Step-by-step Guide: Building a (Generative) Model

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Computational Psychiatry Course Zurich
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GENERATIVE MODELS

Bayes' rule

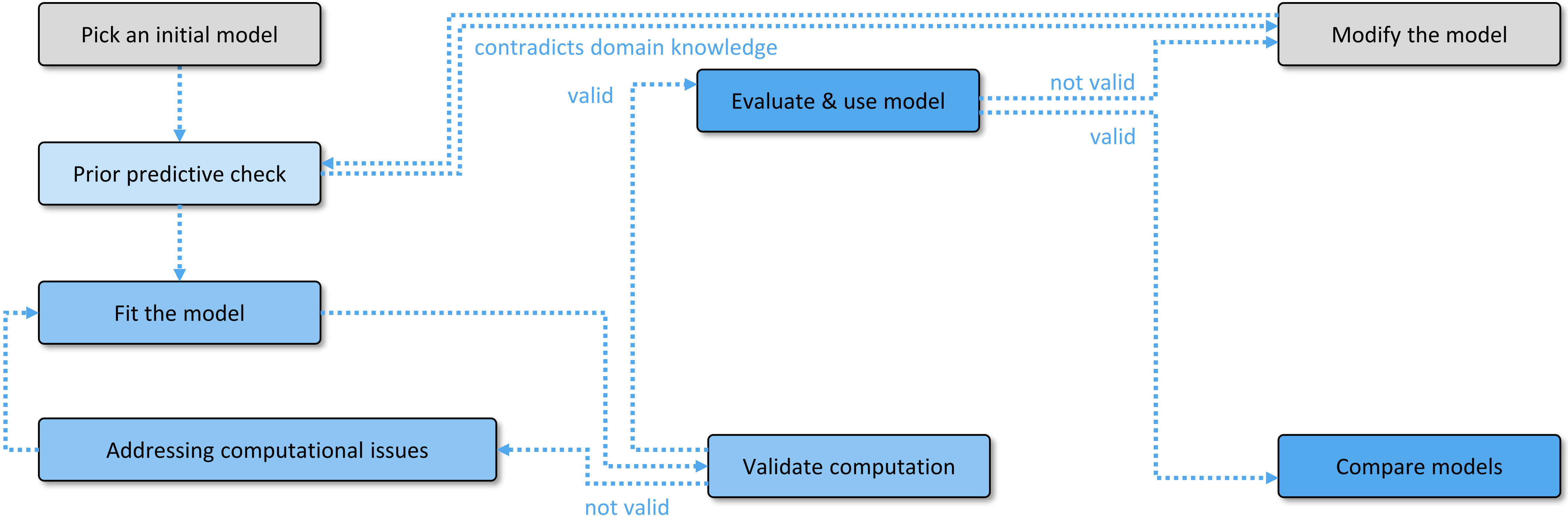
Generative model: likelihood x prior

$$\underbrace{p(\boldsymbol{\theta}|\mathbf{Y},m)}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{Y}|\boldsymbol{\theta},m)}^{\text{likelihood}}\overbrace{p(\boldsymbol{\theta}|m)}^{\text{prior}}}{p(\mathbf{Y}|m)}$$

model evidence
prior predictive distribution
marginal likelihood

$\boldsymbol{\theta}$: parameters
$\mathbf{Y}$: data
m: model

Bayesian workflow



Gabry et al. 2019, *J R Stat Soc A Stat*

Betancourt 2020, https://betanalpha.github.io/assets/case_studies/principled_bayesian_workflow.html

Gelman et al. 2020, *arXiv*

Schad et al. 2020, *arXiv*

Baribault and Collins 2023, *Psychol Methods*

Hess et al. 2025, *Comput Psychiatr*

Figure reproduced from Gelman et al., 2020, *arXiv*

CONSTRUCTING MODELS

Some general tips:

- Adapt what has been done before
- Use **heuristics** to develop computational models (e.g., Rescorla Wagner)
- Ideally, you would like to start from **first principles** (e.g., free energy minimization, Bayes optimal agents)

  Active inference: Lecture (*Wed*), Tutorial (*Sat*)
  Bayesian models of perception: Lecture (*Today*)

- **Transfer of concepts** from artificial intelligence, computer science, and applied mathematics literature (e.g., reinforcement learning, predictive coding)

  Reinforcement learning: Lecture (*Wed*), Tutorial (*Sat*)
  Predictive coding: Lecture (*Wed*)

