

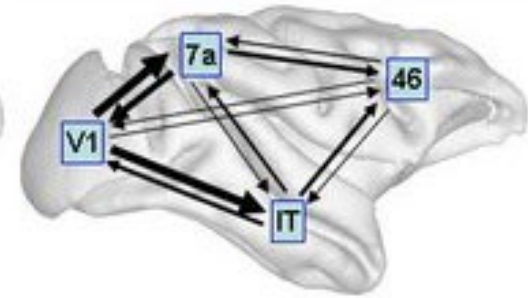
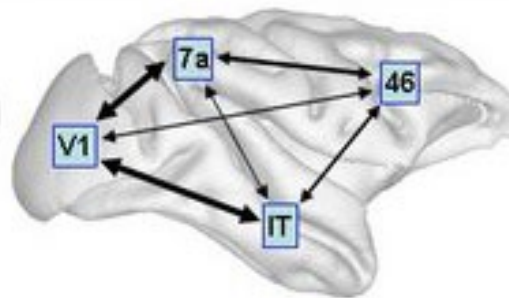
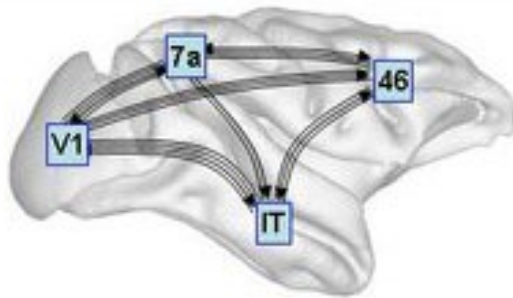
Modeling connectivity: Dynamic Causal Modeling for fMRI

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Institute for Biomedical Engineering
University and ETH Zürich

CP Course 2022, Zürich, Switzerland

Structural, functional & effective connectivity



Sporns 2007, *Scholarpedia*

anatomical/structural

- presence of physical connections

→ *DWI, tractography, tracer studies (animals)*

functional

- statistical dependency between regional time series

→ *correlations, ICA*

effective

- direct influences between neuronal populations

→ *DCM*

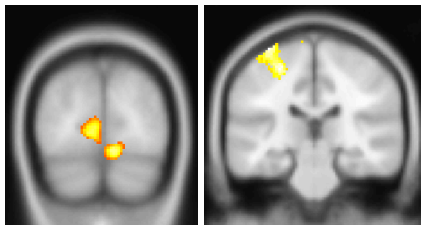
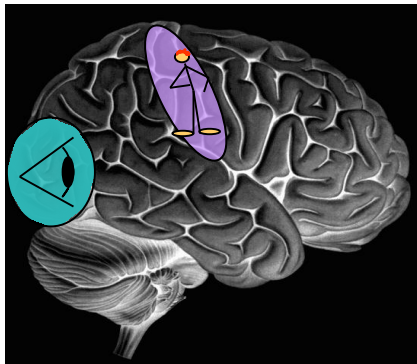
Context-independent

Mechanism - free

Mechanistic

Specialisation vs. Integration

Functional Specialisation

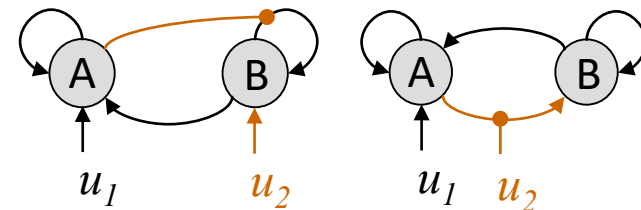
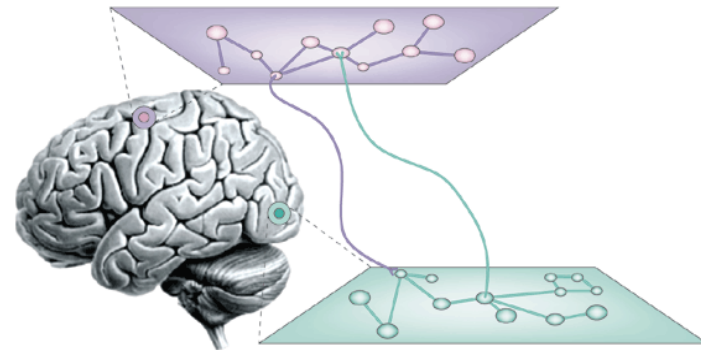


u_1

$u_1 \times u_2$

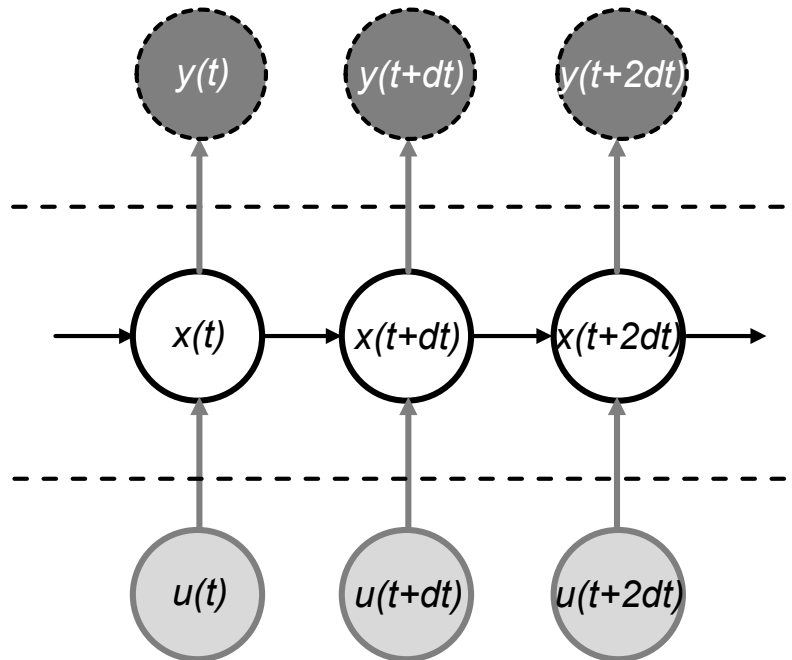
«**Where**, in the brain, did my experimental manipulation have an effect?»

Functional Integration



«**How** did my experimental manipulation propagate through the network?»

A reminder – generative models



Observed data (fMRI)

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

Hidden states (Brain activity)

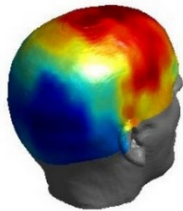
$$\frac{dx}{dt} = f(x, u, \theta) + \omega$$

Inputs (Exp. manipulations)

$$u(t)$$

Dynamic causal modelling

EEG,
MEG

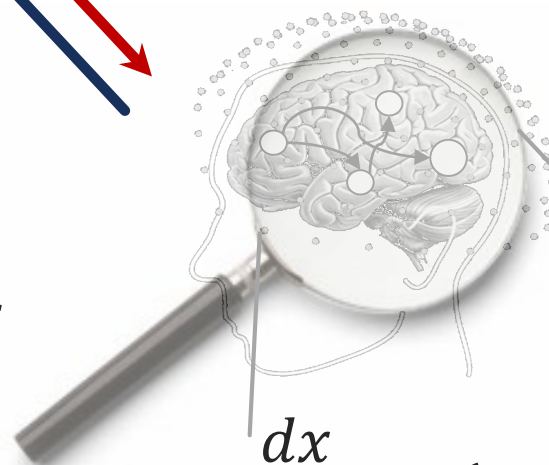
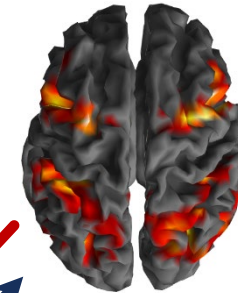


Model inversion:
Estimating
neuronal
mechanisms

Forward model:
Predicting
measured activity

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

fMRI



$$\frac{dx}{dt} = f(x, u, \theta) + \omega$$

State equation:
Describing neuronal
dynamics (and
hemodynamics)

DCM for EEG
→ later today
→ Rosalyn Moran



Dynamic causal modelling



ACADEMIC
PRESS

Available online at www.sciencedirect.com



NeuroImage 19 (2003) 1273–1302

NeuroImage

www.elsevier.com/locate/ynimg

Dynamic causal modelling

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Received 18 October 2002; revised 7 March 2003; accepted 2 April 2003

DCM for fMRI - overview

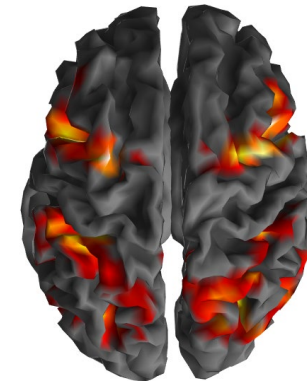
Model inversion:
Estimating
neuronal
mechanisms

Forward model:
Predicting
measured activity

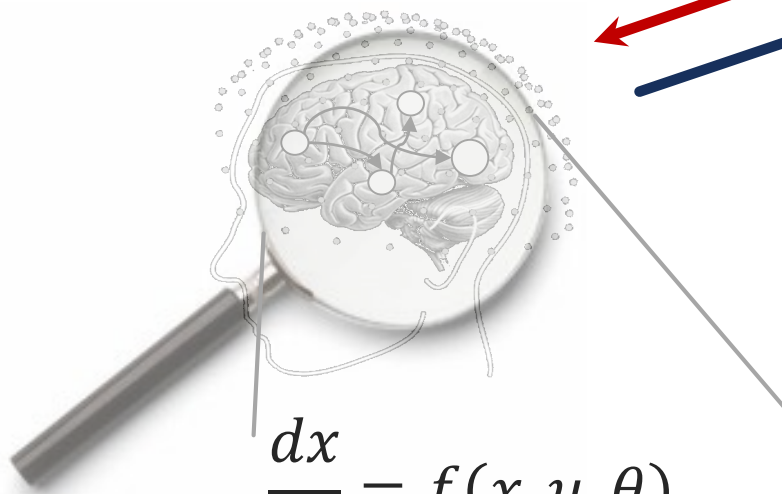
$$y = g(x, \theta) + \varepsilon$$

Neural state equation:
Describing neuronal
dynamics

$$\frac{dx}{dt} = f(x, u, \theta)$$



fMRI



DCM for fMRI - overview

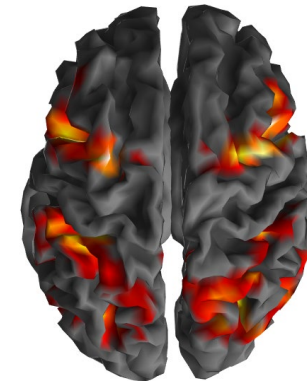
Model inversion:
Estimating
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Forward model:
Predicting
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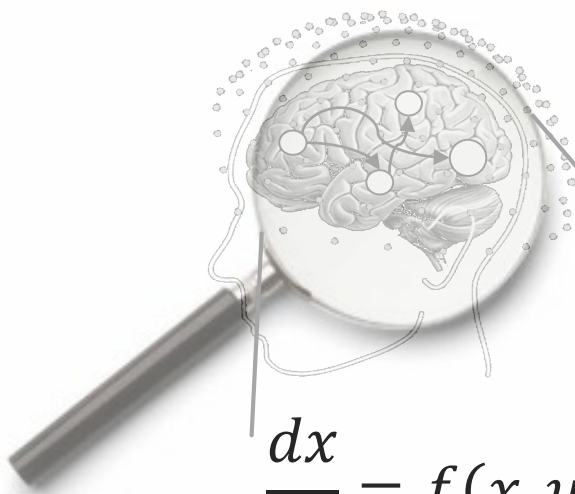
$$y = g(x, \theta) + \varepsilon$$

