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

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Computational Psychiatry Course Zurich
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GENERATIVE MODELS

Bayes' rule

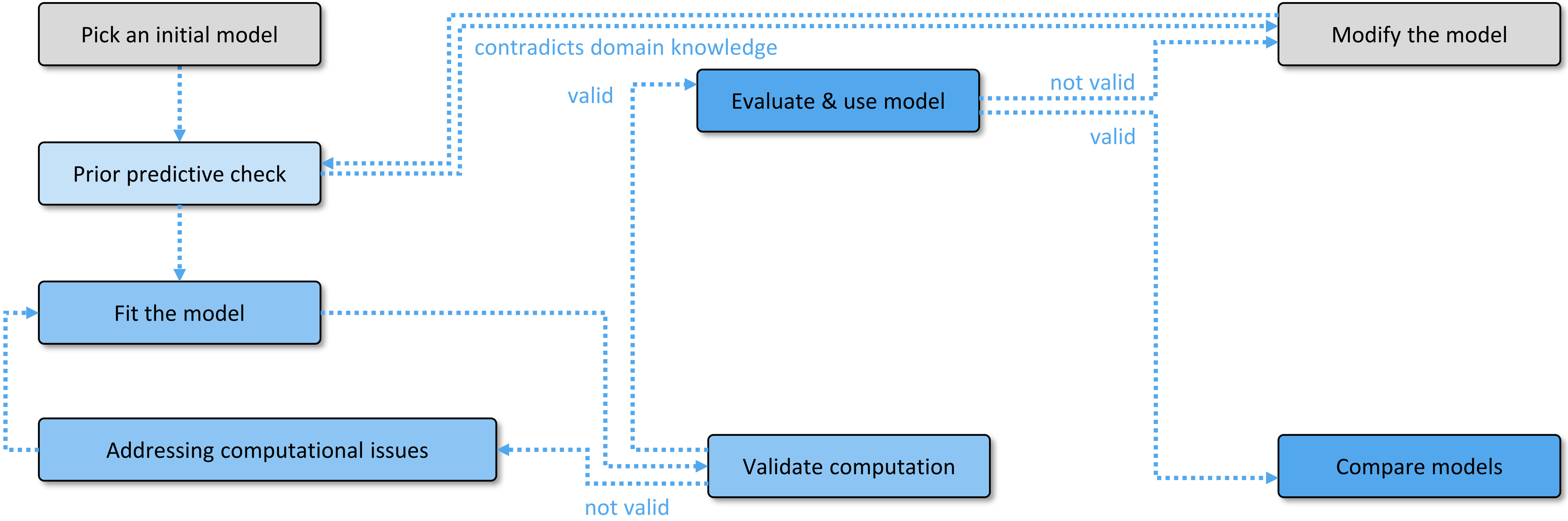
Generative model: likelihood x prior

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

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. 2024, *bioRxiv*

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, Tutorial B*)

  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, Tutorial C*)

  Predictive coding: Lecture (*Wed*)

- …

Adapted from slide by Stefan Frässle

SPECIFY PRIORS

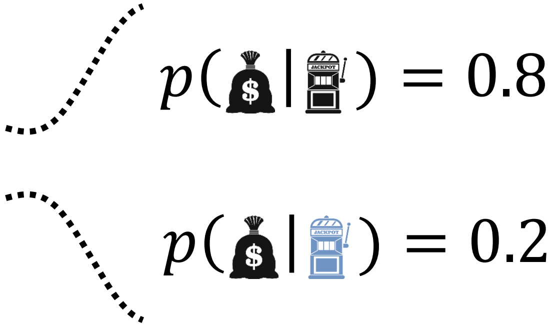
Define a range of *a priori* plausible parameter values

