Objective priors:
 - "non-informative" priors
 - objective constraints (e.g., non-negativity)
- Subjective priors:
 - subjective but not arbitrary
 - can express beliefs that result from understanding of the problem or system
 - can be result of previous empirical results
- Shrinkage priors:
 - emphasize regularization and sparsity
- Empirical priors:
 - learn parameters of prior distributions from the data ("empirical Bayes")
 - rest on a hierarchical model



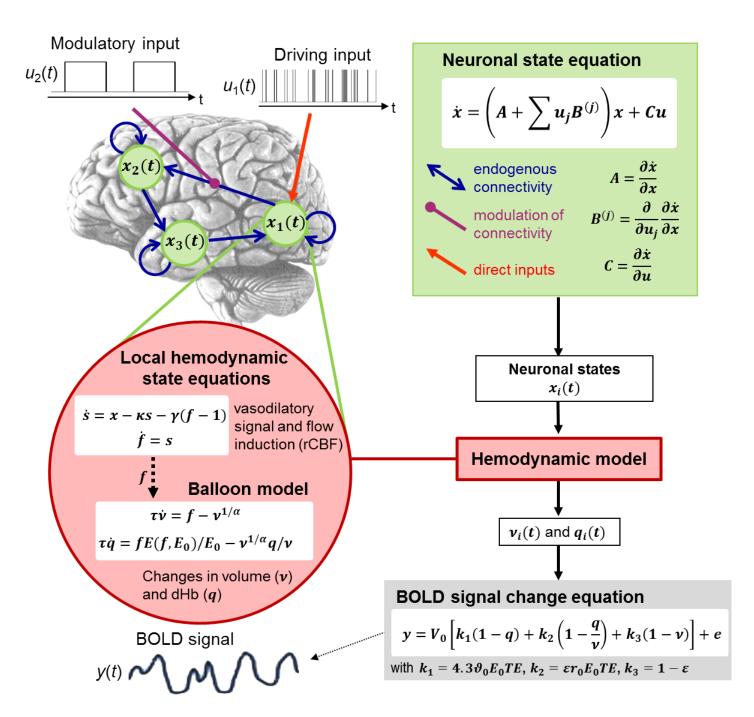
A generative modelling framework for fMRI & EEG: Dynamic causal modeling (DCM)



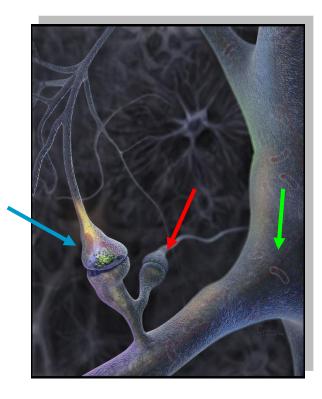
Friston et al. 2003, *NeuroImage*

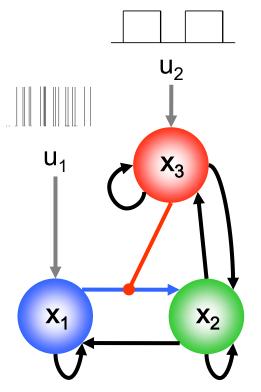
Stephan et al. 2009, NeuroImage

DCM for fMRI



Stephan et al. 2015, *Neuron*

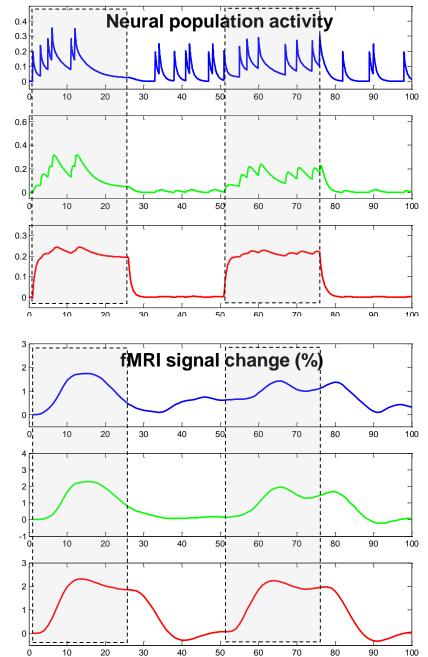




Nonlinear Dynamic Causal Model for fMRI

$$\frac{dx}{dt} = \left(A + \sum_{i=1}^{m} u_i B^{(i)} + \sum_{j=1}^{n} x_j D^{(j)}\right) x + Cu$$

Stephan et al. 2008, NeuroImage



Bayesian system identification

Neural dynamics

Observer function

$$dx/dt = f(x, u, \theta)$$

u(t)

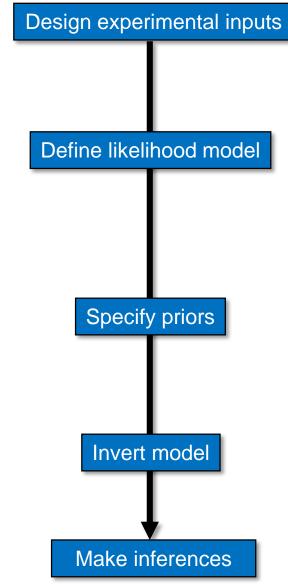
$$y = g(x, \theta) + \varepsilon$$

$$\begin{split} p(y \mid \theta, m) &= N(g(\theta), \Sigma(\theta)) \\ p(\theta, m) &= N(\mu_{\theta}, \Sigma_{\theta}) \end{split}$$

Inference on model structure

Inference on parameters

$$p(y \mid m) = \int p(y \mid \theta, m) p(\theta) d\theta$$
$$p(\theta \mid y, m) = \frac{p(y \mid \theta, m) p(\theta, m)}{p(y \mid m)}$$

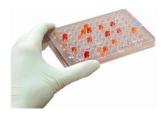


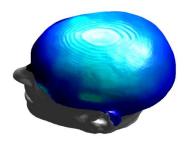
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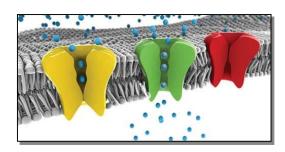
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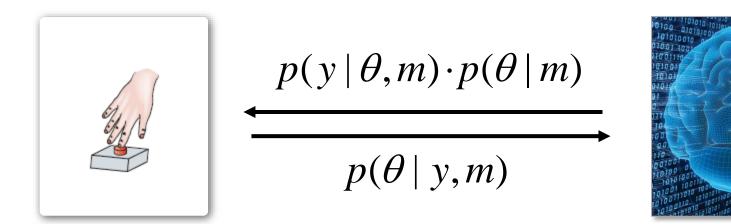
Generative models as "computational assays"