- …

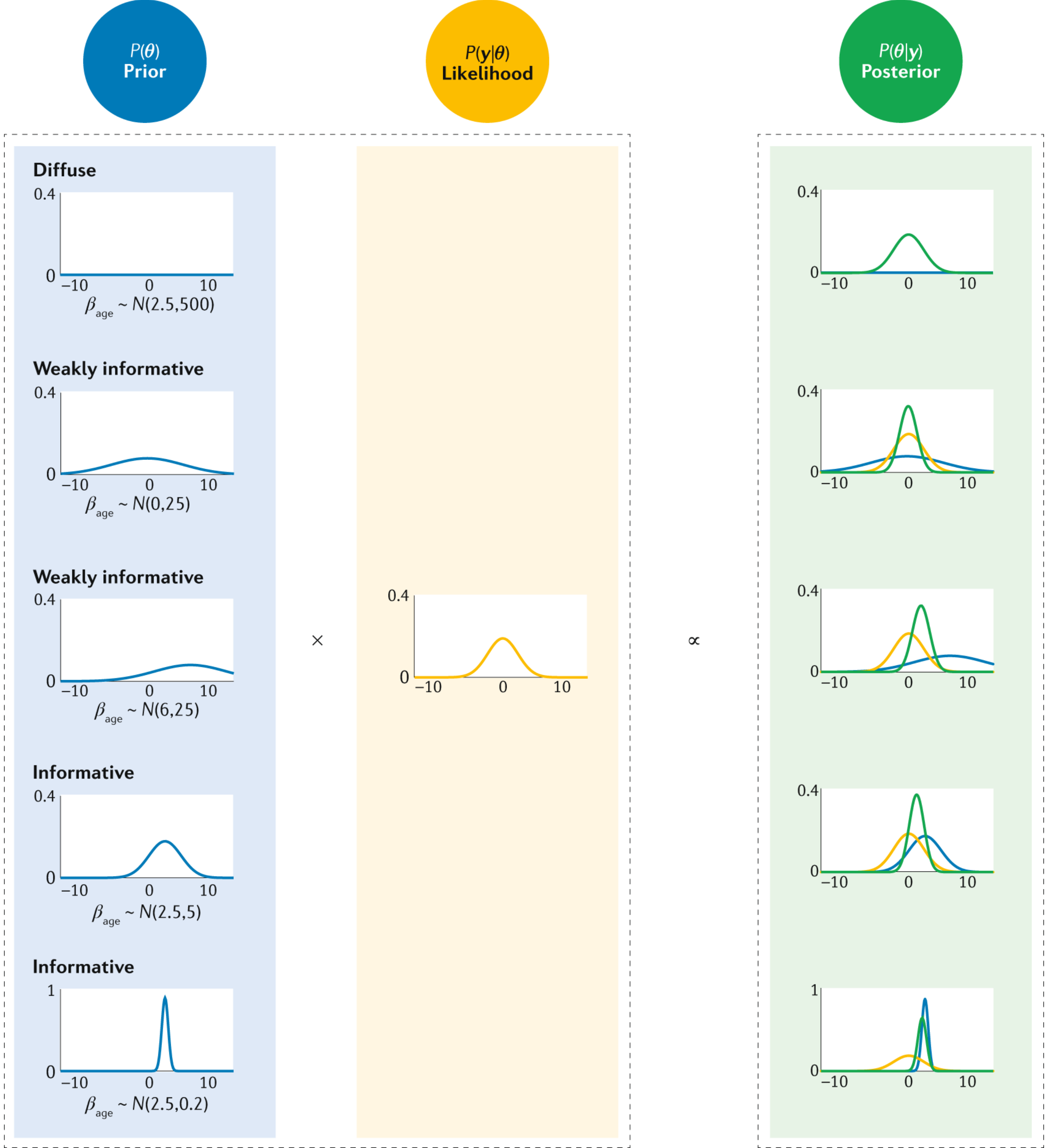
Adapted from slide by Stefan Frässle

PRIOR SPECIFICATION

Define a range of *a priori* plausible parameter values

- Regularisation
- Informativeness
- Prior elicitation
  - Will depend on parametrisation
  - Previous literature
  - Expert knowledge (e.g. volume parameter in BOLD signal models)
  - Empirical priors (beware of double-dipping!)
  - …

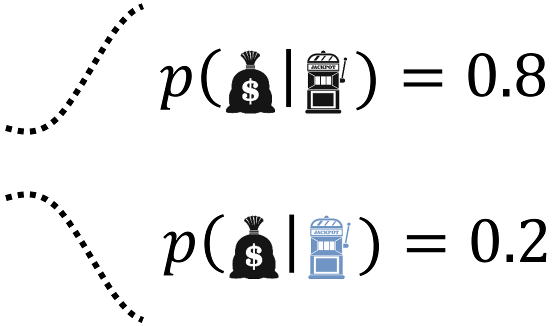
Useful resource: Prior Choice Wiki (https://github.com/stan-dev/stan/wiki/Prior-Choice-Recommendations)

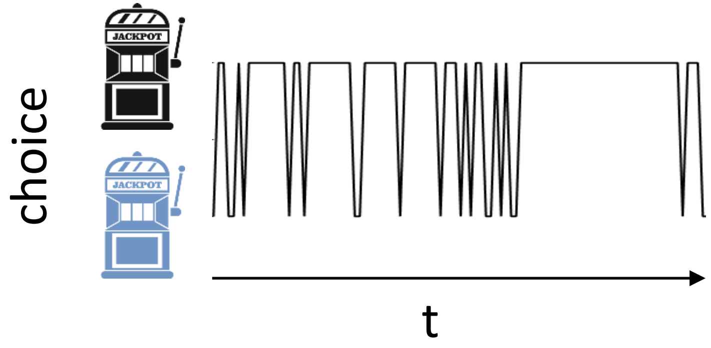


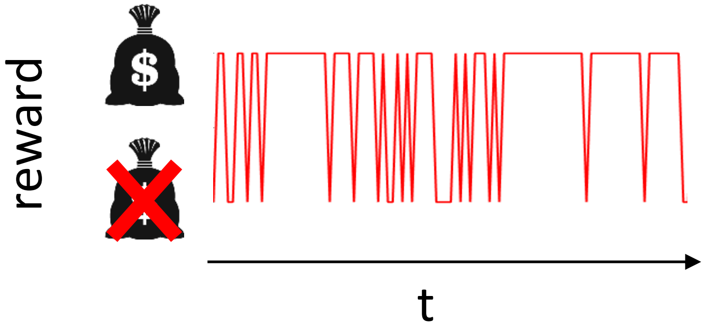
van de Schoot et al. 2021,
Nat Rev Methods Primer

EXAMPLE: MULTI-ARMED BANDIT TASK

- K=2 slot machines
- Series of T choices (trials)
- Slot machines have different (but constant) reward probabilities







Wilson & Collins, 2019, *eLife*

How do individuals learn to maximize their rewards in a case where the most rewarding choice is initially unknown?

Pick initial model

model 1
Random choice

$p_t^1 = b$

$p_t^2 = 1 - b$

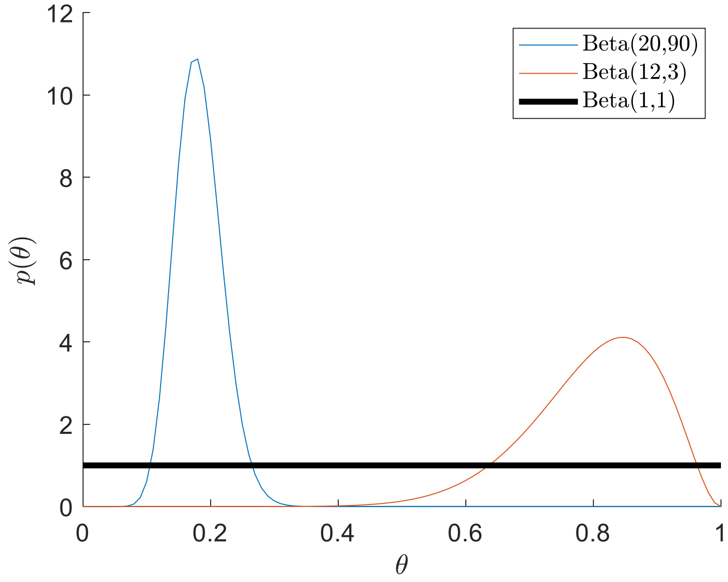
$0 \leq b \leq 1$

$\boldsymbol{\theta} = \{b\}$

Prior elicitation

- Conjugacy: $\underbrace{\text{Beta}}_{\text{posterior}} \propto \underbrace{\text{Binomial}}_{\text{likelihood}} * \underbrace{\text{Beta}}_{\text{prior}}$
- No preference for specific values *a priori*

$$p(\boldsymbol{\theta}) = \text{Beta}(1,1)$$



Prior predictive check

Prior predictive distribution: $p(\mathbf{Y}) = \int \underbrace{p(\mathbf{Y}|\boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\theta})}_{\text{prior}} d\boldsymbol{\theta}$

Use simulations to refine model without using data multiple times

Sample from prior
$\tilde{\boldsymbol{\theta}} \sim p(\boldsymbol{\theta})$

→

Draw simulated data set
$\tilde{\mathbf{y}} \sim p(\mathbf{Y}|\tilde{\boldsymbol{\theta}})$