Neural state equation:
Describing neuronal
dynamics

$$\frac{dx}{dt} = f(x, u, \theta)$$



fMRI





Neuronal state equations

$$\frac{dx}{dt} = f(x, u)$$

Neuronal state equations

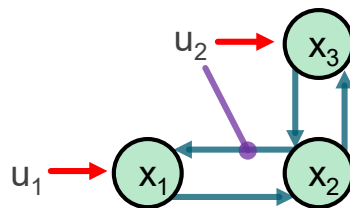
$$\frac{dx}{dt} = f(x, u) \approx f(x_0, 0) + \frac{\partial f}{\partial x} x + \frac{\partial f}{\partial u} u + \frac{\partial^2 f}{\partial x \partial u} ux + \frac{\partial^2 f}{\partial x^2} \frac{x^2}{2} + \dots$$

bilinear model

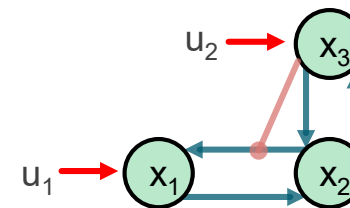
Neuronal state equations

$$\frac{dx}{dt} = f(x, u) \approx \overset{A}{f(x_0, 0)} + \overset{C}{\frac{\partial f}{\partial x} x} + \overset{B}{\frac{\partial f}{\partial u} u} + \overset{D}{\frac{\partial^2 f}{\partial x \partial u} ux} + \frac{\partial^2 f}{\partial x^2} \frac{x^2}{2} + \dots$$

bilinear model

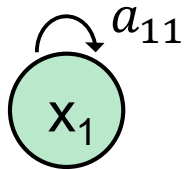


nonlinear model



Neuronal state equations

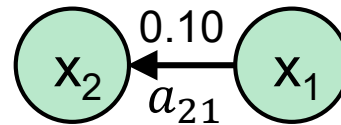
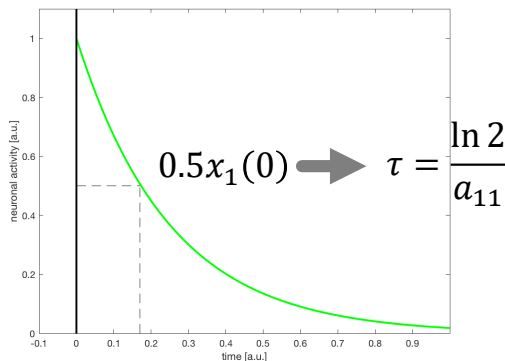
DCM effective connectivity parameters are rate constants



$$\frac{dx_1}{dt} = a_{11}x_1$$



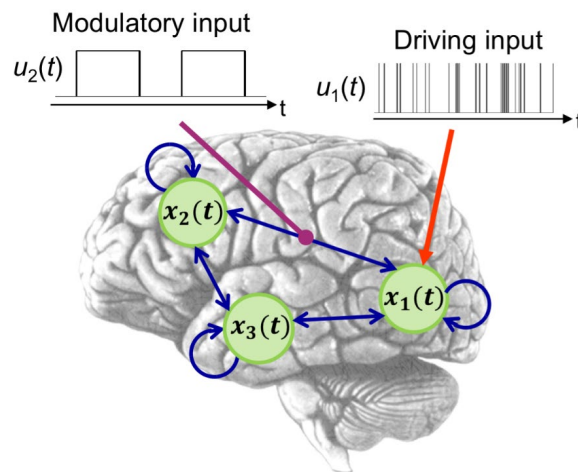
$$x_1(t) = x_1(0) \cdot \exp(a_{11}t)$$



If a_{21} is 0.10s^{-1} , this means that, per unit time, the increase in activity in x_2 corresponds to 10% of the current activity in x_1

Neuronal state equations

Interim summary: bilinear neuronal state equation



State change

External inputs

Current state

$$\frac{dx}{dt} = \underbrace{\left(A + \sum_{j=1}^m u_j B^{(j)} \right)}_{\text{connectivity}} x + C u$$

$$\theta = \{ A, B^{(1)}, \dots, B^{(m)}, C \}$$

Endogenous connectivity

Modulatory connectivity

Driving input weights

DCM for fMRI - overview

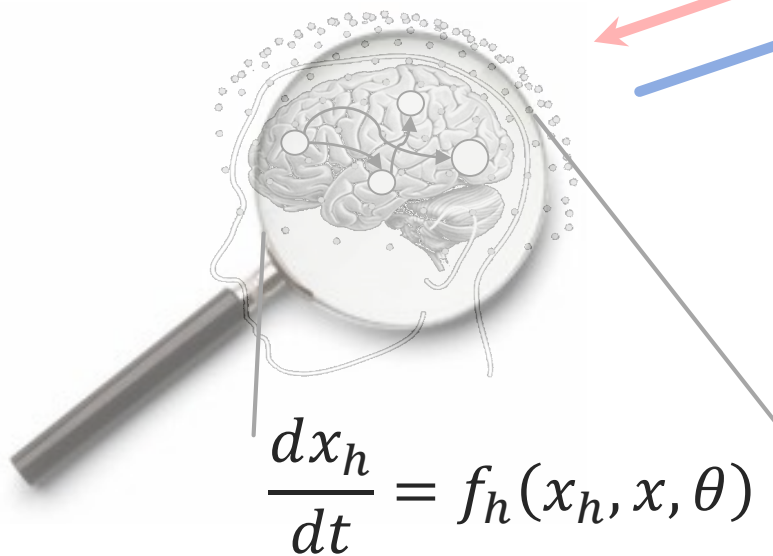
Model inversion:
Estimating
neuronal
mechanisms

Forward model:
Predicting
measured activity

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

Hemodynamic state equation:
Describing hemodynamics

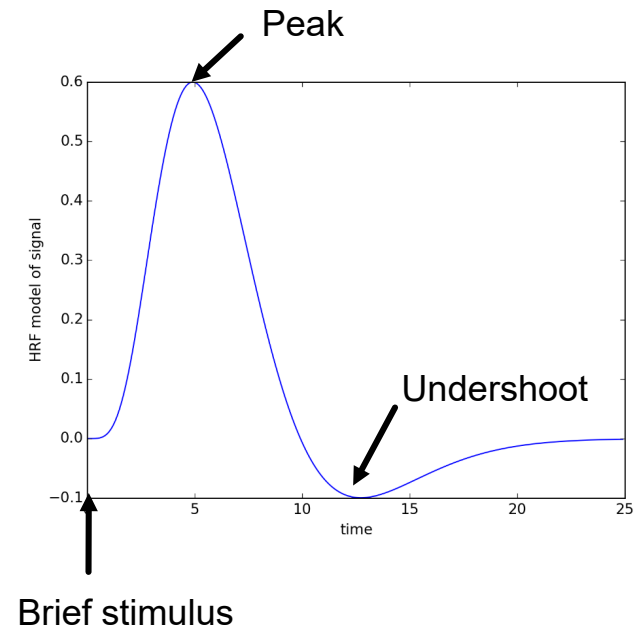
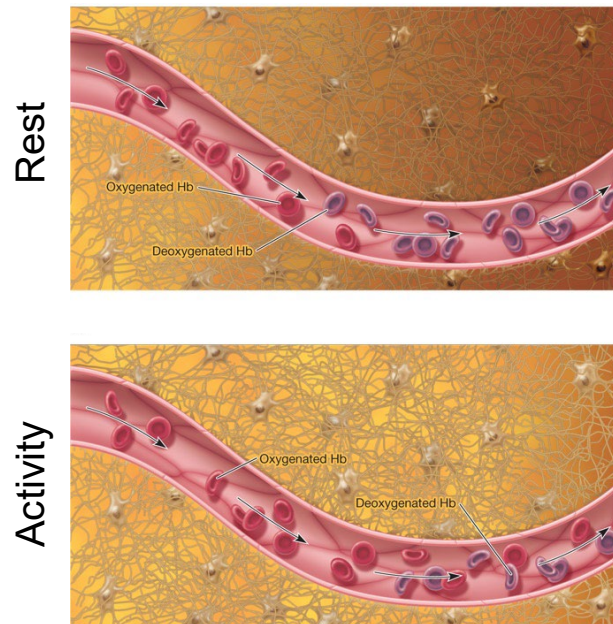
fMRI



The hemodynamic response

Neuronal dynamics only indirectly observable via hemodynamic response

↑ neuronal activity
 ↑ blood flow
 ↑ oxygenated Hb
 ↑ T2*
 ↑ fMRI signal



The hemodynamic model

6 parameters:

$$\theta^h = \{\kappa, \gamma, \tau, \alpha, \rho, \varepsilon\}$$

Important for model fitting,
but typically of no interest
for statistical inference.

Region specific HRF

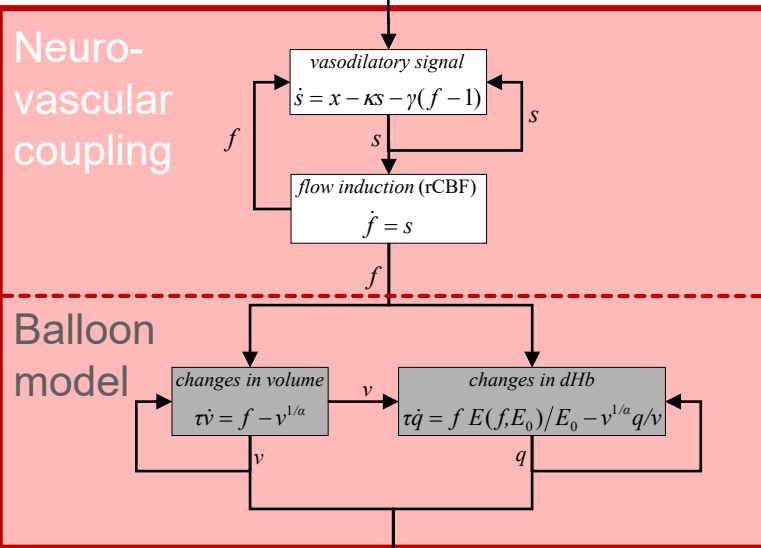
→ Parameters computed
separately for each region

State equation

neural

Inputs u

$$\frac{dx}{dt} = \left(A + \sum_{j=1}^m u_j B^{(j)} \right) x + Cu$$



hemodynamic

$$\lambda(q, v) = \frac{\Delta S}{S_0} \approx V_0 \left[k_1(1 - q) + k_2 \left(1 - \frac{q}{v} \right) + k_3(1 - v) \right]$$

$$k_1 = 4.3 \vartheta_0 E_0 TE$$

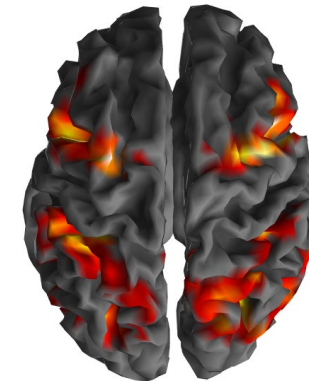
$$k_2 = \varepsilon r_0 E_0 TE$$

$$k_3 = 1 - \varepsilon$$

**BOLD signal
change equation**

DCM for fMRI - overview

Model inversion:
Estimating
neuronal
mechanisms



fMRI

Forward model:
Predicting
measured activity

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

Neural state equation:
Describing neuronal
dynamics

$$\frac{dx}{dt} = f(x, u, \theta) + \omega$$



The BOLD signal equation

Resting blood
volume

Deoxyhemoglobin
content

Blood
volume

$$\lambda(q, v) = \frac{\Delta S}{S_0} \approx V_0 \left[k_1(1 - q) + k_2 \left(1 - \frac{q}{v} \right) + k_3(1 - v) \right]$$