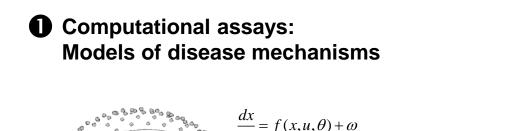




 $p(y \mid \theta, m) \cdot p(\theta \mid m)$ $p(\theta \mid y, m)$

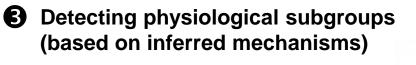


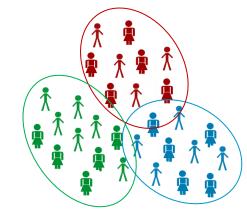




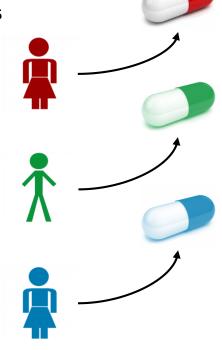
Translational Neuromodeling

4 Individual treatment prediction





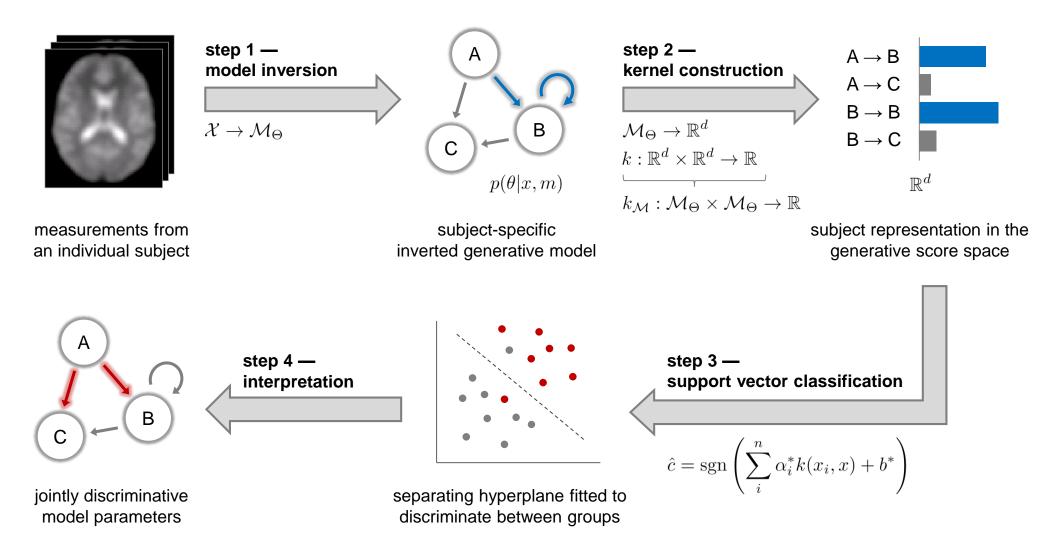
disease mechanism A
disease mechanism B
disease mechanism C



Stephan et al. 2015, Neuron

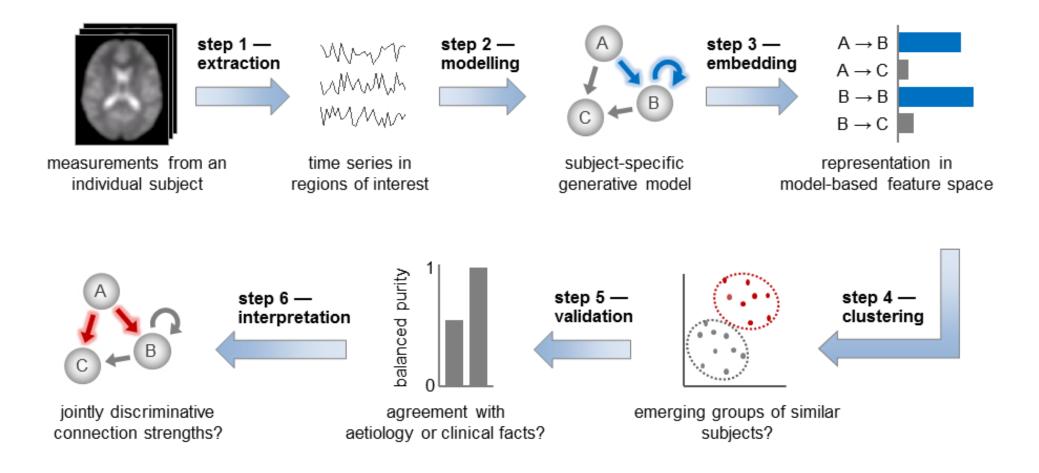
Application to brain activity and behaviour of individual patients

Generative embedding (supervised)

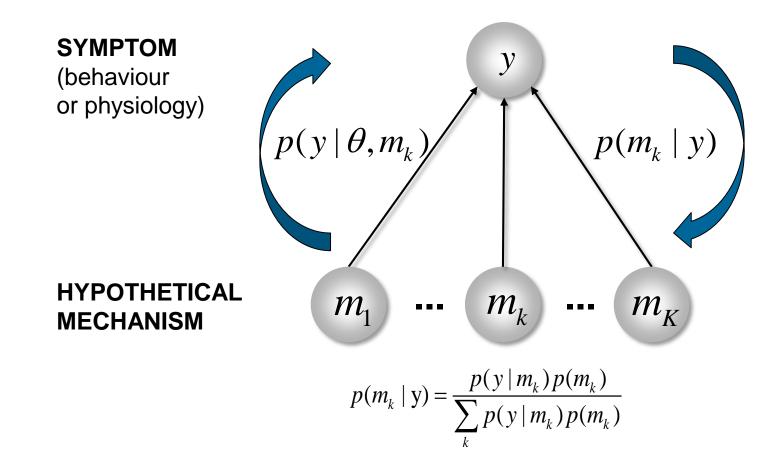


Brodersen et al. 2011, PLoS Comput. Biol.

Generative embedding (unsupervised)



Differential diagnosis by model selection



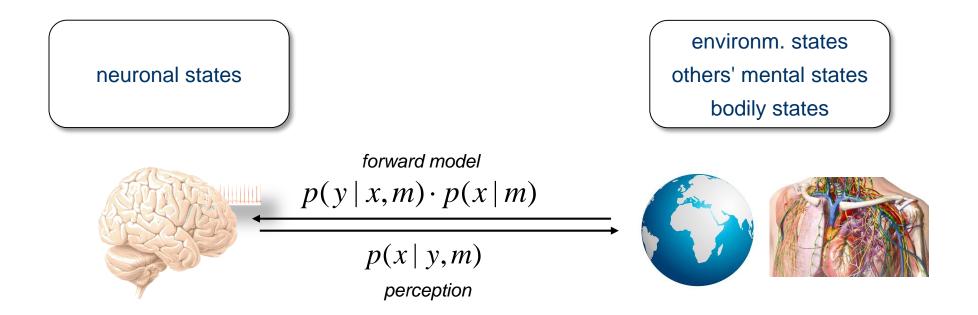
Stephan et al. 2017, NeuroImage

Why should I know about Bayesian inference?