→

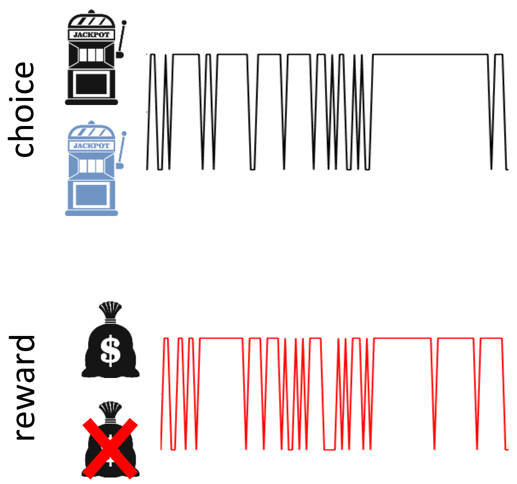
Examine characteristics of interest

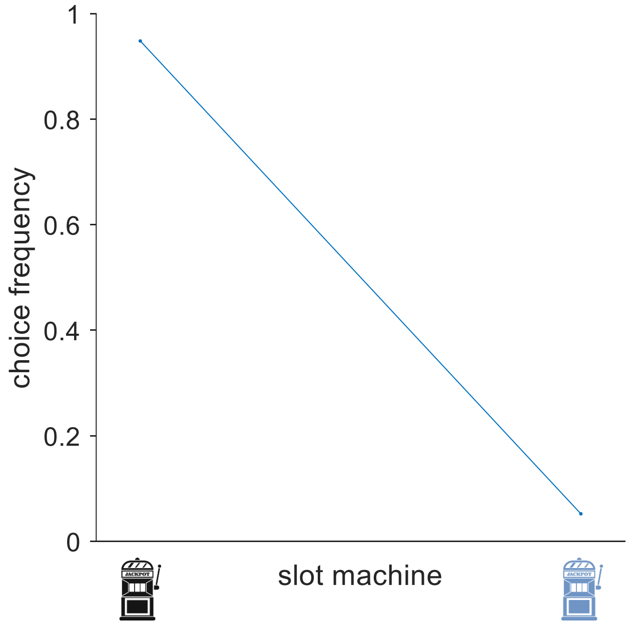
model 1
Random Choice

$$p(\mathbf{y}|\boldsymbol{\theta}) = B(T, \boldsymbol{\theta})$$

$$p(\boldsymbol{\theta}) = Beta(1,1)$$

$$\tilde{\boldsymbol{\theta}} = 0.94$$





PRIOR PREDICTIVE CHECK

likelihood prior

Prior predictive distribution: $p(\mathbf{Y}) = \int p(\mathbf{Y}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$

Use simulations to refine model without using data multiple times

Sample from prior $\tilde{\boldsymbol{\theta}} \sim p(\boldsymbol{\theta})$ → Draw simulated data set $\tilde{\mathbf{y}} \sim p(\mathbf{Y}|\tilde{\boldsymbol{\theta}})$ → Examine characteristics of interest

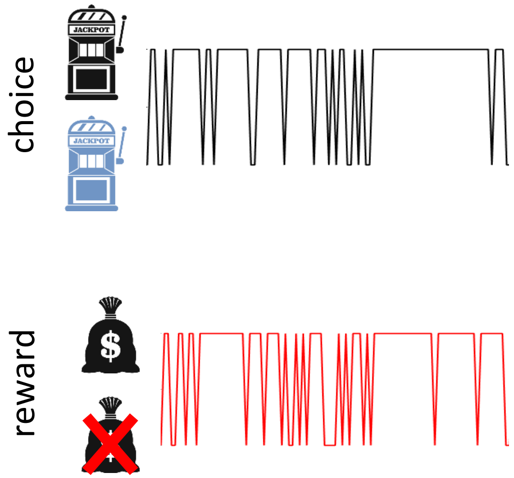
N

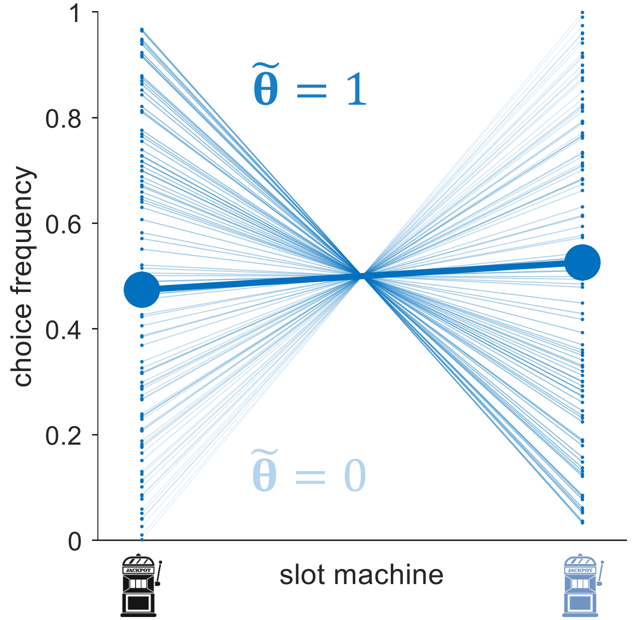
model 1

Random Choice

$$p(\mathbf{y}|\boldsymbol{\theta}) = B(T, \boldsymbol{\theta})$$

$$p(\boldsymbol{\theta}) = Beta(1,1)$$





PRIOR PREDICTIVE CHECK

Prior predictive distribution: $p(\mathbf{Y}) = \int \underbrace{p(\mathbf{Y}|\boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\theta})}_{\text{prior}} d\boldsymbol{\theta}$

Use simulations to refine model without using data multiple times

Sample from prior $\tilde{\boldsymbol{\theta}} \sim p(\boldsymbol{\theta})$ → Draw simulated data set $\tilde{\mathbf{y}} \sim p(\mathbf{Y}|\tilde{\boldsymbol{\theta}})$ → Examine characteristics of interest

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model 1

Random Choice

$$p(\mathbf{y}|\boldsymbol{\theta}) = B(T, \boldsymbol{\theta})$$

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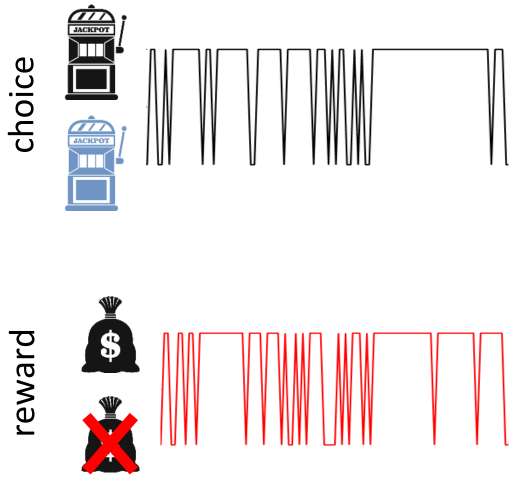
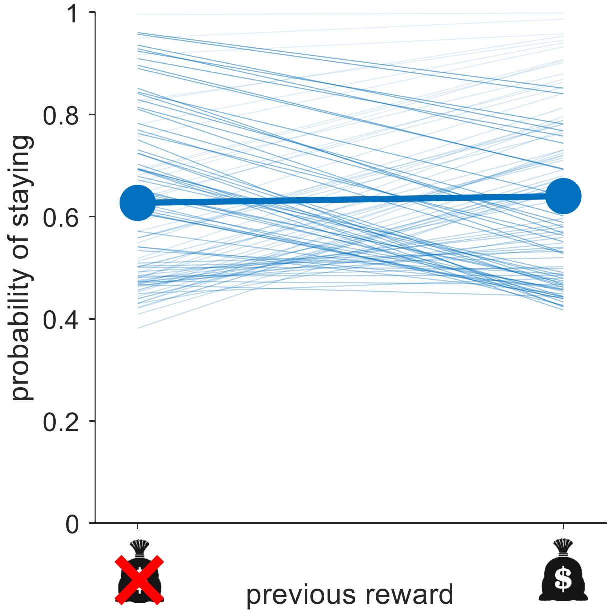




PRIOR PREDICTIVE CHECK

Prior predictive distribution: $p(\mathbf{Y}) = \int \underbrace{p(\mathbf{Y}|\boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\theta})}_{\text{prior}} d\boldsymbol{\theta}$

Use simulations to refine model without using data multiple times

Sample from prior

Draw simulated data set

Examine characteristics of

N

"Are the simulated data under the chosen prior consistent with domain knowledge?"