BOLD-Signal Parameters:

$$k_1 = 4.3 \vartheta_0 E_0 TE$$

$$k_2 = \varepsilon r_0 E_0 TE$$

$$k_3 = 1 - \varepsilon$$

$$V_0 = 0.04 \quad E_0 = 0.32 - 0.4$$

At 1.5 Tesla

At 3 Tesla

At 7 Tesla

$$\vartheta_0 \approx 40.3 \text{ s}^{-1}$$

$$\vartheta_0 \approx 80.6 \text{ s}^{-1}$$

$$\vartheta_0 \approx 188 \text{ s}^{-1}$$

$$r_0 \approx 25 \text{ s}^{-1}$$

$$r_0 \approx 110 \text{ s}^{-1}$$

$$r_0 \approx 340 \text{ s}^{-1}$$

$$TE \approx 0.04 \text{ s}$$

$$TE \approx 0.035 \text{ s}$$

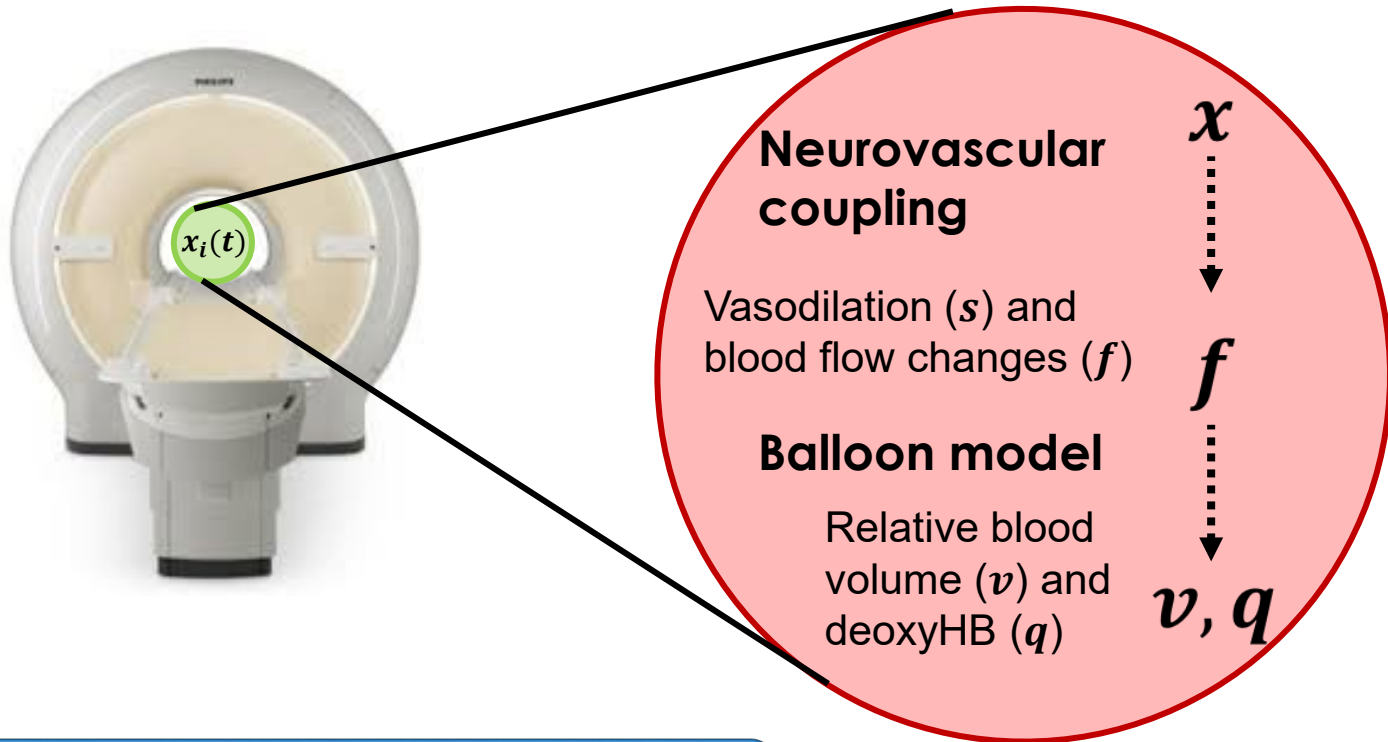
$$TE \approx 0.025 \text{ s}$$

$$\varepsilon \approx 1.28$$

$$\varepsilon \approx 0.47$$

$$\varepsilon \approx 0.026$$

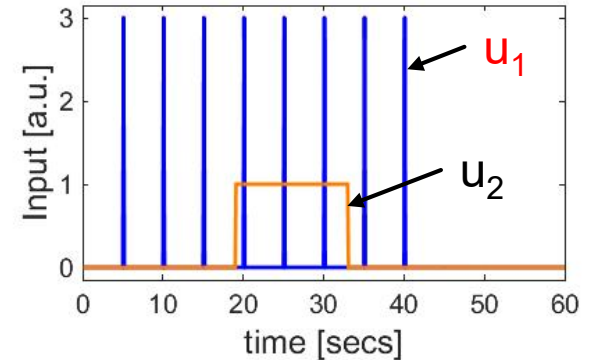
From neural activity to the BOLD signal: summary



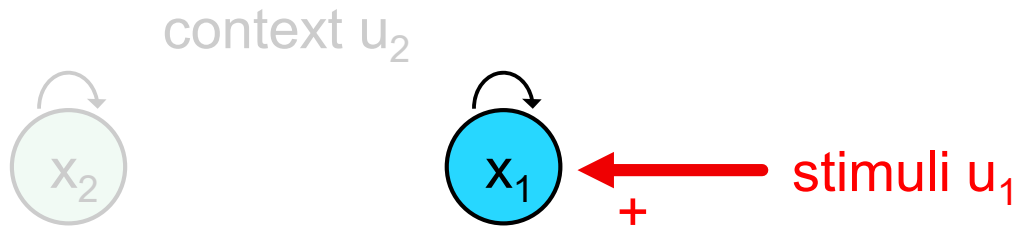
BOLD signal is a **direct function** of v and q

$$y = \frac{\Delta S}{S_0} = g(v, q) + \varepsilon$$

Simulation example: What can DCM explain?



Example: single node

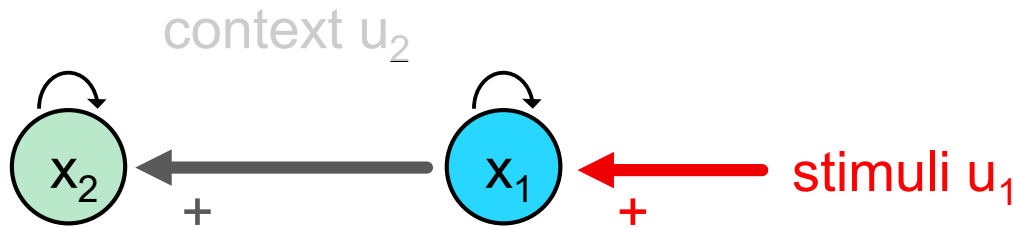


$$\frac{dx}{dt} = (A + u_2 B^{(2)})x + C u_1$$

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \left(\begin{bmatrix} a_{11} & 0 \\ 0 & a_{22} \end{bmatrix} + u_2 \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \right) \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} c_{11} & 0 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

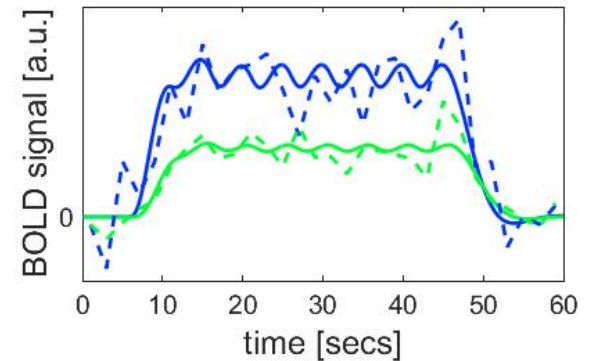
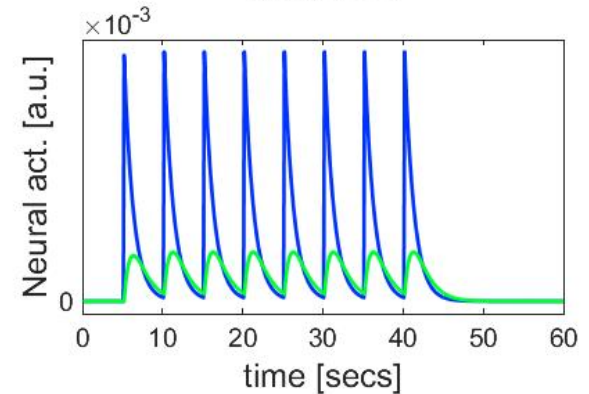
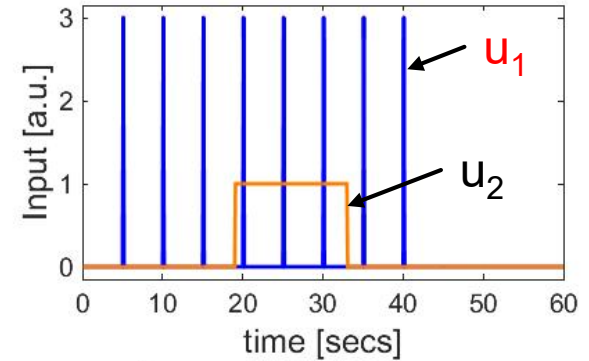
Simulation example: What can DCM explain?

Example: two connected node



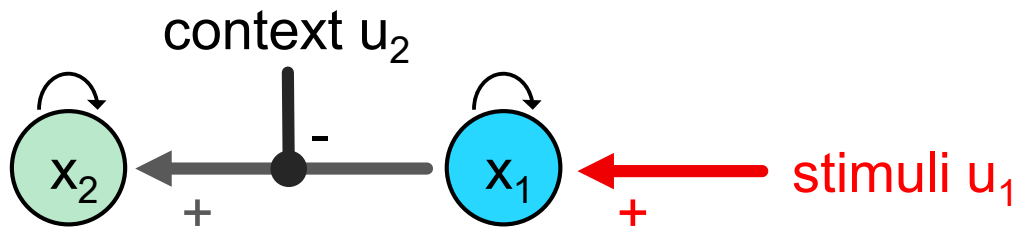
$$\frac{dx}{dt} = (A + u_2 B^{(2)})x + C u_1$$

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \left(\begin{bmatrix} a_{11} & 0 \\ a_{21} & a_{22} \end{bmatrix} + u_2 \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \right) \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} c_{11} & 0 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$



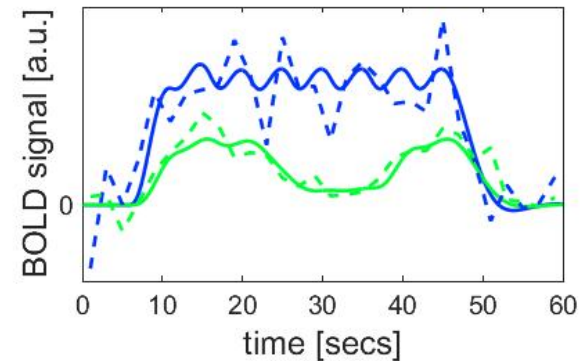
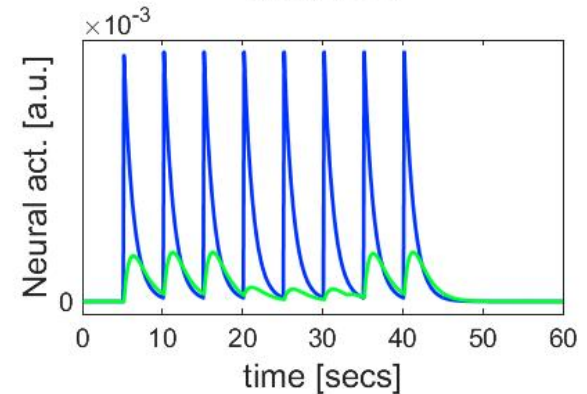
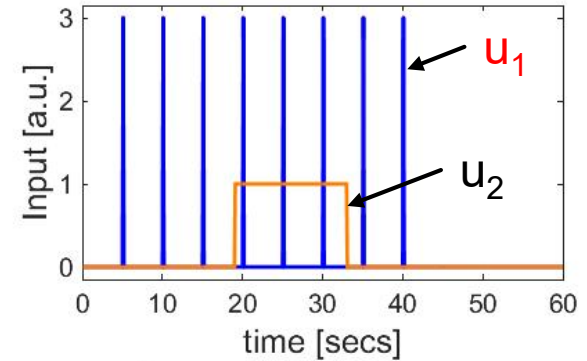
Simulation example: What can DCM explain?