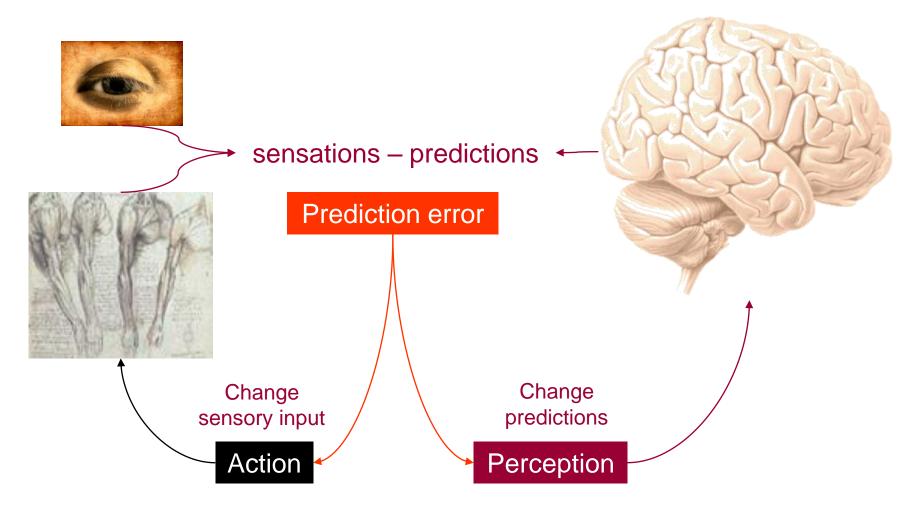
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Perception = inversion of a hierarchical generative model



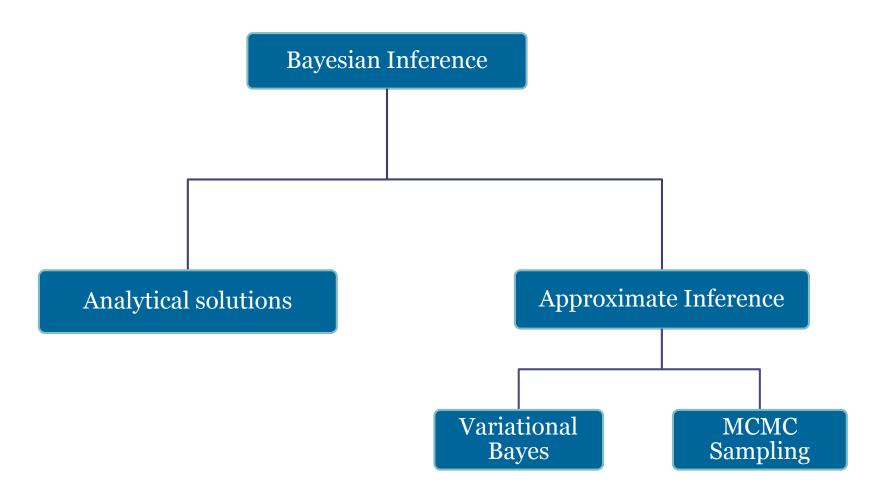
Free energy principle: predictive coding & active inference



Maximizing the evidence (of the brain's generative model) = minimizing the surprise about the data (sensory inputs).

Friston et al. 2006, *J Physiol Paris*

How is the posterior computed = how is a generative model inverted?



How is the posterior computed = how is a generative model inverted?

- compute the posterior analytically
 - requires conjugate priors
- variational Bayes (VB)
 - often hard work to derive, but fast to compute
 - uses approximations (approx. posterior, mean field)
 - problems: local minima, potentially inaccurate approximations
- Sampling: Markov Chain Monte Carlo (MCMC)
 - theoretically guaranteed to be accurate (for infinite computation time)
 - problems: may require very long run time in practice, convergence difficult to prove

Conjugate priors

- for a given likelihood function, the choice of prior determines the algebraic form of the posterior
- for some probability distributions a prior can be found such that the posterior has the same algebraic form as the prior
- such a prior is called "conjugate" to the likelihood
- examples:
 - Normal × Normal \propto Normal
 - Beta x Binomial ∞ Beta
 - Dirichlet \times Multinomial \propto Dirichlet

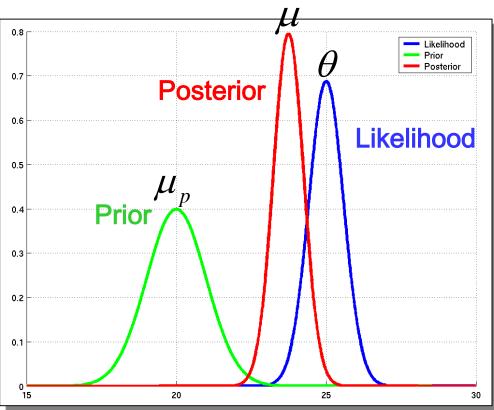
 $p(\boldsymbol{\theta} \mid \mathbf{y}) \propto p(\mathbf{y} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta})$ same form

Posterior mean & variance of univariate Gaussians

Likelihood & Prior $p(y \mid \theta) = N(\theta, \sigma_{\rho}^2)$ $p(\theta) = N(\mu_p, \sigma_p^2)$ 0.8 0.7 Posterior: $p(\theta \mid y) = N(\mu, \sigma^2)$ 0.6 $\frac{1}{\sigma^2} = \frac{1}{\sigma_e^2} + \frac{1}{\sigma_p^2}$ 0.5 $\mu = \sigma^2 \left(\frac{1}{\sigma_e^2} \theta + \frac{1}{\sigma_p^2} \mu_p \right)$ 0.3 0.2

Posterior mean = variance-weighted combination of prior mean and data mean

$$y = \theta + \varepsilon$$



Same thing – but expressed as precision weighting

Likelihood & prior

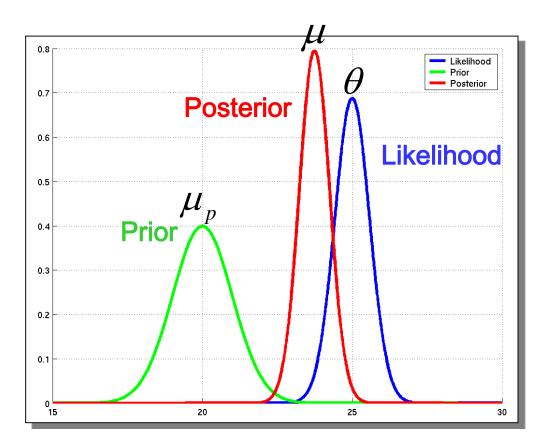
$$p(y | \theta) = N(\theta, \lambda_e^{-1})$$
$$p(\theta) = N(\mu_p, \lambda_p^{-1})$$

Posterior:
$$p(\theta \mid y) = N(\mu, \lambda^{-1})$$

$$\lambda = \lambda_e + \lambda_p$$
$$\mu = \frac{\lambda_e}{\lambda}\theta + \frac{\lambda_p}{\lambda}\mu_p$$

Relative precision weighting

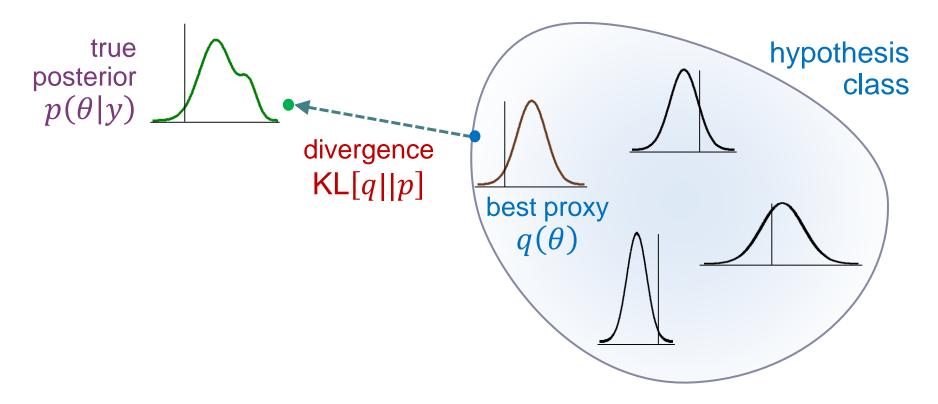
$$y = \theta + \varepsilon$$



Variational Bayes (VB)

Idea: find an approximate density $q(\theta)$ that is maximally similar to the true posterior $p(\theta|y)$.