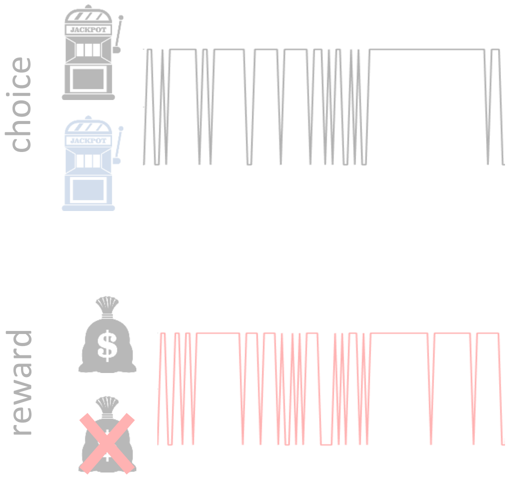
Gabry et al. 2019, *J R Stat Soc A Stat*

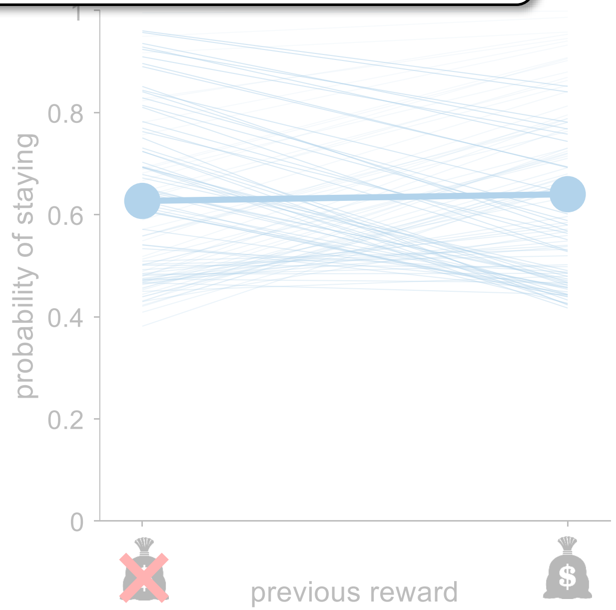
model 1

Random Choice

$p(\mathbf{y}|\boldsymbol{\theta}) = B(T, \boldsymbol{\theta})$

$p(\boldsymbol{\theta}) = Beta(1,1)$





Modify the model space

model 1
Random choice

$$p_t^1 = b$$
$$p_t^2 = 1 - b$$

$$0 \le b \le 1$$

$$\boldsymbol{\theta} = \{b\}$$

model 2
Noisy win-stay-lose-switch

$$p_t^1 = \begin{cases} 1 - \dfrac{\varepsilon}{2} & \text{if } (c_{t-1} = 1 \text{ and } r_{t-1} = 1) \text{ OR } (c_{t-1} \ne 1 \text{ and } r_{t-1} = 0) \\ \dfrac{\varepsilon}{2} & \text{if } (c_{t-1} \ne 1 \text{ and } r_{t-1} = 1) \text{ OR } (c_{t-1} = 1 \text{ and } r_{t-1} = 0) \end{cases}$$

$$\boldsymbol{\theta} = \{\varepsilon\}$$

model 3
Rescorla Wagner

$$Q_{t+1}^1 = Q_t^1 + \alpha(r_t - Q_t^1) \quad \text{and} \quad p_t^1 = \frac{\exp(\beta Q_t^1)}{\sum_{i=1}^K \exp(\beta Q_t^i)}$$

$$\boldsymbol{\theta} = \{\alpha, \beta\}$$

Wilson & Collins, 2019, *eLife*

Repeat prior predictive check

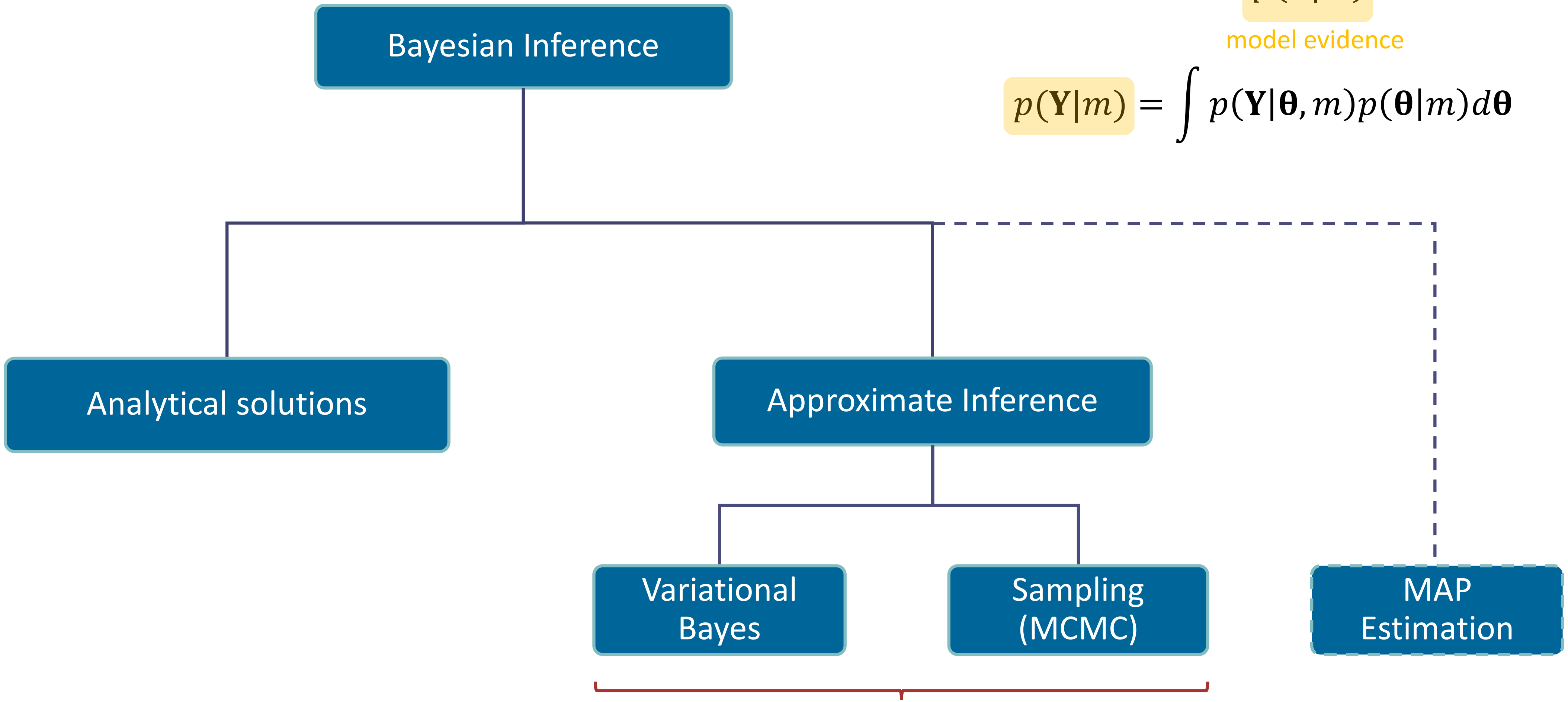
Do our models make distinct predictions?