Example: modulation of connection



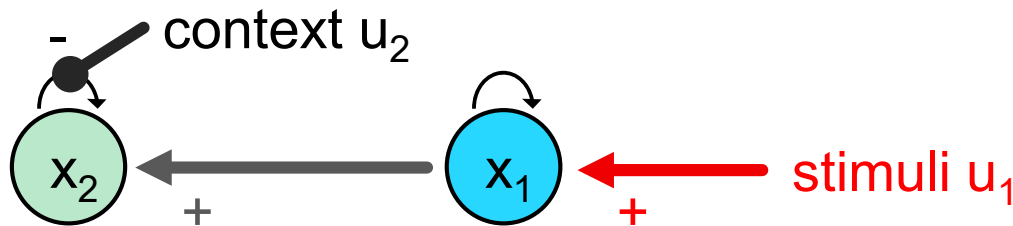
$$\frac{dx}{dt} = (A + u_2 B^{(2)})x + C u_1$$

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \left(\begin{bmatrix} a_{11} & 0 \\ a_{21} & a_{22} \end{bmatrix} + u_2 \begin{bmatrix} 0 & 0 \\ b_{21}^{(2)} & 0 \end{bmatrix} \right) \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} c_{11} & 0 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$



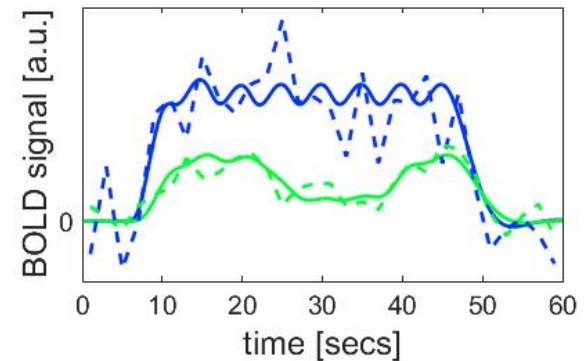
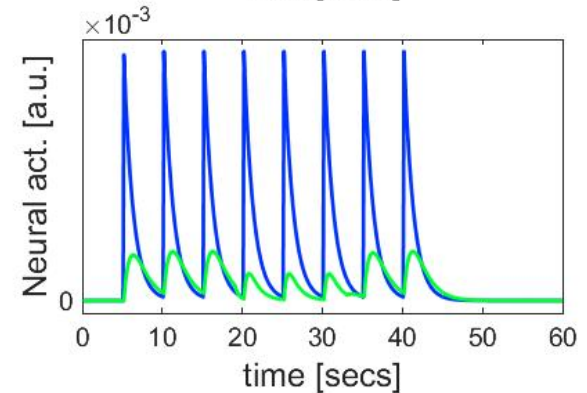
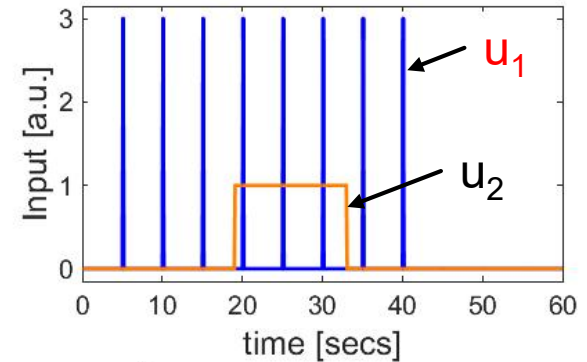
Simulation example: What can DCM explain?

Example: modulation of inhibitory self-connection



$$\frac{dx}{dt} = (A + u_2 B^{(2)})x + C u_1$$

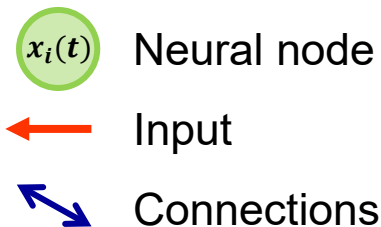
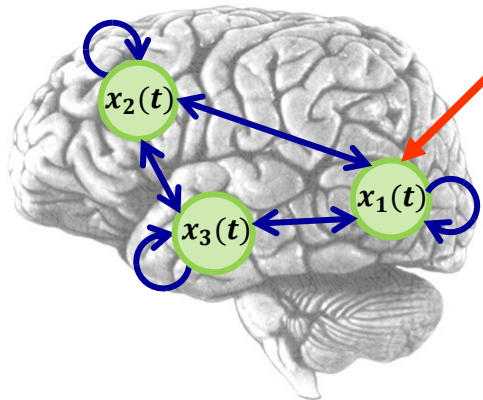
$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \left(\begin{bmatrix} a_{11} & 0 \\ a_{21} & a_{22} \end{bmatrix} + u_2 \begin{bmatrix} 0 & 0 \\ 0 & b_{22}^{(2)} \end{bmatrix} \right) \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} c_{11} & 0 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$



DCM for fMRI

A simple model of
a neural network

...



... described as a
dynamical system

...

$$\dot{x} = f(x, u, \theta)$$

... causes the data
(BOLD signal).

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

Simulate the system with input u and
parameters θ

→ BOLD signal time course y that can be
compared to measured data.

DCM for fMRI - overview

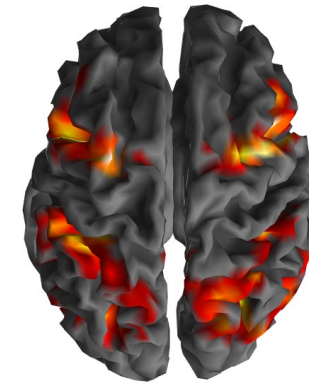
Model inversion:
Estimating
neuronal
mechanisms

Forward model:
Predicting
measured activity

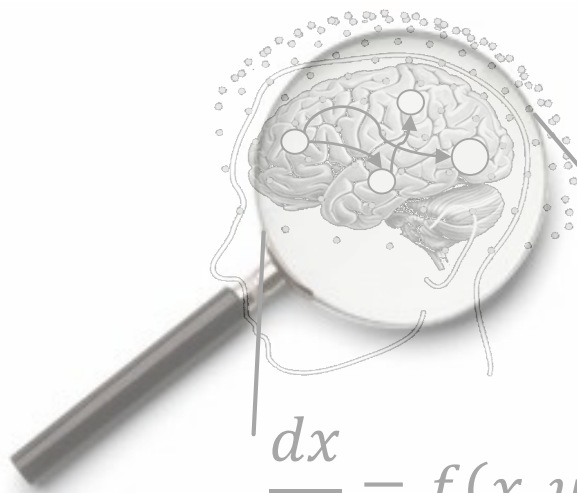
$$y = g(x, \theta) + \varepsilon$$

Neural state equation:
Describing neuronal
dynamics

$$\frac{dx}{dt} = f(x, u, \theta) + \omega$$



fMRI

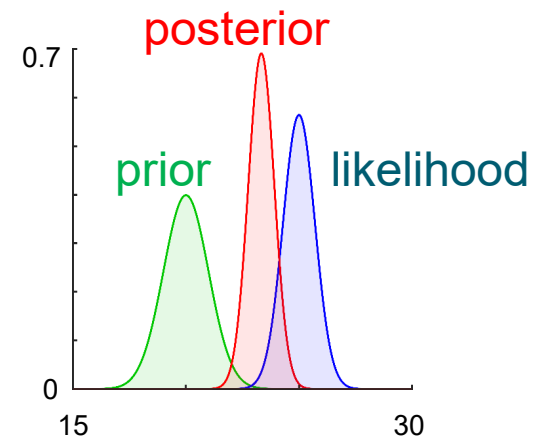


Bayes' theorem

$$\text{posterior } p(\theta|y, m) = \frac{\text{likelihood } p(y|\theta, m) \text{ prior } p(\theta|m)}{\text{model evidence } p(y|m)}$$



Reverend Thomas Bayes
(1702-1761)



The likelihood function for DCM

$$p(y(t)|\theta, m) = \mathcal{N}(y(t); g(\theta^n, \theta^h, u(t)), \theta^\sigma)$$

likelihood

Assume data is normally distributed around the prediction from the dynamical model (Gaussian noise)

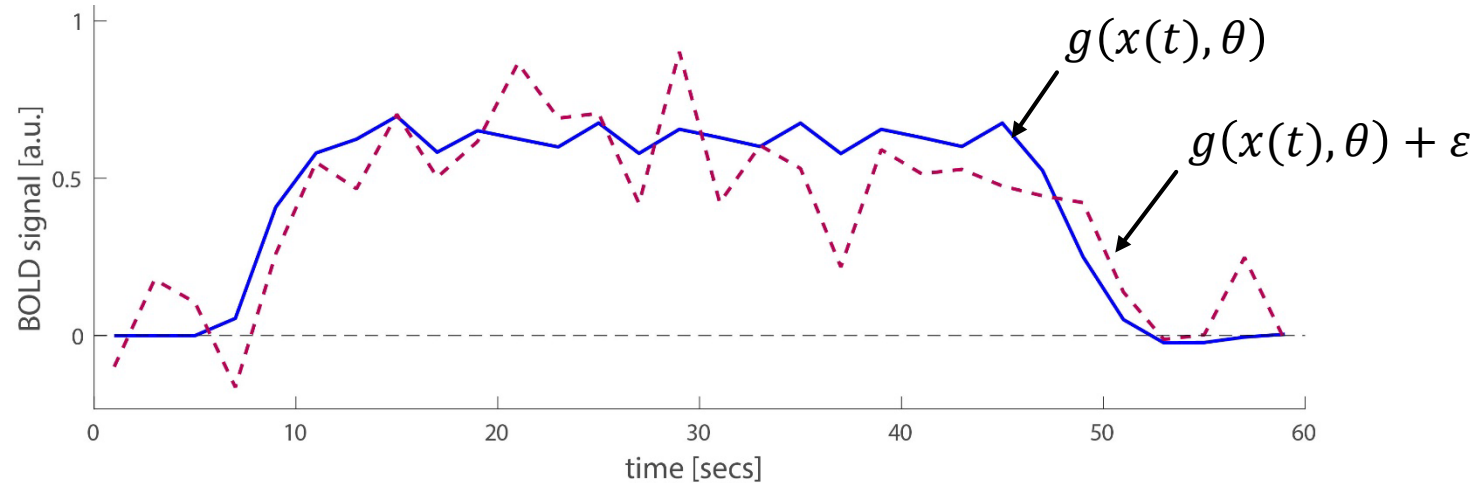
$$y(t) = g(x(t), \theta) + \varepsilon$$
$$\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$$

Data is prediction plus
Gaussian noise

The likelihood function for DCM

$$p(y(t)|\theta, m) = \mathcal{N}(y(t); g(\theta^n, \theta^h, u), \theta^\sigma)$$