This is often done by assuming a particular form for q (fixed form VB) and then optimizing its sufficient statistics.



Kullback–Leibler (KL) divergence

- asymmetric measure of the difference between two probability distributions P and Q
- Interpretations of $D_{KL}(P||Q)$:
 - "Bayesian surprise" when Q=prior, P=posterior: measure of the information gained when one updates one's prior beliefs to the posterior P
 - a measure of the information lost when Q is used to approximate P
- non-negative: ≥ 0 (zero when P=Q)

$$D_{\mathrm{KL}}(P||Q) = \sum_{i} P(i) \ln \frac{P(i)}{Q(i)}.$$

$$D_{\mathrm{KL}}(P||Q) = \int_{-\infty}^{\infty} p(x) \ln \frac{p(x)}{q(x)} \mathrm{d}x,$$

Variational calculus

Standard calculus Newton, Leibniz, and others

- functions $f: x \mapsto f(x)$
- derivatives $\frac{d_f}{d_x}$

Example: maximize the likelihood expression $p(y|\theta)$ w.r.t. θ Variational calculus Euler, Lagrange, and others

• functionals $F: f \mapsto F(f)$

• derivatives
$$\frac{dF}{df}$$

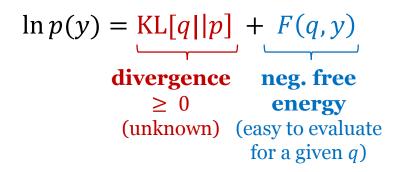
Example: maximize the entropy H[p]w.r.t. a probability distribution p(x)



Leonhard Euler (1707 – 1783)

Swiss mathematician, 'Elementa Calculi Variationum'

Variational Bayes

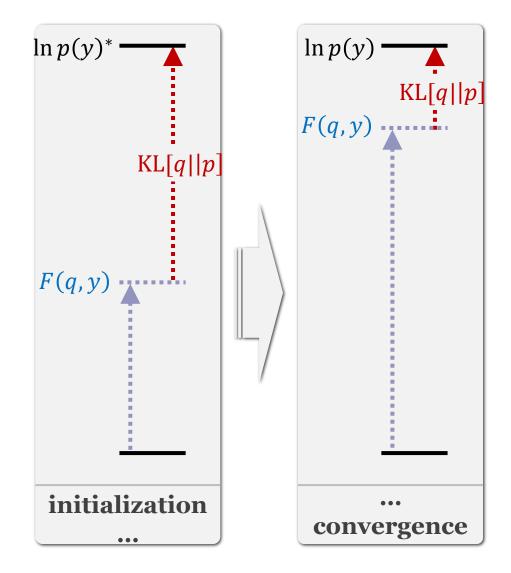


F(q) is a functional wrt. the approximate posterior $q(\theta)$.

Maximizing F(q, y) is equivalent to:

- minimizing KL[q||p]
- tightening F(q, y) as a lower bound to the log model evidence

When F(q, y) is maximized, $q(\theta)$ is our best estimate of the posterior.



Derivation of the (negative) free energy approximation

- See whiteboard!
- (or Appendix to Stephan et al. 2007, NeuroImage 38: 387-401)

Mean field assumption

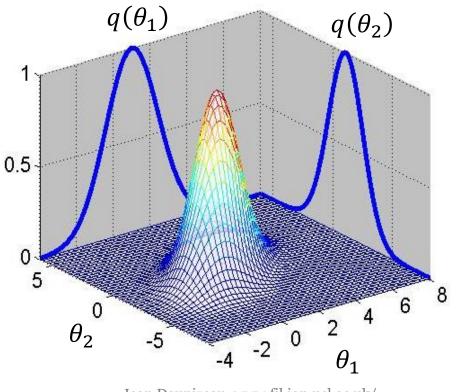
Factorize the approximate posterior $q(\theta)$ into independent partitions:

$$q(\theta) = \prod_i q_i(\theta_i)$$

where $q_i(\theta_i)$ is the approximate posterior for the *i*th subset of parameters.

For example, split parameters and hyperparameters:

$$p(\theta, \lambda \mid y) \approx q(\theta, \lambda) = q(\theta)q(\lambda)$$



Jean Daunizeau, www.fil.ion.ucl.ac.uk/ ~jdaunize/presentations/Bayes2.pdf

VB in a nutshell (under mean-field approximation)

 Neg. free-energy approx. to model evidence.

$$\ln p(y|m) = F + KL[q(\theta,\lambda), p(\theta,\lambda|y)]$$
$$F = \langle \ln p(y|\theta,\lambda) \rangle_{q} - KL[q(\theta,\lambda), p(\theta,\lambda|m)]$$

Mean field approx.

$$p(\theta, \lambda | y) \approx q(\theta, \lambda) = q(\theta)q(\lambda)$$

 Maximise neg. free energy wrt. q = minimise divergence, by maximising variational energies

$$q(\theta) \propto \exp(I_{\theta}) = \exp\left[\left\langle \ln p(y,\theta,\lambda) \right\rangle_{q(\lambda)}\right]$$
$$q(\lambda) \propto \exp(I_{\lambda}) = \exp\left[\left\langle \ln p(y,\theta,\lambda) \right\rangle_{q(\theta)}\right]$$

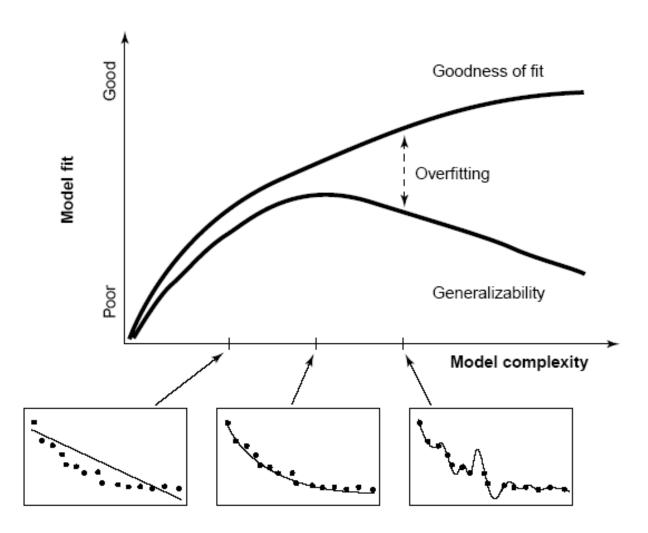
 Iterative updating of sufficient statistics of approx. posteriors by gradient ascent.