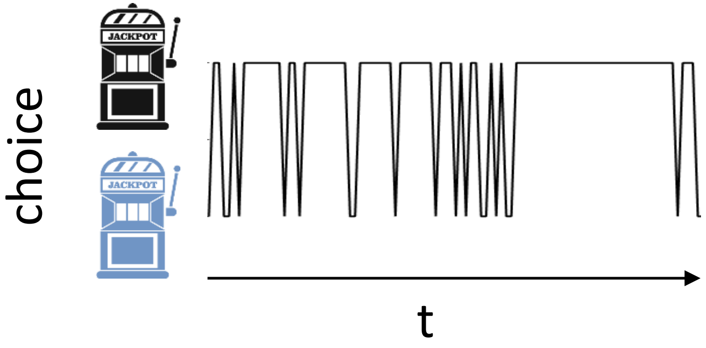
- Regularisation
- Informativeness
- Prior elicitation
  - Will depend on parametrisation
  - Previous literature
  - Expert knowledge (e.g. volume parameter in BOLD signal models)
  - Empirical priors (beware of double-dipping!)
  - …

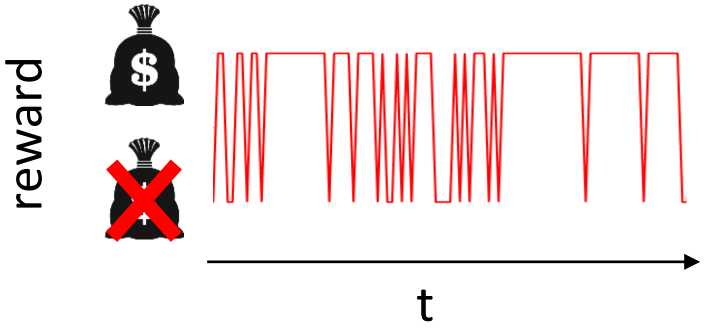
Useful resource: Prior Choice Wiki (https://github.com/stan-dev/stan/wiki/Prior-Choice-Recommendations)

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

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

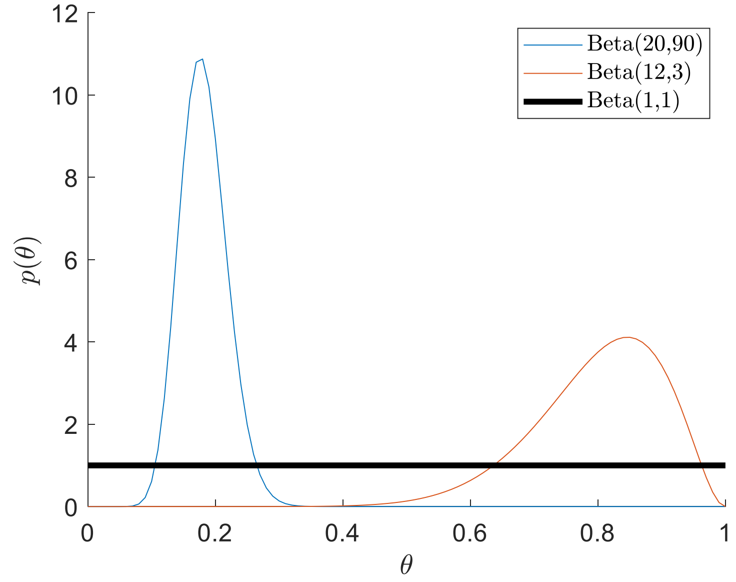
$$0 \leq b \leq 1$$

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

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

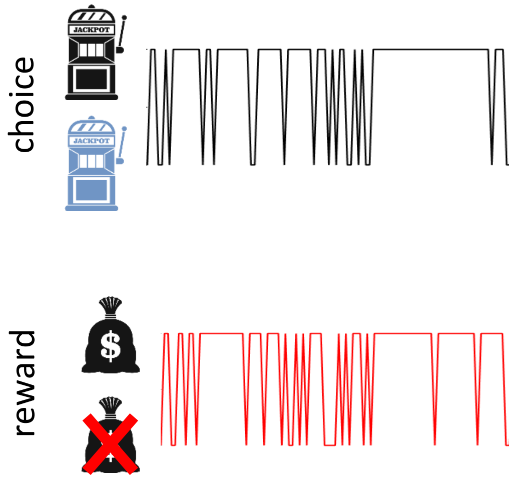
Sample from prior
$\tilde{\boldsymbol{\theta}} \sim p(\boldsymbol{\theta})$
→
Draw simulated data set
$\tilde{\mathbf{y}} \sim p(\mathbf{Y}|\tilde{\boldsymbol{\theta}})$
→
Examine characteristics of interest