INFERENCE ON MODEL PARAMETERS

posterior, likelihood, prior, model evidence:

$$\underbrace{p(\boldsymbol{\theta}|\mathbf{Y},m)}_{\text{posterior}} = \frac{\overbrace{p(\mathbf{Y}|\boldsymbol{\theta},m)}^{\text{likelihood}}\overbrace{p(\boldsymbol{\theta}|m)}^{\text{prior}}}{\underbrace{p(\mathbf{Y}|m)}_{\text{model evidence}}}$$

$$p(\mathbf{Y}|m) = \int p(\mathbf{Y}|\boldsymbol{\theta},m)p(\boldsymbol{\theta}|m)d\boldsymbol{\theta}$$



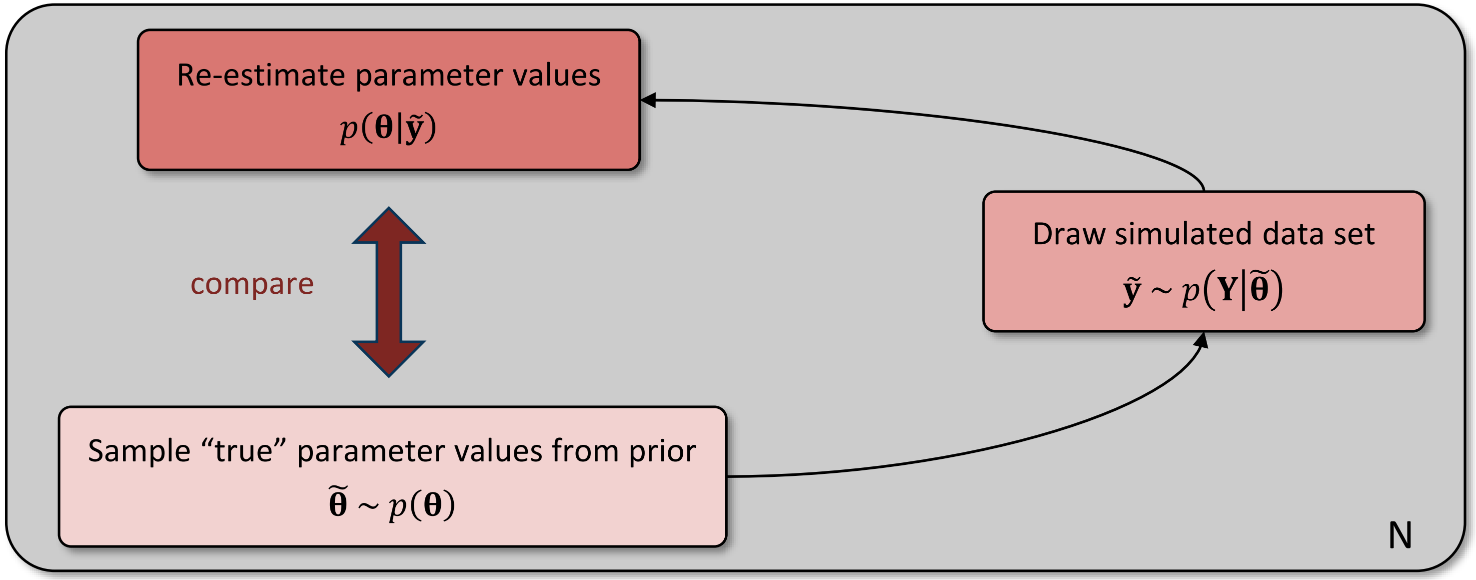
VB & MCMC: Lecture (*Today*)

Adapted from slide by Klaas Enno Stephan

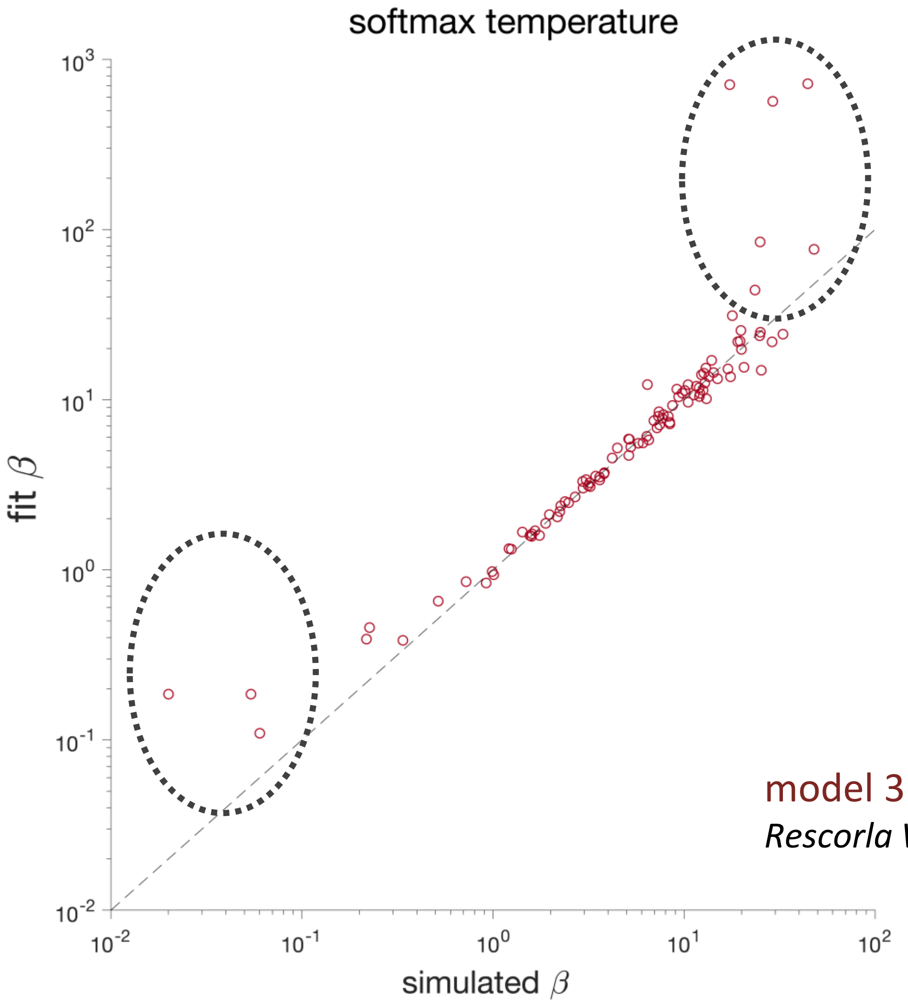
Validate computation

Ensure that the inference on latent variables is reliable

- Identifiability: can we identify the value of a parameter from measured data?
  - Structural identifiability: $f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}') \leftrightarrow \boldsymbol{\theta} = \boldsymbol{\theta}'$
  - Practical identifiability