Model comparison and selection

Given competing hypotheses on structure & functional mechanisms of a system, which model is the best?

Which model represents the best balance between model fit and model complexity?

For which model m does p(y|m) become maximal?



Pitt & Miyung (2002) TICS

Bayesian model selection (BMS)

- First step of inference: define model space *M*
- Inference on model structure *m*:

 $|M| \in [1,\infty[$

Posterior model probability $p(m \mid y) = \frac{p(y \mid m) p(m)}{p(y)}$ $= \frac{p(y \mid m) p(m)}{\sum_{m} p(y \mid m) p(m)}$

• For a uniform prior on *m*, model evidence sufficient for model selection

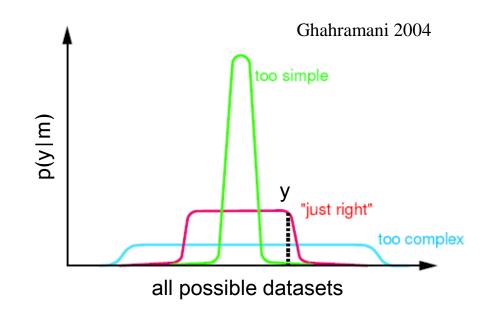
Model evidence: $p(y | m) = \int p(y | \theta, m) p(\theta | m) d\theta$

Bayesian model selection (BMS)

Model evidence:

$$p(y \mid m) = \int p(y \mid \theta, m) p(\theta \mid m) \ d\theta$$

- probability that data were generated by model *m*, averaging over all possible parameter values (as specified by the prior)
- ⇒ accounts for both accuracy and complexity of the model



Various approximations:

- negative free energy (F)
- Akaike Information Criterion (AIC)
- Bayesian Information Criterion (BIC)

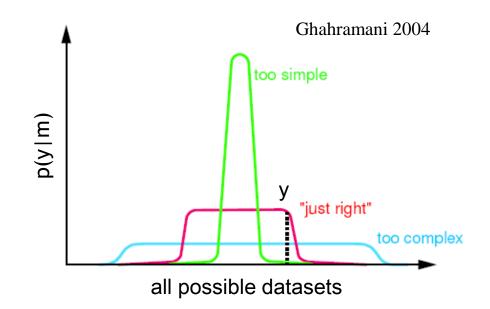
Bayesian model selection (BMS)

Model evidence:

$$p(y \mid m) = \int p(y \mid \theta, m) p(\theta \mid m) \ d\theta$$

"If I randomly sampled from my prior and plugged the resulting value into the likelihood function, how close would the predicted data be – on average – to my observed data?"

accounts for both accuracy and complexity of the model

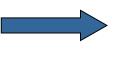


Various approximations:

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Approximations to the model evidence

Logarithm is a monotonic function



Maximizing log model evidence = Maximizing model evidence

Log model evidence = balance between fit and complexity $\log p(y | m) = accuracy(m) - complexity(m)$ $= \log p(y | \theta, m) - complexity(m)$ No. of parameters Akaike Information Criterion: $AIC = \log p(y | \theta, m) - (p)$ Bayesian Information Criterion: $BIC = \log p(y | \theta, m) - \frac{p}{2} \log N$ No. of data points

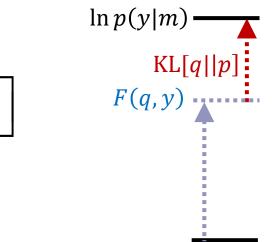
The (negative) free energy approximation ${\it F}$

F is a lower bound on the log model evidence:

$$\log p(y | m) = F + KL[q(\theta), p(\theta | y, m)]$$

Like AIC/BIC, *F* is an accuracy/complexity tradeoff:

$$F = \underbrace{\langle \log p(y | \theta, m) \rangle}_{accuracy} - \underbrace{KL[q(\theta), p(\theta | m)]}_{complexity}$$



The (negative) free energy approximation

• Log evidence is thus expected log likelihood (wrt. q) plus 2 KL's:

$$\log p(y | m) = \langle \log p(y | \theta, m) \rangle - KL[q(\theta), p(\theta | m)] + KL[q(\theta), p(\theta | y, m)]$$

$$F = \log p(y|m) - KL[q(\theta), p(\theta|y,m)]$$
$$= \langle \log p(y|\theta,m) \rangle - KL[q(\theta), p(\theta|m)]$$
$$\underbrace{\operatorname{complexity}}_{complexity}$$

The complexity term in F

In contrast to AIC & BIC, the complexity term of the negative free energy F accounts for parameter interdependencies.
 Under Gaussian assumptions about the posterior (Laplace approximation):

$$KL[q(\theta), p(\theta \mid m)] = \frac{1}{2} \ln |C_{\theta|y}| + \frac{1}{2} (\mu_{\theta|y} - \mu_{\theta})^T C_{\theta}^{-1} (\mu_{\theta|y} - \mu_{\theta})$$

- The complexity term of *F* is higher
 - the more independent the prior parameters (\uparrow effective DFs)
 - the more dependent the posterior parameters
 - the more the posterior mean deviates from the prior mean

Bayes factors

To compare two models, we could just compare their log evidences.

But: the log evidence is just some number – not very intuitive!

A more intuitive interpretation of model comparisons is made possible by Bayes factors:

$$B_{12} = \frac{p(y \mid m_1)}{p(y \mid m_2)}$$

positive value, [0; ∞ [

Kass & Raftery classification:

B ₁₂	p(m₁ y)	Evidence
1 to 3	50-75%	weak
3 to 20	75-95%	positive
20 to 150	95-99%	strong
≥ 150	≥ 99%	Very strong

Fixed effects BMS at group level

Group Bayes factor (GBF) for 1...K subjects:

$$GBF_{ij} = \prod_{k} BF_{ij}^{(k)}$$

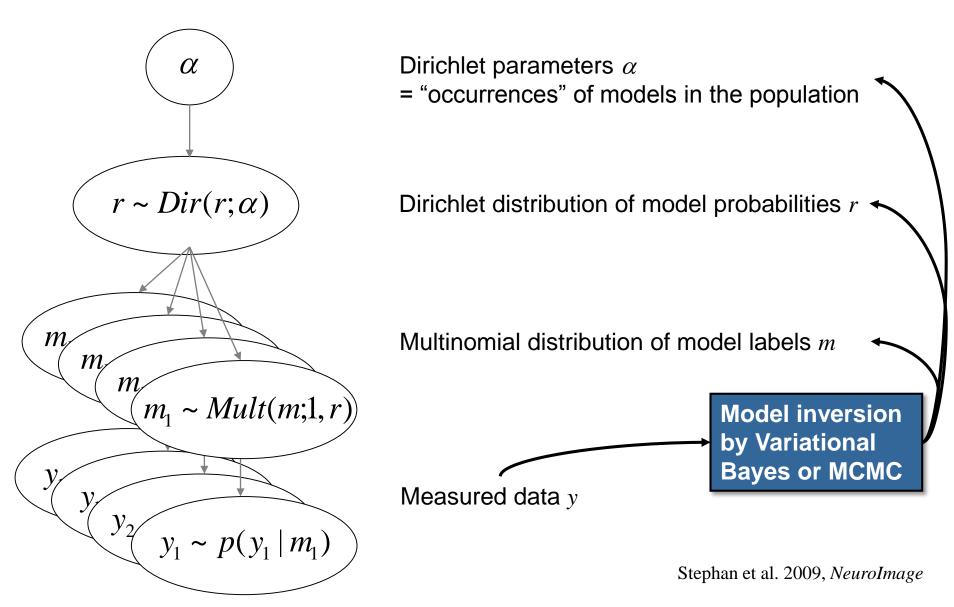
Average Bayes factor (ABF):