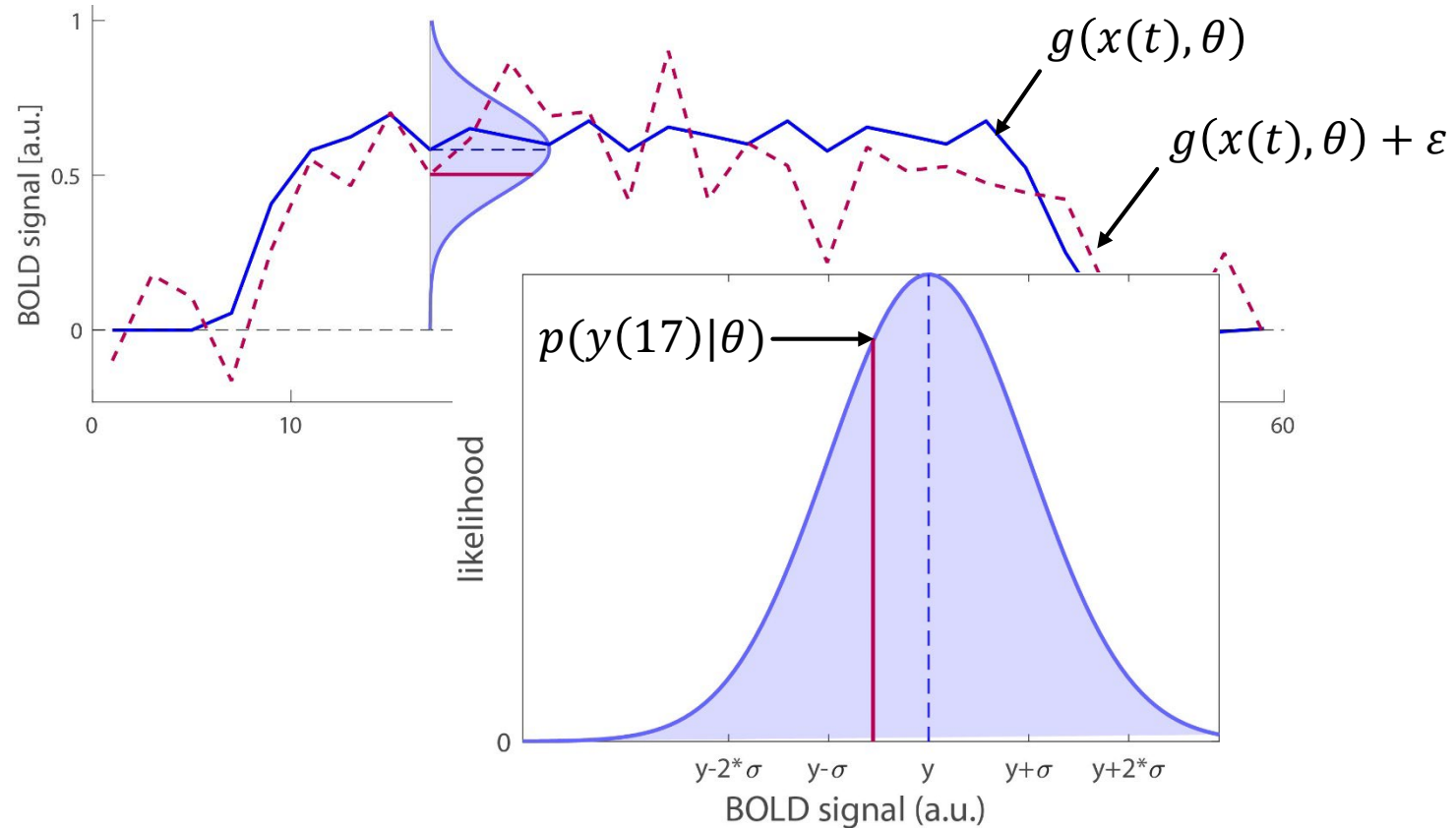
likelihood



The likelihood function for DCM

$$p(y(t)|\theta, m) = \mathcal{N}(y(t); g(\theta^n, \theta^h, u), \theta^\sigma)$$

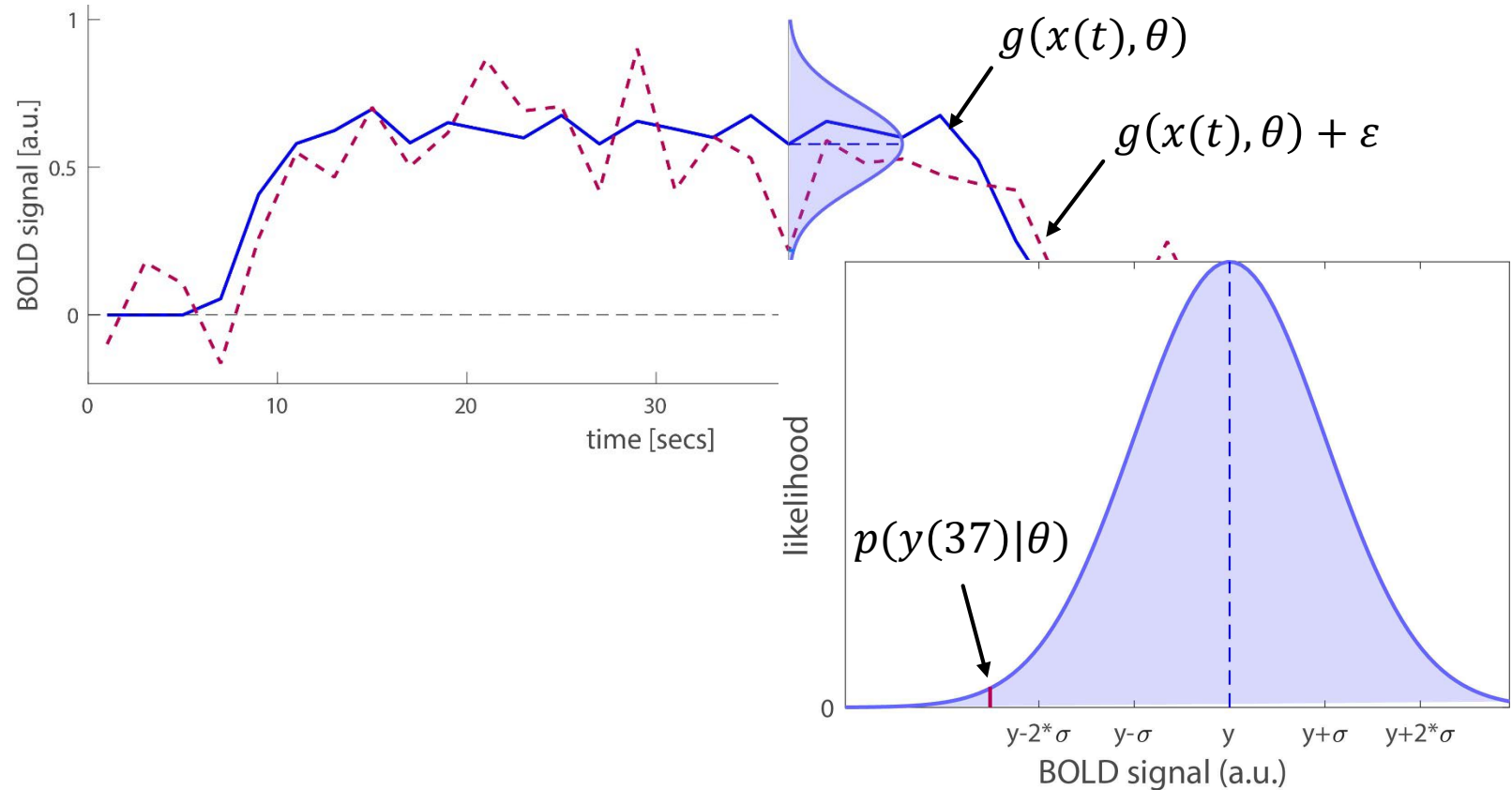
likelihood



The likelihood function for DCM

$$p(y(t)|\theta, m) = \mathcal{N}(y(t); g(\theta^n, \theta^h, u), \theta^\sigma)$$

likelihood



Priors

$$p(\theta|y, m) = \frac{p(y|\theta, m) \overset{\text{prior}}{p(\theta|m)}}{p(y|m)}$$

Neuronal parameters:

- self-connections: principled (to “ensure” that the system is stable)
- other parameters (between—region connections, modulation, inputs): shrinkage priors

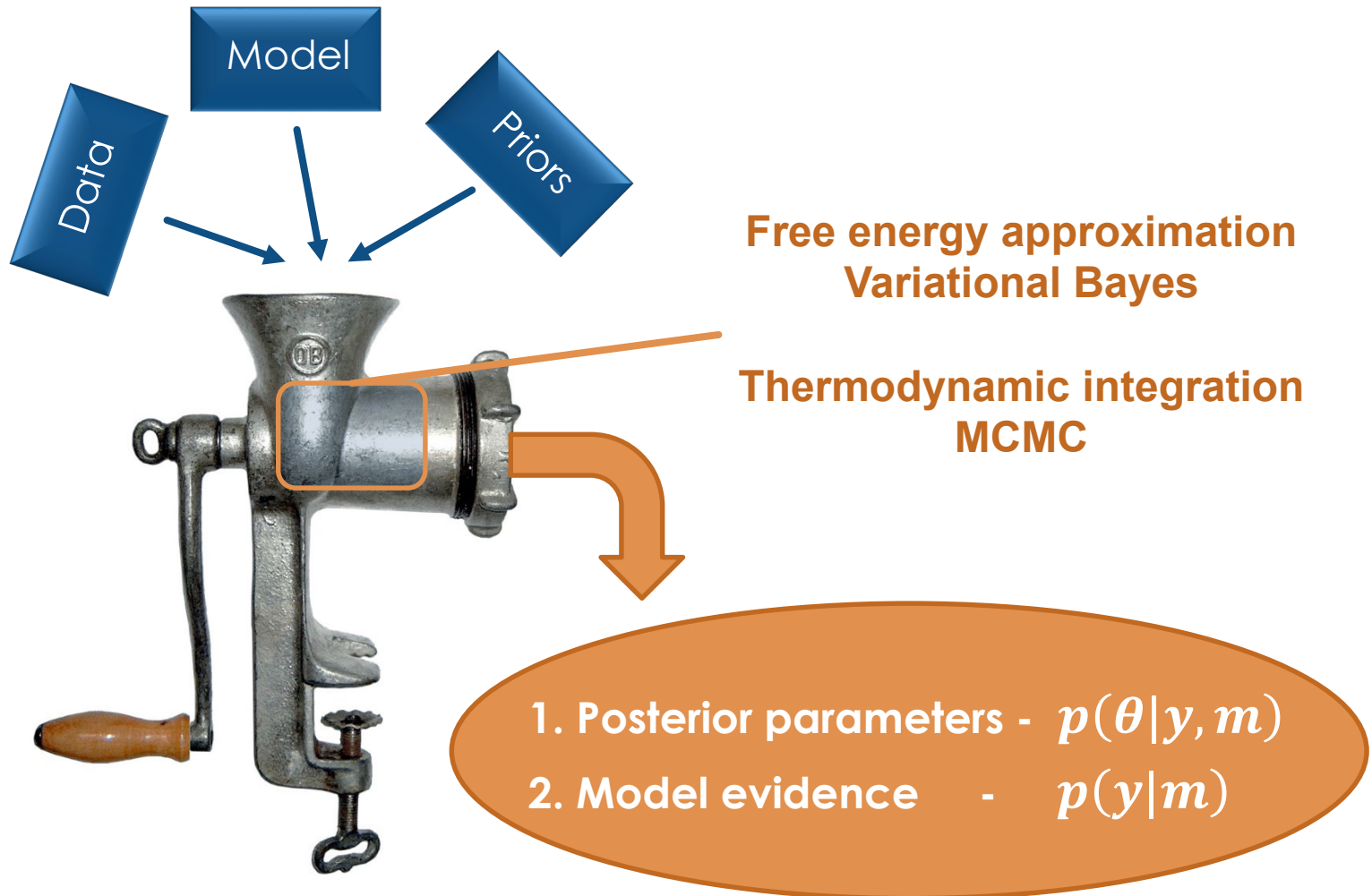
Hemodynamic parameters:

- empirical

Noise prior:

- assume relatively noisy data
(not default in SPM12 → set DCM.options.hE = 0; DCM.options.hC = 1)