PRACTICAL IDENTIFIABILITY: PARAMETER RECOVERY



model 3
Rescorla Wagner

Wilson & Collins, 2019, *eLife*

VALIDATE COMPUTATION

Ensure that the inference on latent variables is reliable

- Identifiability: can we identify the value of a parameter from measured data?
  - Structural identifiability: $f(\boldsymbol{\theta}) = f(\boldsymbol{\theta}') \leftrightarrow \boldsymbol{\theta} = \boldsymbol{\theta}'$
  - Practical identifiability (formal and practical limitations!)
- Simulation-based calibration Talts et al. 2020 *arXiv*

$$\underbrace{p(\boldsymbol{\theta})}_{\text{prior}} = \int \underbrace{p(\boldsymbol{\theta}|\tilde{\mathbf{y}})}_{\text{posterior}} \underbrace{p(\tilde{\mathbf{y}}|\tilde{\boldsymbol{\theta}})\, p(\tilde{\boldsymbol{\theta}})}_{\text{joint}} \, d\tilde{\boldsymbol{\theta}}\, d\tilde{\mathbf{y}}$$

  - any deviation between data-averaged posterior and prior indicates a problem
- Convergence diagnostics
  - Gradient-based optimisation techniques
  - Sampling methods: trace plots, auto-correlation functions, potential scale reduction factor $\hat{R}$
    Gelman and Rubin 1992 *Stat Sci*

Bayesian workflow

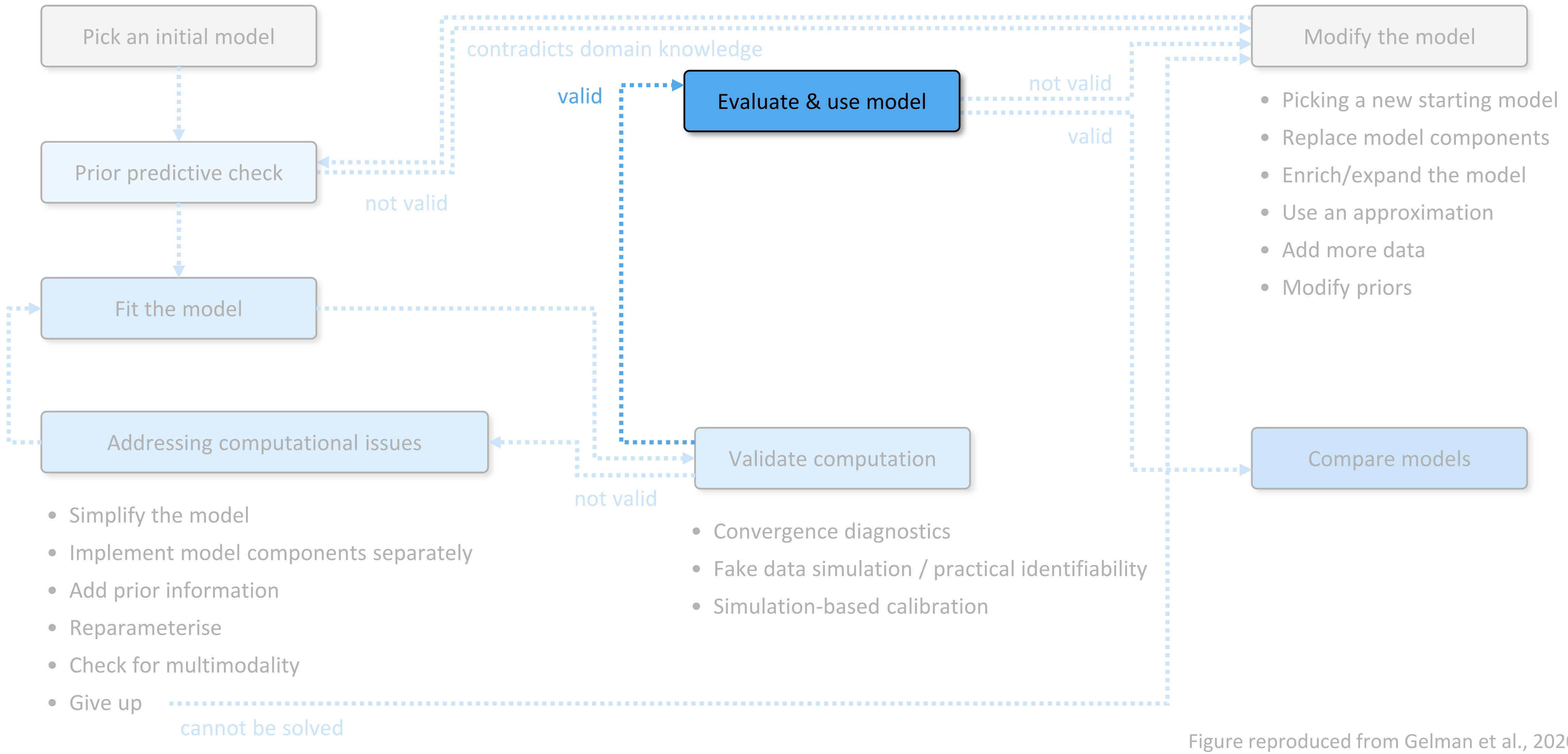
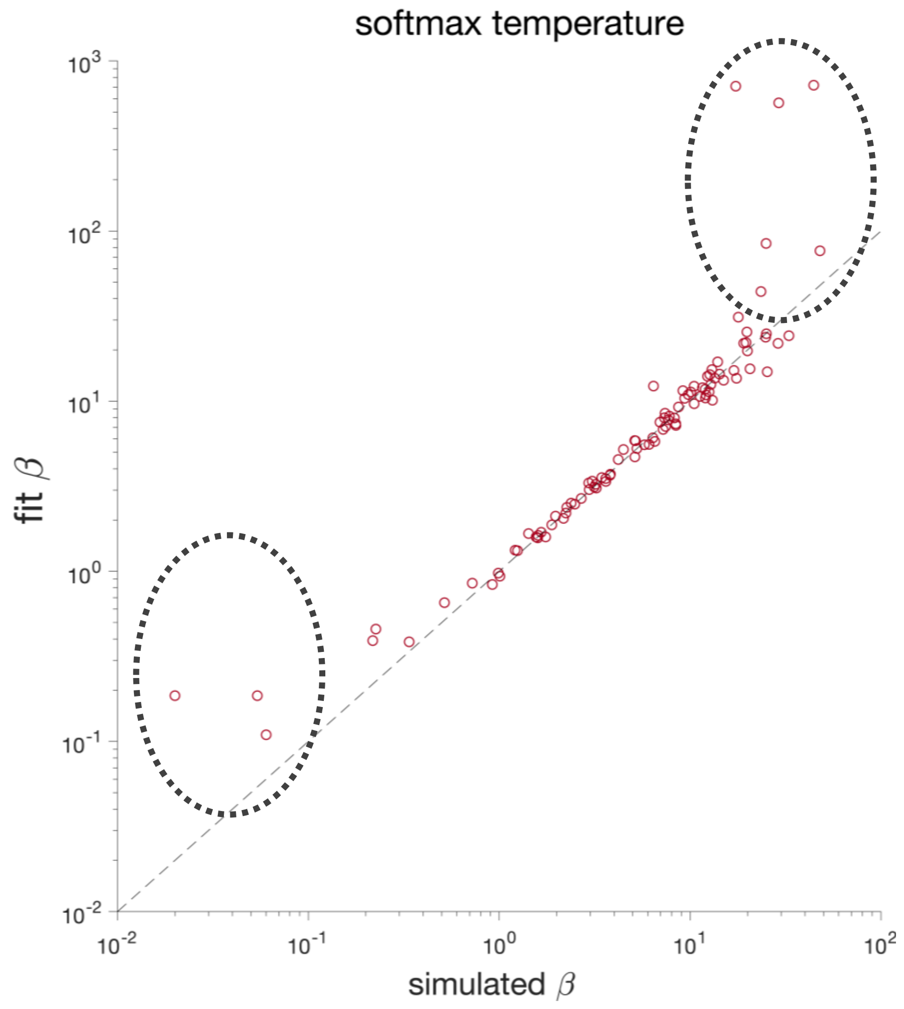