$$ABF_{ij} = \sqrt[K]{\prod_{k} BF_{ij}^{(k)}}$$

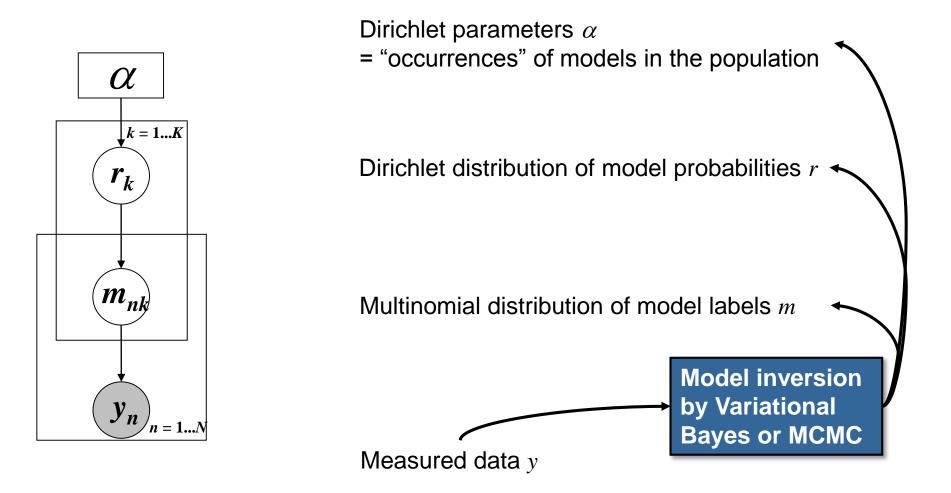
Problems:

- blind with regard to group heterogeneity
- sensitive to outliers

Random effects BMS for heterogeneous groups



Random effects BMS for heterogeneous groups



Stephan et al. 2009, NeuroImage

Four equivalent options for reporting model ranking by random effects BMS

1. Dirichlet parameter estimates

2. **expected posterior probability** of obtaining the k-th model for any randomly selected subject

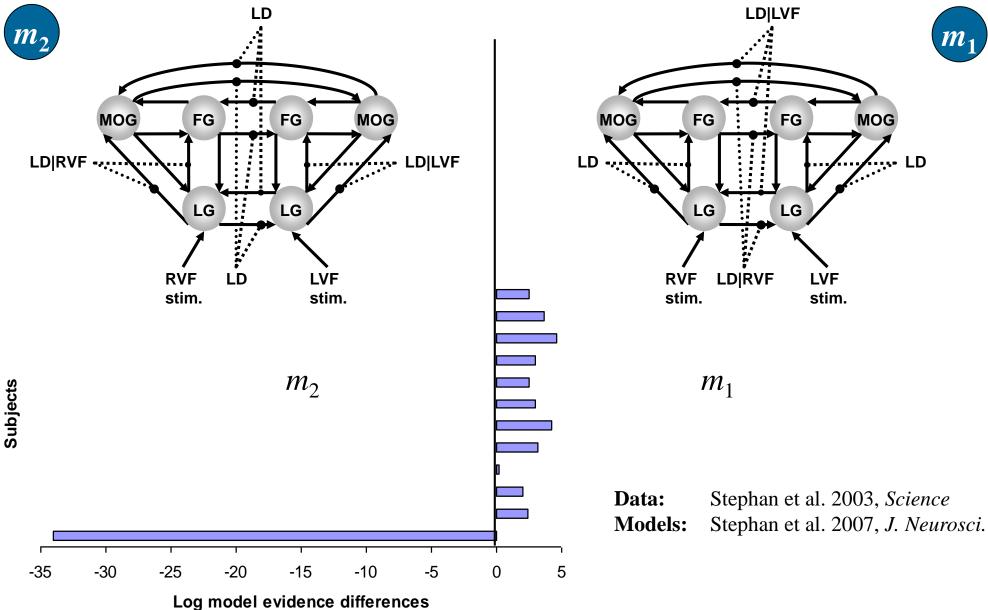
$$\langle r_k \rangle_q = \alpha_k / (\alpha_1 + \ldots + \alpha_K)$$

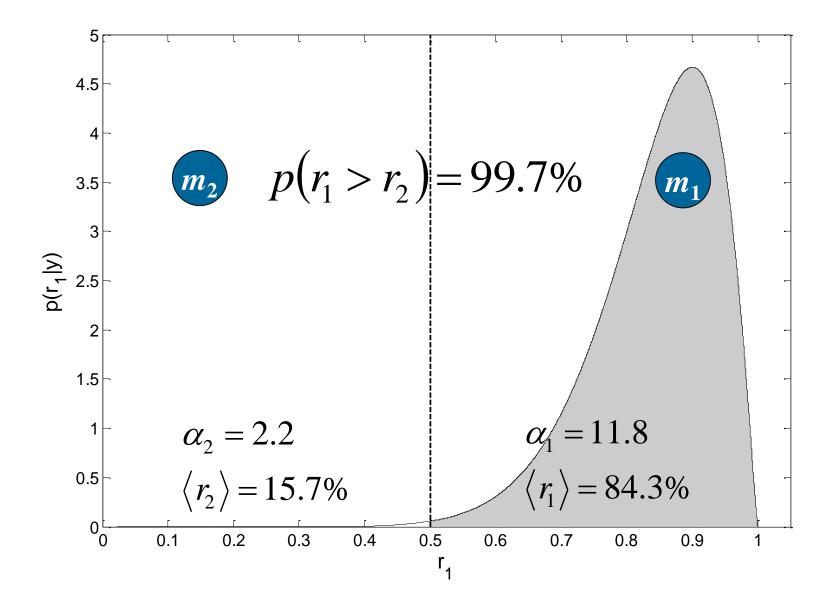
α

- 3. **exceedance probability** that a particular model *k* is more likely than any other model (of the *K* models tested), given the group data
- 4. protected exceedance probability: see below

$$\exists k \in \{1...K\}, \forall j \in \{1...K \mid j \neq k\}:$$
$$\varphi_k = p(r_k > r_j \mid y; \alpha)$$