Model estimation: running the machinery

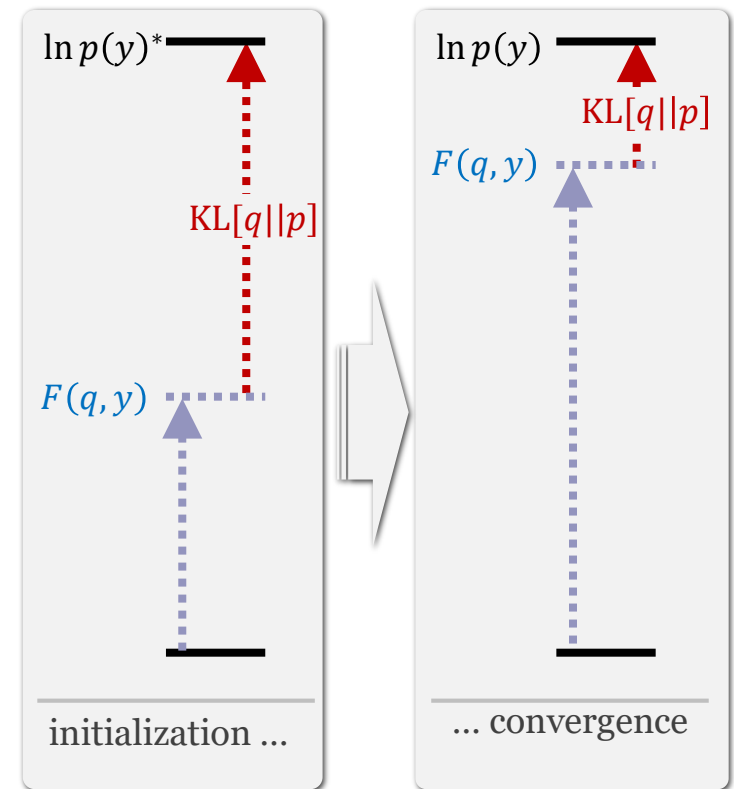


Inversion – variational Free Energy approximation to model evidence

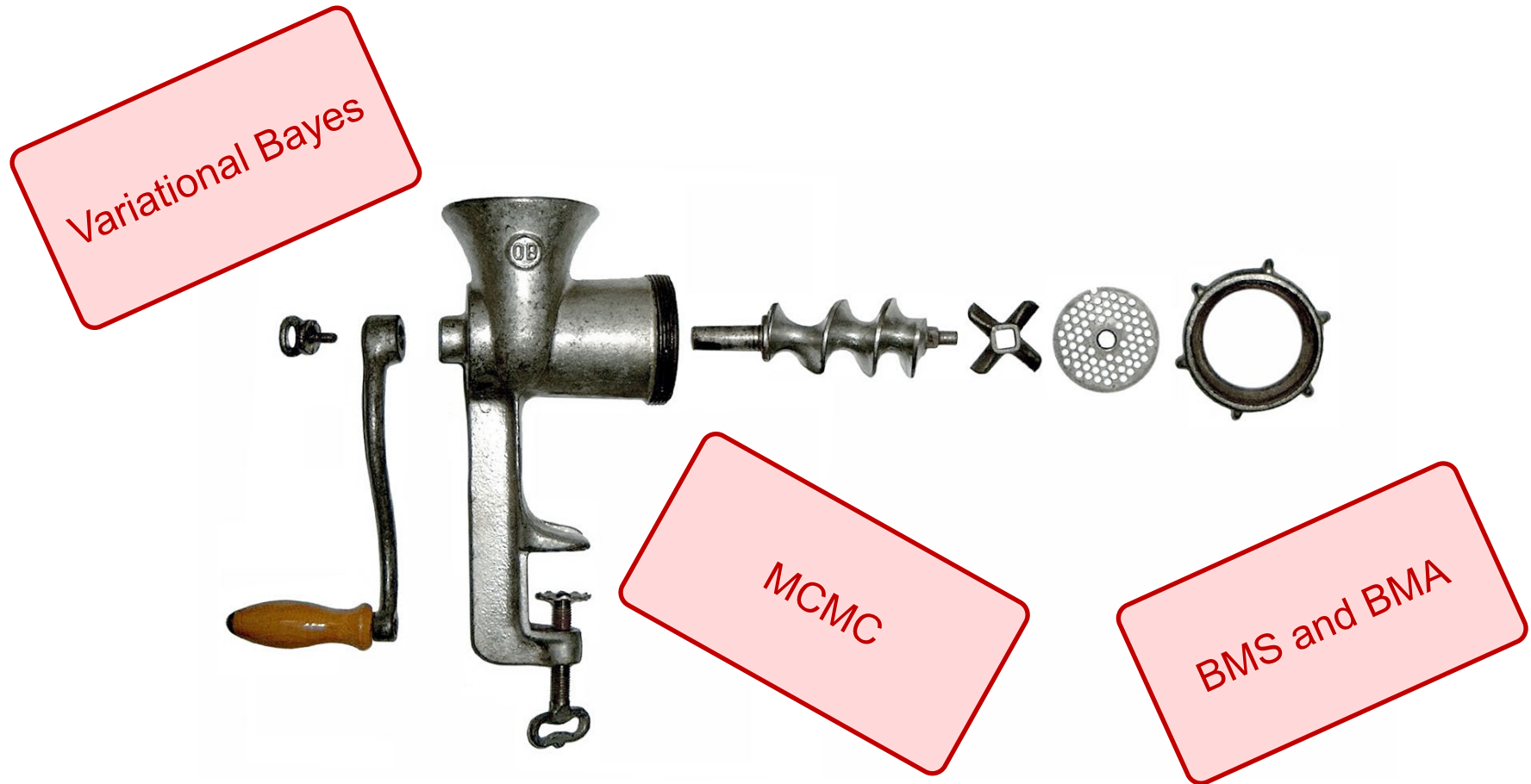
model evidence

$$\ln p(y) = \underbrace{\text{KL}[q||p]}_{\substack{\text{divergence} \\ \geq 0 \\ \text{(unknown)}}} + \underbrace{F(q, y)}_{\substack{\text{neg. free energy} \\ \text{(easy to evaluate} \\ \text{for a given } q)}}$$

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

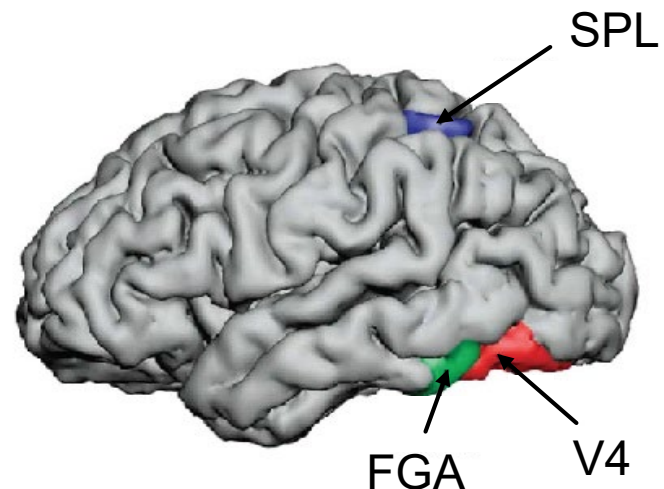


Model estimation: running the machinery



Model selection example: Synesthesia

- Specific sensory stimuli lead to unusual, additional experiences
- Grapheme-color synesthesia: **color**
- Involuntary, automatic; stable over time, prevalence ~4%
- Potential cause: aberrant **cross-activation/coupling** between brain areas
 - grapheme encoding area (FGA)
 - color area (V4)
 - superior parietal lobule (SPL)

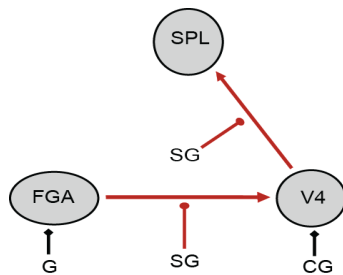


Hubbard, 2007

Bottom-up or Top-down “cross-activation”?

Bottom-up

(Ramachandran & Hubbard, 2001)

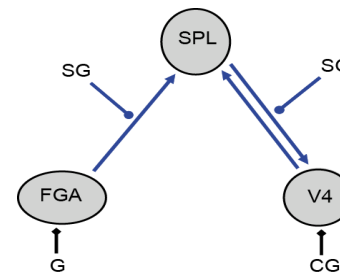


Projectors

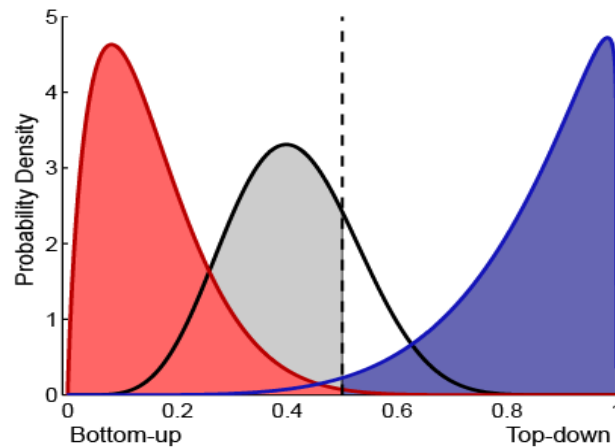
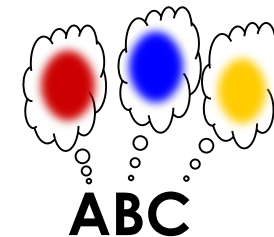
ABC

Top-down

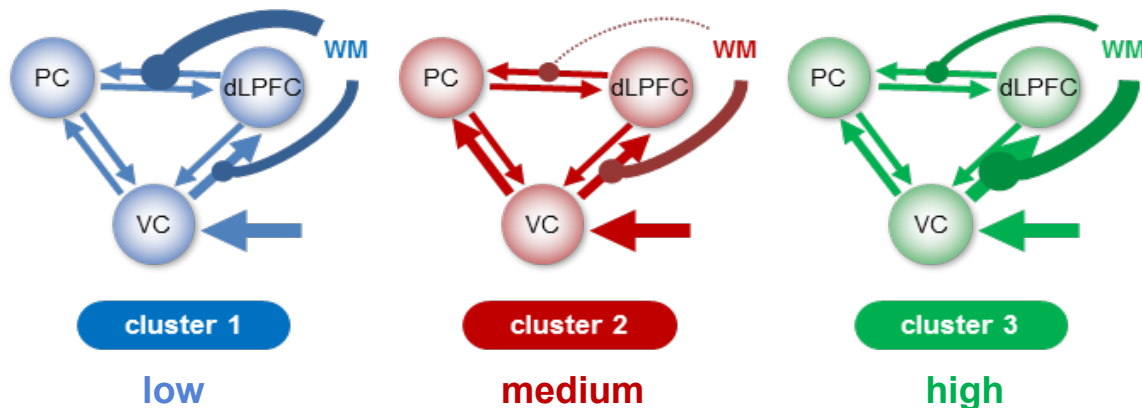
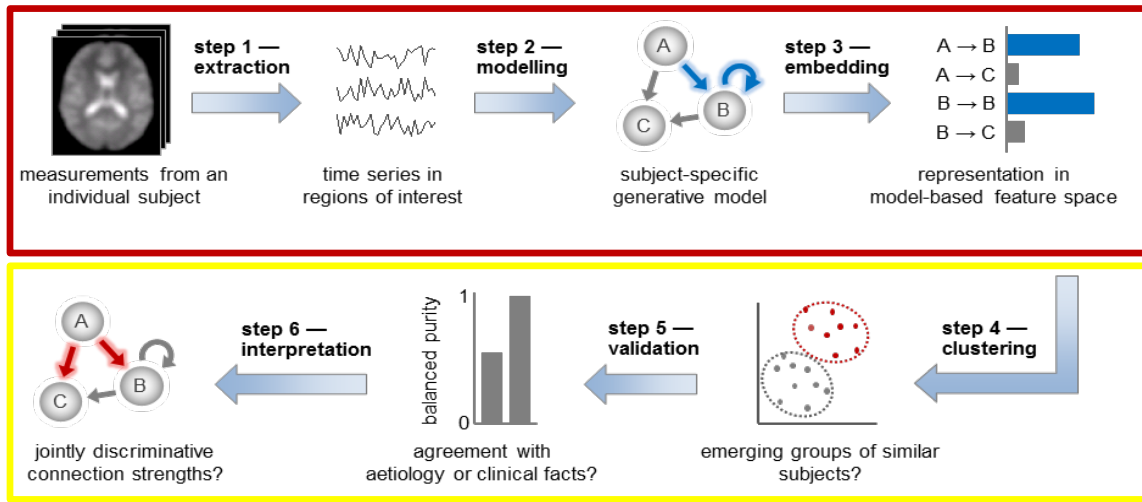
(Grossenbacher & Lovelace, 2001)