Figure reproduced from Gelman et al., 2020, *arXiv*

EVALUATE MODEL

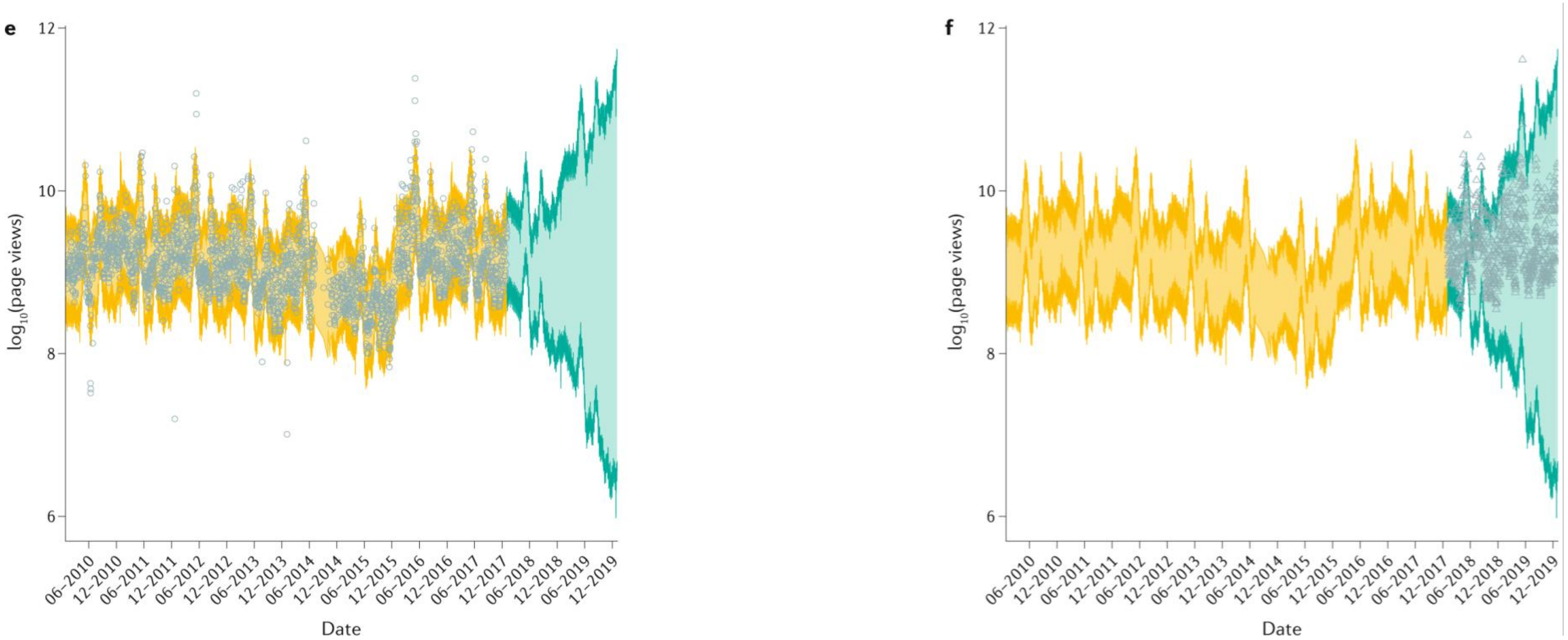
Things to consider:

- Goodness of fit (always plot data and model fit)
- Check the range of the estimated parameters (identifiability)
- Posterior predictive check $p(\tilde{\mathbf{y}}|\mathbf{y}) = \int \underbrace{p(\tilde{\mathbf{y}}|\boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\theta}|\mathbf{y})}_{\text{posterior}} d\boldsymbol{\theta}$
- Risk of overfitting!
  - Cross validation
  - Holdout test set
- Sensitivity analyses
  - Influence of prior
  - Influence of individual data points (e.g. $\hat{k}$-diagnostics)



POSTERIOR PREDICTIVE CHECK

Posterior predictive distribution: $p(\tilde{\mathbf{y}}|\mathbf{y}) = \int \underbrace{p(\tilde{\mathbf{y}}|\boldsymbol{\theta})}_{\text{likelihood}} \underbrace{p(\boldsymbol{\theta}|\mathbf{y})}_{\text{posterior}} d\boldsymbol{\theta}$