Example: Hemispheric interactions during vision

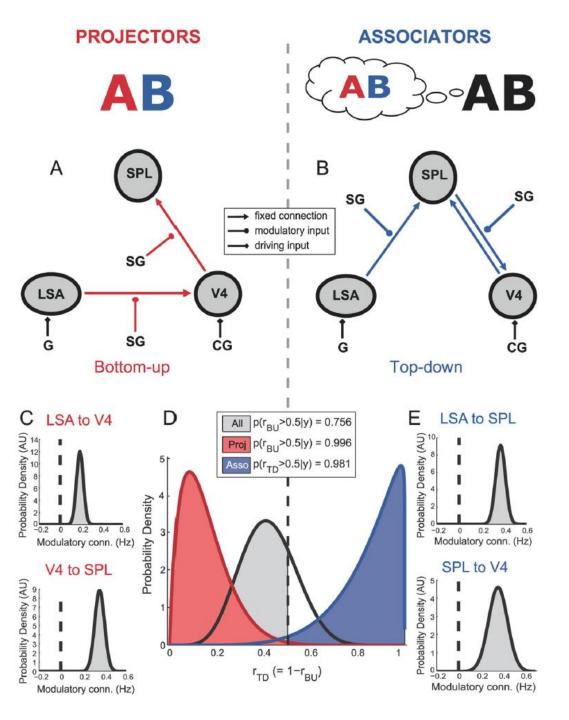




Stephan et al. 2009a, NeuroImage

Example: Synaesthesia

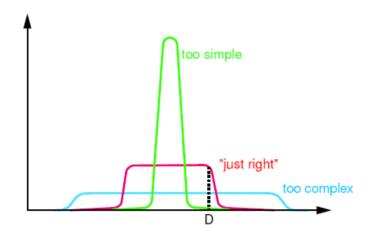
- "projectors" experience color externally colocalized with a presented grapheme
- "associators" report an internally evoked association
- across all subjects: no evidence for either model
- but BMS results map precisely onto projectors (bottom-up mechanisms) and associators (top-down)



van Leeuwen et al. 2011, J. Neurosci.

Overfitting at the level of models

- \uparrow #models \Rightarrow \uparrow risk of overfitting
- solutions:
 - regularisation: definition of model space = choosing priors p(m)
 - family-level BMS
 - Bayesian model averaging (BMA)



posterior model probability:

$$p(m \mid y) = \frac{p(y \mid m) p(m)}{\sum_{m} p(y \mid m) p(m)}$$

BMA:

$$p(\theta | y)$$

 $= \sum_{m} p(\theta | y, m) p(m | y)$

Model space partitioning: comparing model families

- partitioning model space into K subsets or families:
- pooling information over all models in these subsets allows one to compute the probability of a model family, given the data
- effectively removes uncertainty about any aspect of model structure, other than the attribute of interest (which defines the partition)

$$M = \left\{ f_1, \dots, f_K \right\}$$

 $p(f_k)$

Stephan et al. 2009, *NeuroImage* Penny et al. 2010, *PLoS Comput. Biol.*

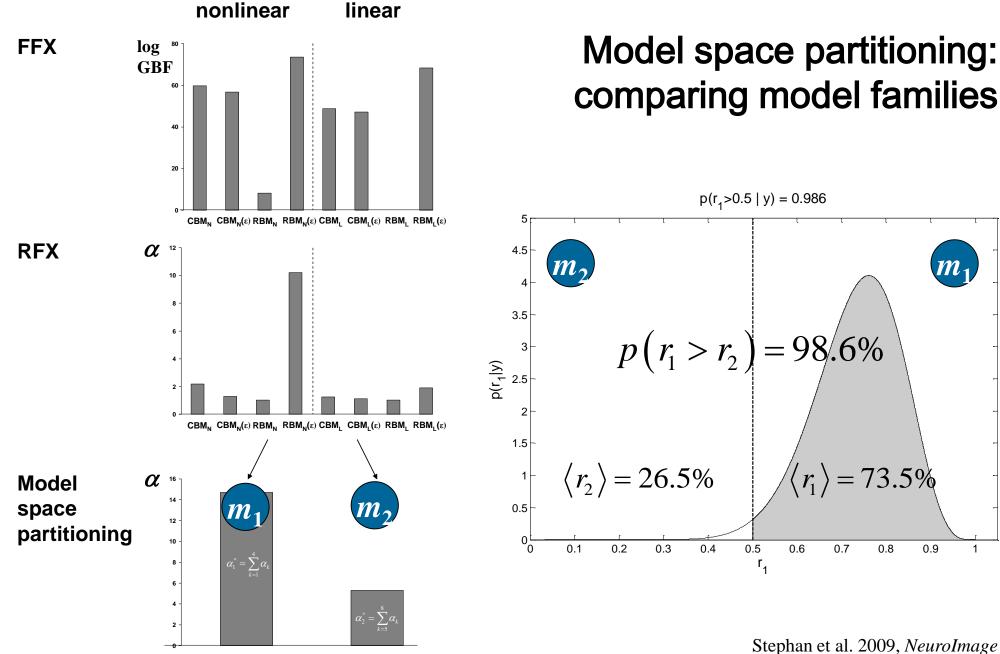
Family-level inference: random effects – a special case

• When the families are of equal size, one can simply sum the posterior model probabilities within families by exploiting the agglomerative property of the Dirichlet distribution:

$$(r_1, r_2, ..., r_K) \sim Dir(\alpha_1, \alpha_2, ..., \alpha_K)$$

$$\Rightarrow r_1^* = \sum_{k \in N_1} r_k, r_2^* = \sum_{k \in N_2} r_k, ..., r_J^* = \sum_{k \in N_J} r_k$$

$$\sim Dir\left(\alpha_1^* = \sum_{k \in N_1} \alpha_k, \alpha_2^* = \sum_{k \in N_2} \alpha_k, ..., \alpha_J^* = \sum_{k \in N_J} \alpha_k\right)$$



nonlinear models linear models

Bayesian Model Averaging (BMA)

- abandons dependence of parameter inference on a single model and takes into account model uncertainty
- uses the entire model space considered (or an optimal family of models)
- averages parameter estimates, weighted by posterior model probabilities
- represents a particularly useful alternative
 - when none of the models (or model subspaces) considered clearly outperforms all others
 - when comparing groups for which the optimal model differs

single-subject BMA:

$$p(\theta \mid y) = \sum_{m} p(\theta \mid y, m) p(m \mid y)$$

group-level BMA: $p(\theta_n \mid y_{1..N})$ $= \sum p(\theta_n \mid y_n, m) p(m \mid y_{1..N})$

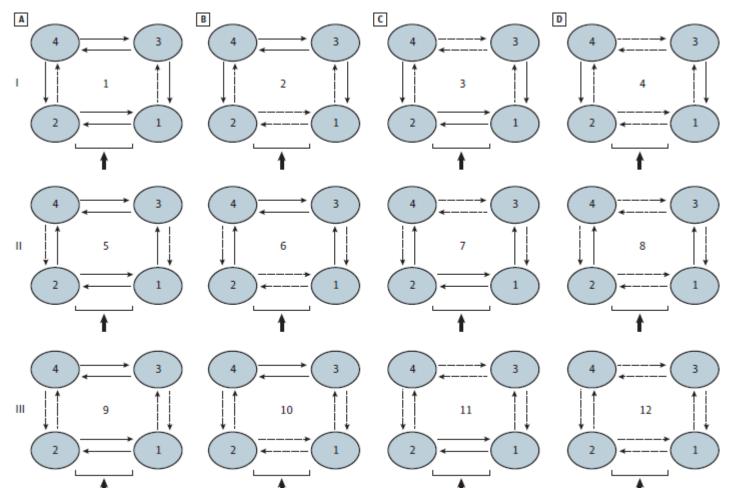
т

NB: $p(m|y_{1..N})$ can be obtained by either FFX or RFX BMS



- 17 at-risk mental state (ARMS) individuals
- 21 first-episode patients (13 non-treated)
- 20 controls