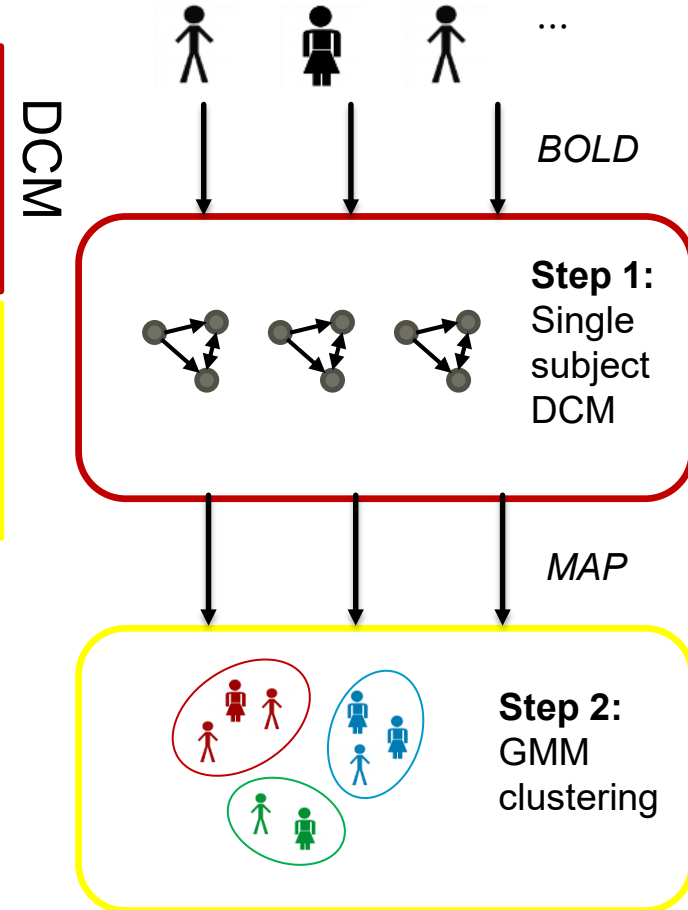
Associators



Example: DCM for physiologically plausible feature extraction (generative embedding)



negative symptoms (NS) subscale of the PANSS score



What questions can we answer using DCM?

Model comparison

What is the functional architecture of a network of brain regions?

→ Synesthesia

Are optimal models different between groups?

→ Synesthesia

Which connections are modulated by experimental manipulations?

Parameter inference

Are parameters different between individuals/groups?

Use parameters as physiologically informed summary statistics

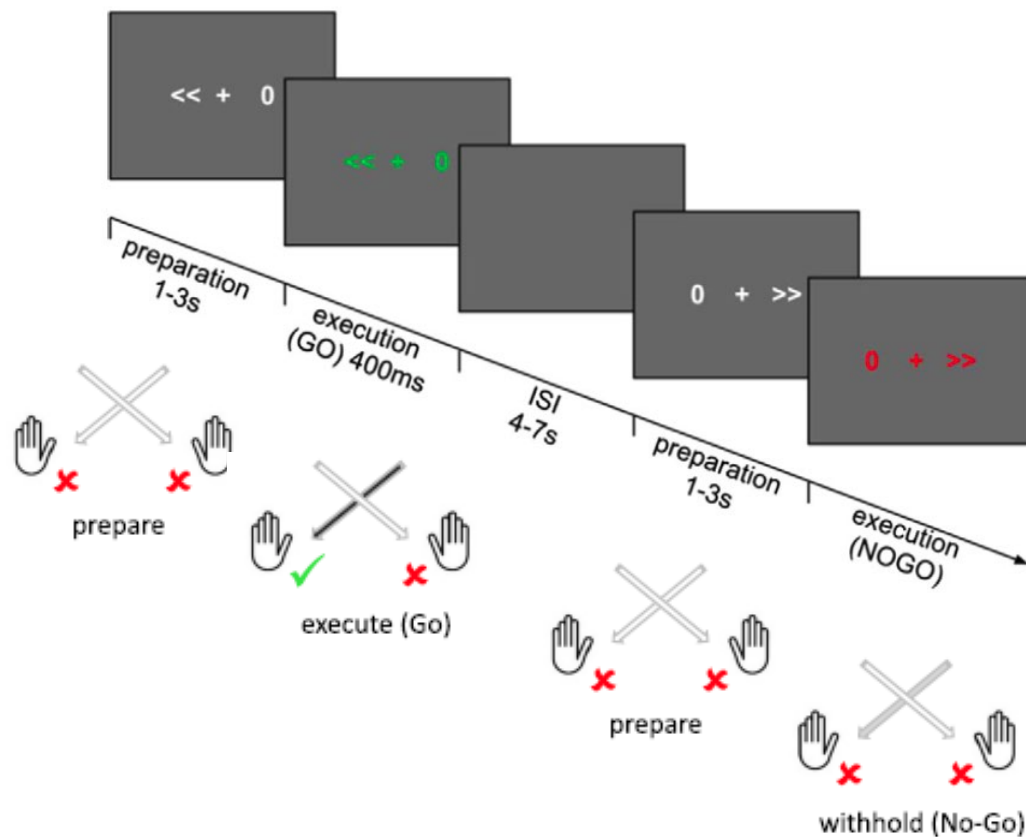
→ Generative embedding

... and of course many more!

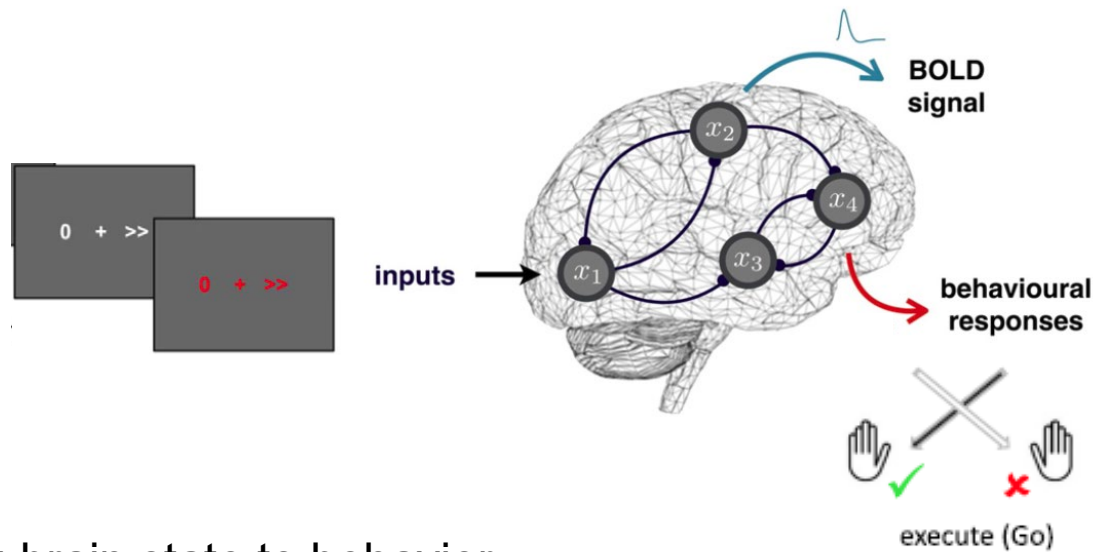
Limitations

- DCMs only have inputs, no outputs
 - Limits the study of behavioral paradigms
- Local minima
 - Variational approximation can get stuck in local minima of free energy
- Size of networks
 - Standard inversion too slow for large networks (>10 nodes).
- Regularization through fixed priors:
 - Regularization based on other data → empirical Bayes.

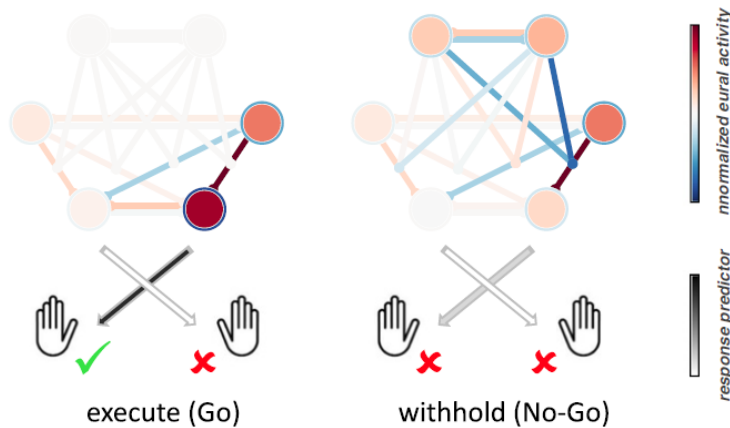
Behavioral DCM – a step towards a neurocomputational model



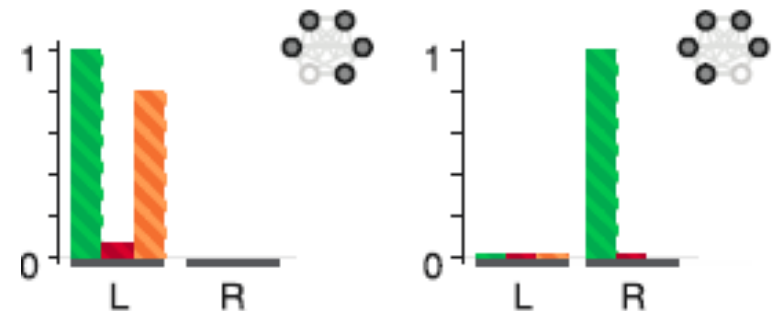
Behavioral DCM – a step towards a neurocomputational model



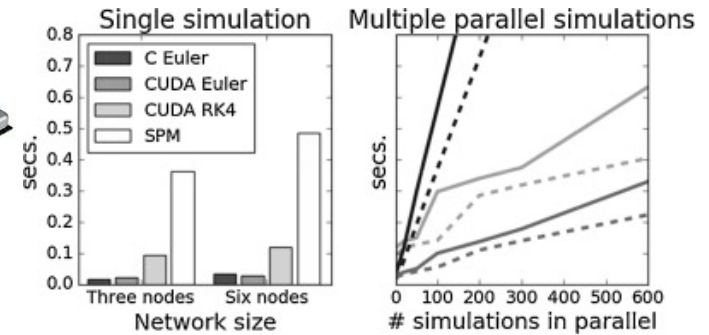
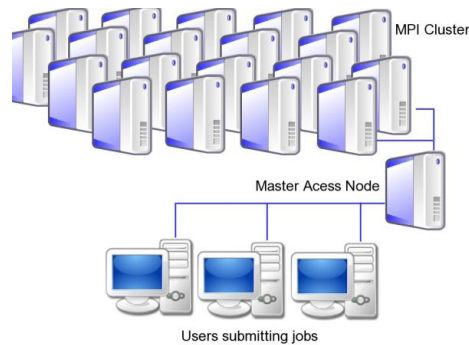
Mapping brain state to behavior



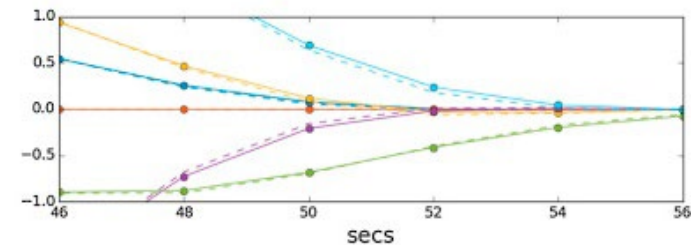
Lesion simulations



MCMC inversion of DCMs: Massively Parallel DCM - mpdcm



$$\left. \begin{array}{l} \dot{x} = f(x, u_1, \theta_1) \\ \dot{x} = f(x, u_2, \theta_2) \\ \vdots \\ \dot{x} = f(x, u_1, \theta_1) \end{array} \right\} \text{mpdcm_integrate(dcms)} \left\{ \begin{array}{l} y_1 \\ y_2 \\ \vdots \\ y_3 \end{array} \right.$$



- Fast inversion of DCMs
 - MCMC based inversion possible
- **Thermodynamic Integration** (alternative to negative Free Energy)