van de Schoot et al. 2021, *Nat Rev Methods Primer*

BAYESIAN WORKFLOW

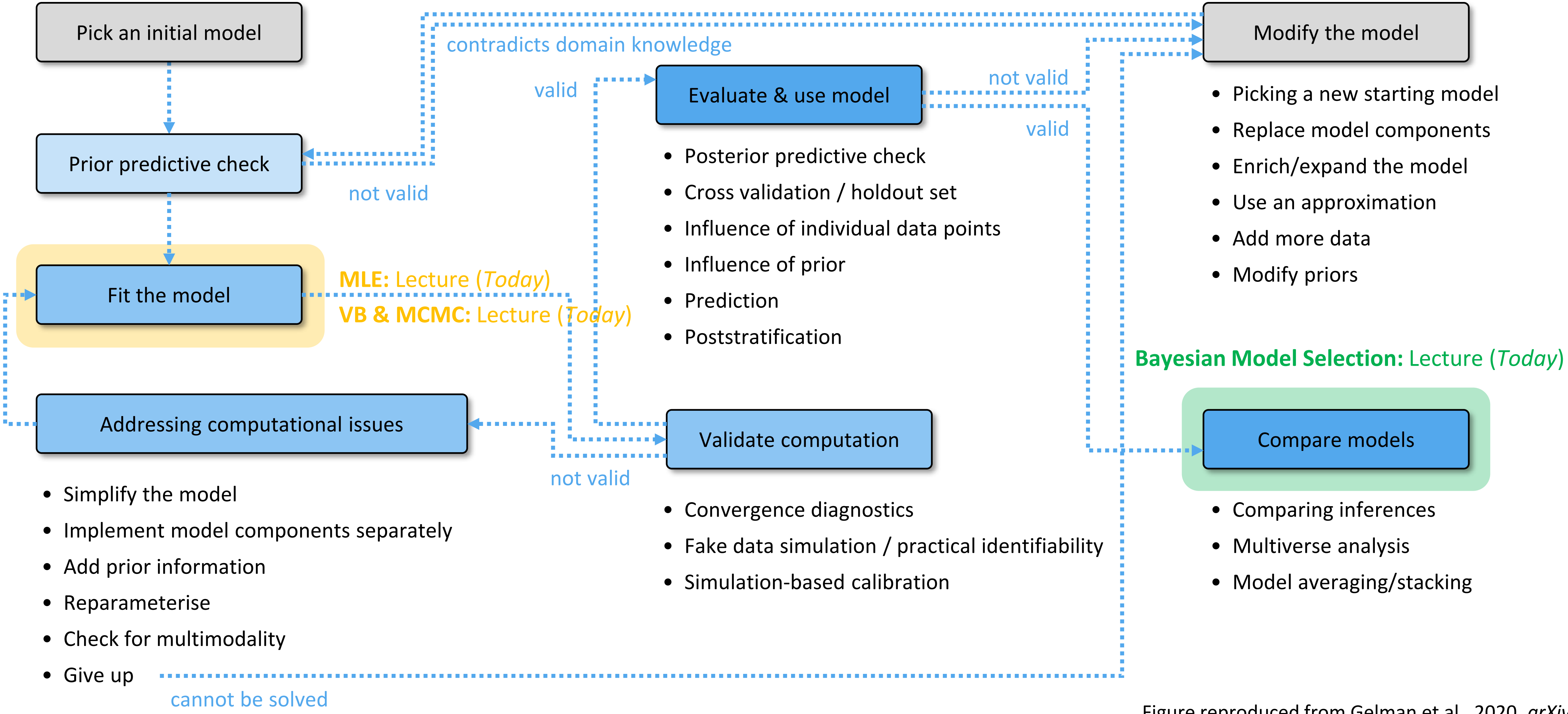


Figure reproduced from Gelman et al., 2020, *arXiv*

computational psychiatry

Bayesian Workflow for Generative Modeling in Computational Psychiatry

RESEARCH ARTICLE

]u[ubiquity press

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ABSTRACT

Computational (generative) modelling of behaviour has considerable potential for clinical applications. In order to unlock the potential of generative models, reliable statistical inference is crucial. For this, Bayesian workflow has been suggested which, however, has

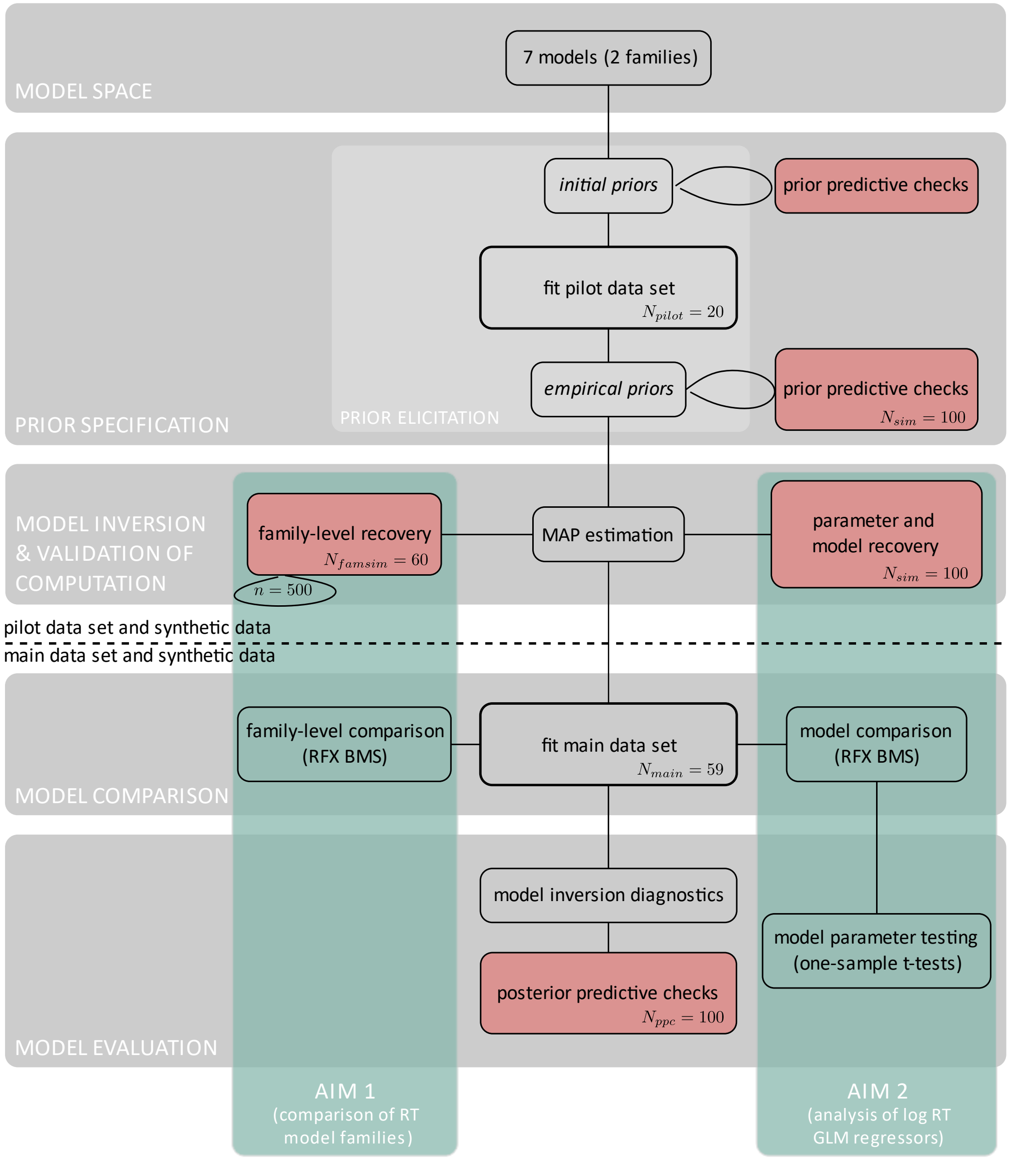
peer-reviewed publication

+ data set

+ analysis code

+ statistical analysis plan

Bayesian Workflow for Generative Modeling in Computational Psychiatry



peer-reviewed publication

+ data set

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Thank You

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Further reading

Bayesian Workflow
[Gabry et al. 2019, *J R Stat Soc A Stat*; Betancourt 2020; Gelman et al. 2020, *arXiv*; Schad et al. 2020, *arXiv*; Baribault and Collins 2023, *Psychol Methods*; Hess et al. 2025, *Comput Psychiatr*; …]

Bayesian Statistics and Modelling
[Etz et al. 2018, *Psychon B Rev*; van de Schoot et al. 2021, *Nat Rev Methods Primers*; Bürkner et al. 2023, *Statist Surv*; …]

Bayesian Cognitive Modelling
[Lee 2008, *Psychon B Rev*; …]

Role of Priors
[Dienes 2011, *Perspect Psychol Sci*; Berger 2006, *Bayesian Anal*; Goldstein et al. 2006, *Bayesian Anal*; Rouder et al. 2016, *Collabra*, Gelman et al. 2017, *Entropy*; …]

Prior Elicitation
[Lee and Vanpaemel 2018, Psychon B Rev; …]

Validation of Computation
[Talts et al. 2020, *arXiv*; Gelman and Rubin 1992, *Stat Sci*; Wilson & Collins 2019, *eLife*; …]

Fitting a Model
[van de Schoot et al. 2014, *Child Dev*; …]

Model Evaluation
[Gelman et al. 2012, *Bayesian Data Analysis*; …]

Bayesian Model Comparison
[Kass & Raftery 1995, *J Am Stat Asoc*; Penny et al. 2004, 2012, *NeuroImage*; Stephan et al. 2009, *NeuroImage*; Penny et al. 2010, *PLoS Comp Biol*; Rigoux et al. 2014, *NeuroImage*; Vandekerckhove et al. 2015, *The Oxford Handbook of Computational and Mathematical Psychology*; …]