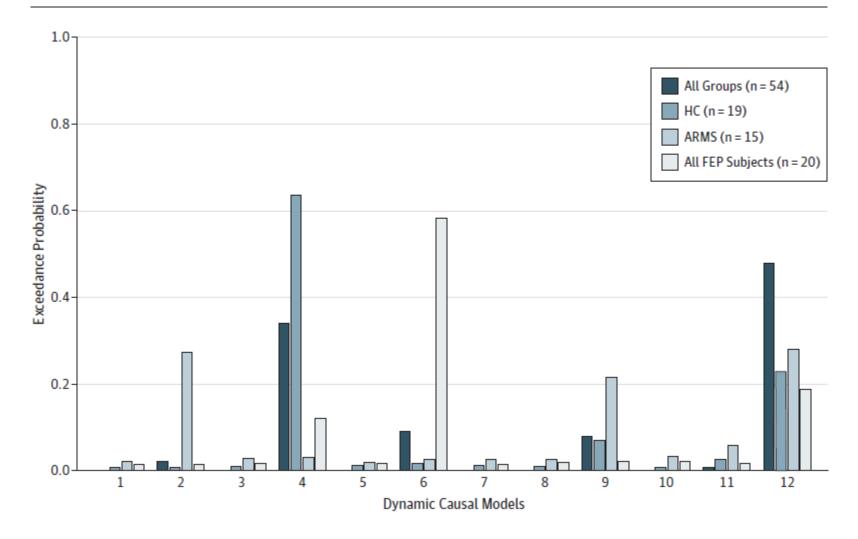
Prefrontal-parietal connectivity during working memory in schizophrenia



Driving input
 Driving input
 Endogenous connection
 Modulatory input

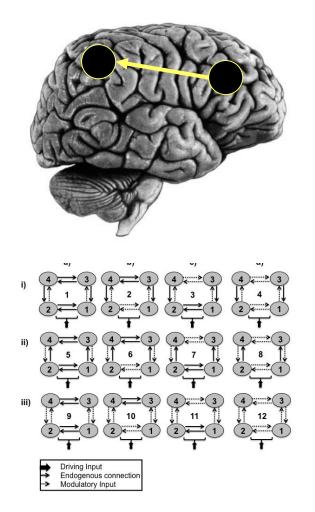
Schmidt et al. 2013, JAMA Psychiatry

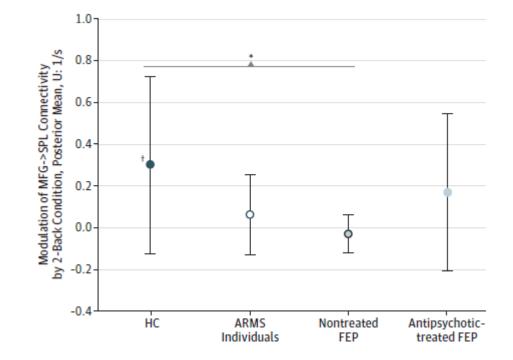
BMS results for all groups



Schmidt et al. 2013, JAMA Psychiatry

BMA results: $PFC \rightarrow PPC$ connectivity





17 ARMS, 21 first-episode (13 non-treated), 20 controls

Protected exceedance probability: Using BMA to protect against chance findings

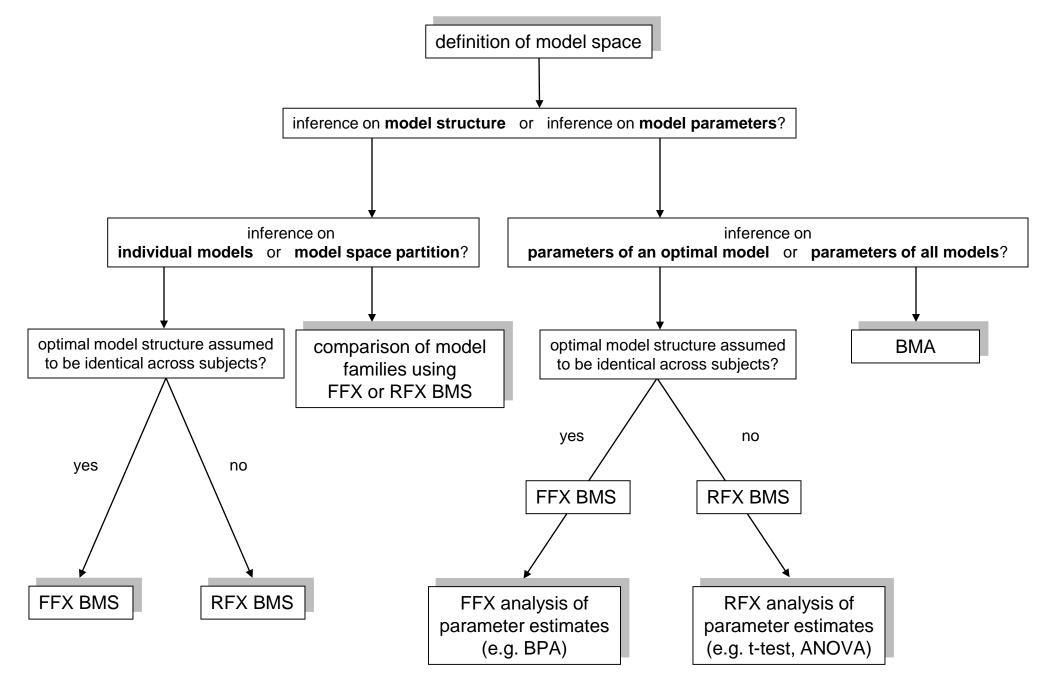
- EPs express our confidence that the posterior probabilities of models are different under the hypothesis H_1 that models differ in probability: $r_k \neq 1/K$
- does not account for possibility "null hypothesis" H_0 : $r_k=1/K$
- **Bayesian omnibus risk (BOR)** of wrongly accepting H_1 over H_0 :

$$P_{o} = \frac{1}{1 + \frac{p(m|H_{1})}{p(m|H_{0}).}}$$

• **protected EP**: Bayesian model averaging over H_0 and H_1 :

$$\begin{split} \widetilde{\varphi}_{k} &= P(r_{k} \geq r_{k' \neq k} | y) \\ &= P(r_{k} \geq r_{k' \neq k} | y, H_{1}) P(H_{1} | y) + P(r_{k} \geq r_{k' \neq k} | y, H_{0}) P(H_{0} | y) \\ &= \varphi_{k}(1 - P_{0}) + \frac{1}{K} P_{0} \end{split}$$

Rigoux et al. 2014, NeuroImage



Stephan et al. 2010, NeuroImage

Further reading

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Thank you