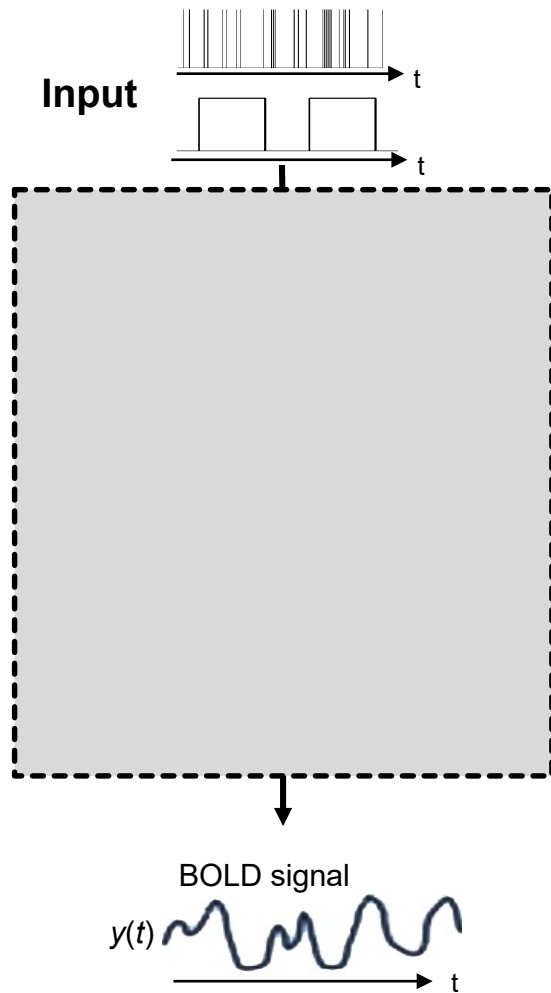
Recent additions to DCM for fMRI

- Massively parallel dynamic causal modelling
 - **mpdcm** Aponte et al., J Neuroscience Methods, 2016
- Regression dynamic causal modelling
 - **rDCM** Frässle et al., Neuroimage, 2017
- Hierarchical unsupervised generative embedding
 - **HUGE** Yu et al., Neuroimage, 2019

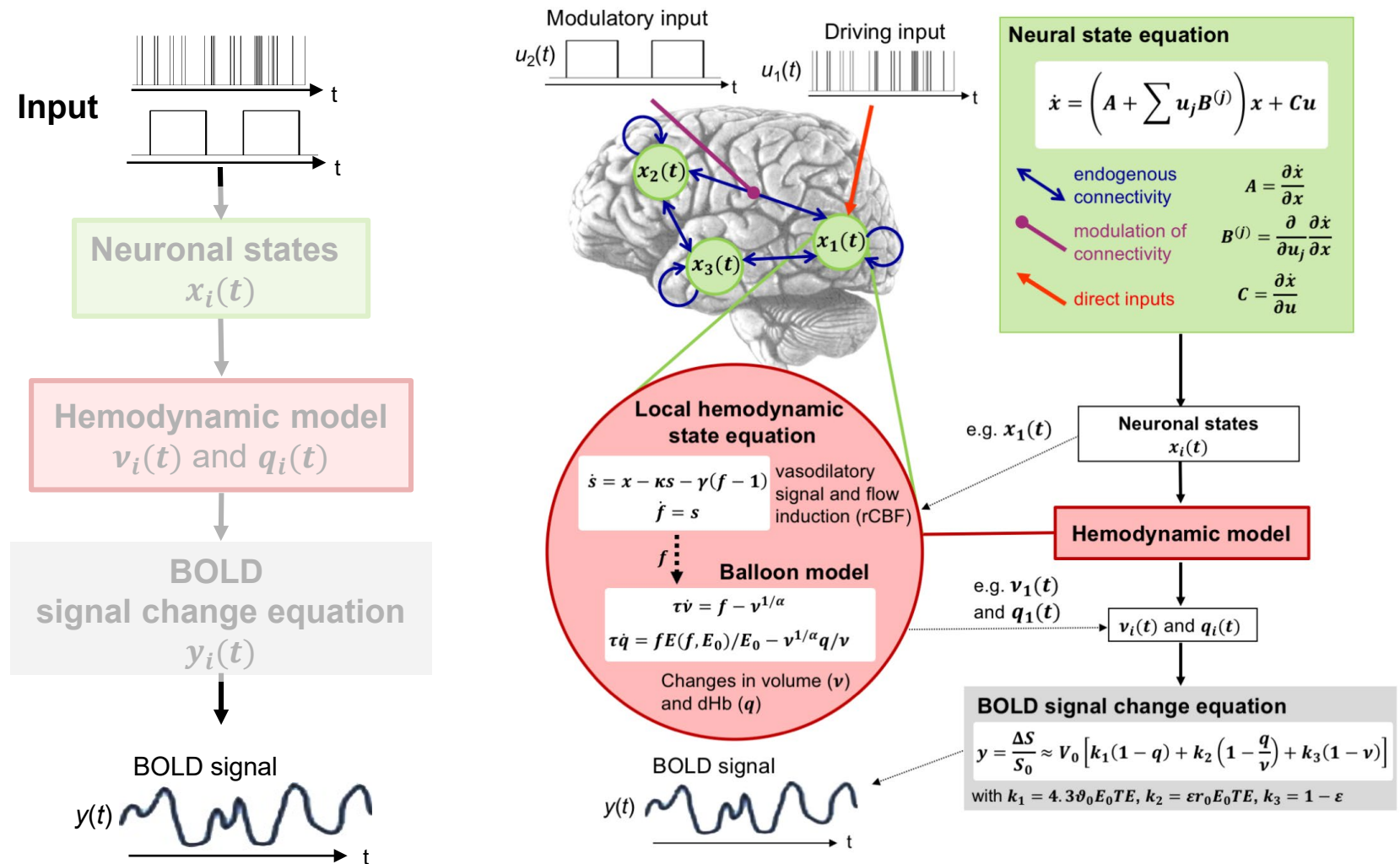
Modeling Connectivity:
Advanced DCM for
fMRI
→ Stefan Frässle

Available in TAPAS:
www.translationalneuromodeling.org/tapas

Summary – generative model



Summary – generative model



Summary - Bayesian system identification

Neural (and hemo-)
dynamics

Observer function

$u(t)$



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

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

$$p(y | \theta, m) = N(g(\theta), \Sigma(\theta))$$

$$p(\theta, m) = N(\mu_\theta, \Sigma_\theta)$$

Inference on
model structure

Inference on
parameters

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

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

Design experimental inputs

Define likelihood model

Specify priors

Invert model

Make inferences

DCM software note

Basic functionality for DCM for fMRI is provided within

SPM

<https://www.fil.ion.ucl.ac.uk/spm/>



Thank you!

Many thanks to Stefan Frässle,
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List with suggested DCM literature in Appendix of this presentation!

DCM literature (1)

- **Aponte EA, Raman S, Sengupta B, Penny WD, Stephan KE, Heinzle J (2016). mpdcm: A Toolbox for Massively Parallel Dynamic Causal Modeling. Journal of Neuroscience Methods 257: 7-16.**
- **Aponte EA, Yao Y, Raman S, Frässle S, Heinzle J, Penny WD, Stephan KE (2021). An introduction to thermodynamic integration and application. Cognitive Neurodynamics 16: 1-15.**
- Brodersen KH, Schofield TM, Leff AP, Ong CS, Lomakina EI, Buhmann JM, Stephan KE (2011) Generative embedding for model-based classification of fMRI data. PLoS Computational Biology 7: e1002079.
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- Daunizeau J, David, O, Stephan KE (2011) Dynamic Causal Modelling: A critical review of the biophysical and statistical foundations. Neurolmage 58: 312-322.
- Daunizeau J, Stephan KE, Friston KJ (2012) Stochastic Dynamic Causal Modelling of fMRI data: Should we care about neural noise? Neurolmage 62: 464-481.
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- Friston K, Penny W (2011) Post hoc Bayesian model selection. Neuroimage 56: 2089-2099.
- Friston KJ, Kahan J, Biswal B, Razi A (2014) A DCM for resting state fMRI. Neuroimage 94:396-407.
- Frässle S, Yao Y, Schöbi S, Aponte EA, Heinzle J, Stephan KE (in press) Generative models for clinical applications in computational psychiatry. Wiley Interdisciplinary Reviews: Cognitive Science.
- **Frässle S, Lomakina EI, Razi A, Friston KJ, Buhmann JM, Stephan KE (2017) Regression DCM for fMRI. Neurolmage 155:406-421.**

DCM literature (2)

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- Li B, Daunizeau J, Stephan KE, Penny WD, Friston KJ (2011). Stochastic DCM and generalised filtering. *NeuroImage* 58: 442-457
- Marreiros AC, Kiebel SJ, Friston KJ (2008) Dynamic causal modelling for fMRI: a two-state model. *NeuroImage* 39:269-278.
- Penny WD, Stephan KE, Mechelli A, Friston KJ (2004a) Comparing dynamic causal models. *NeuroImage* 22:1157-1172.
- Penny WD, Stephan KE, Mechelli A, Friston KJ (2004b) Modelling functional integration: a comparison of structural equation and dynamic causal models. *NeuroImage* 23 Suppl 1:S264-274.
- Penny WD, Stephan KE, Daunizeau J, Joao M, Friston K, Schofield T, Leff AP (2010) Comparing Families of Dynamic Causal Models. *PLoS Computational Biology* 6: e1000709.
- Penny WD (2012) Comparing dynamic causal models using AIC, BIC and free energy. *Neuroimage* 59: 319-330
- **Raman S, Deserno L, Schlagenhauf F, Stephan KE (2016). A hierarchical model for integrating unsupervised generative embedding and empirical Bayes. *Journal of Neuroscience Methods* 269: 6-20.**
- Rigoux L, Stephan KE, Friston KJ, Daunizeau J (2014). Bayesian model selection for group studies – revisited. *NeuroImage* 84: 971-985.
- **Rigoux L and Daunizeau J (2015). Dynamic causal modelling of brain–behaviour relationships. *NeuroImage* 117:202-221**
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- Stephan KE, Weiskopf N, Drysdale PM, Robinson PA, Friston KJ (2007) Comparing hemodynamic models with DCM. *NeuroImage* 38:387-401.
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DCM literature (3)

- Stephan KE, Weiskopf N, Drysdale PM, Robinson PA, Friston KJ (2007) Comparing hemodynamic models with DCM. *NeuroImage* 38:387-401.
- Stephan KE, Kasper L, Harrison LM, Daunizeau J, den Ouden HE, Breakspear M, Friston KJ (2008) Nonlinear dynamic causal models for fMRI. *NeuroImage* 42:649-662.
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- Stephan KE, Tittgemeyer M, Knösche TR, Moran RJ, Friston KJ (2009b) Tractography-based priors for dynamic causal models. *NeuroImage* 47: 1628-1638.
- **Stephan KE, Penny WD, Moran RJ, den Ouden HEM, Daunizeau J, Friston KJ (2010) Ten simple rules for Dynamic Causal Modelling. *NeuroImage* 49: 3099-3109.**
- Stephan KE, Mathys C (2014). Computational approaches to psychiatry. *Current Opinion in Neurobiology* 25: 85-92.
- **Yao Y, Raman SS, Schiek M, Leff A, Frässle S, Stephan KE (2018) Variational Bayesian Inversion for Hierarchical Unsupervised Generative Embedding (HUGE). *NeuroImage*, 179: 604-619**
- **Zeidman P, Jafarian A, Corbin N, Seghier ML, Razi A, Price CJ, Friston KJ (2019) A guide to group effective connectivity analysis, part 1: First level analysis with DCM for fMRI. *NeuroImage*, DOI: 10.1016/j.neuroimage.2019.06.031**
- **Zeidman P, Jafarian A, Seghier ML, Litvak V, Cagnan H, Price CJ, Friston KJ (2019) A guide to group effective connectivity analysis, part 2: Second level analysis with PEB. *NeuroImage*, DOI: 10.1016/j.neuroimage.2019.06.032**