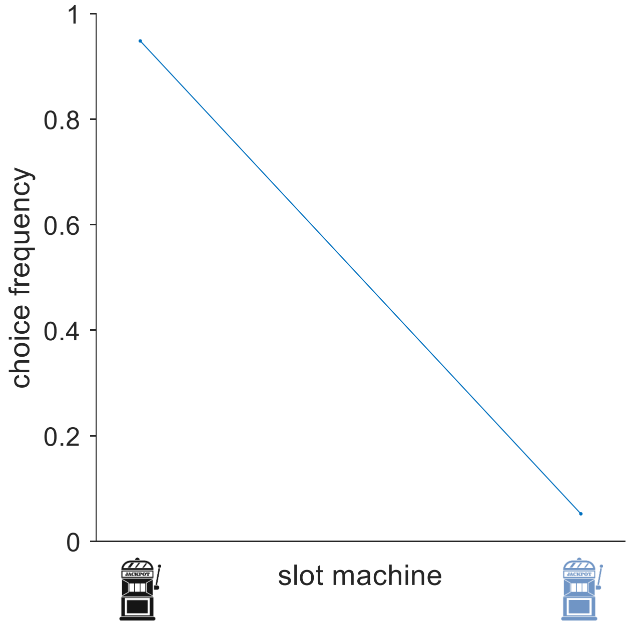
model 1
Random Choice

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

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

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





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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

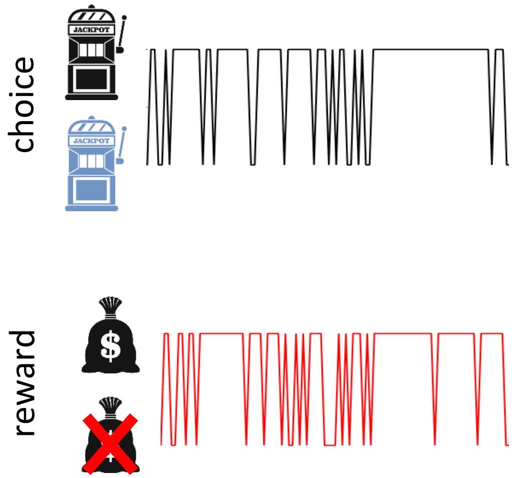
N

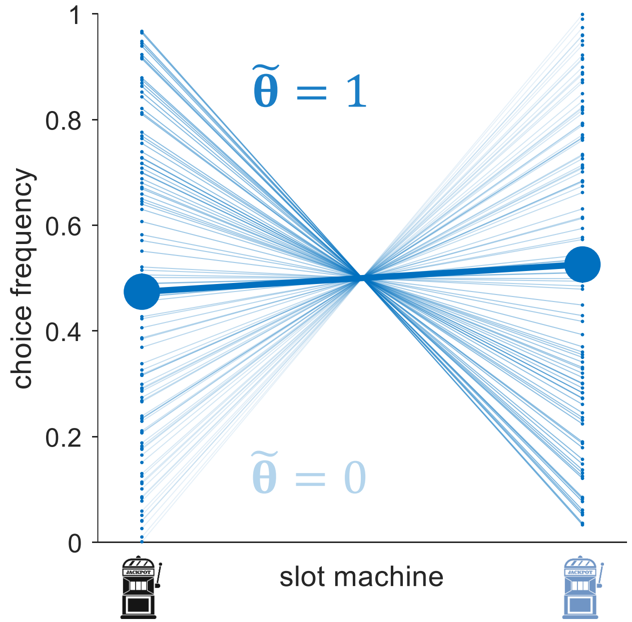
model 1

Random Choice

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

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





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model 1

Random Choice

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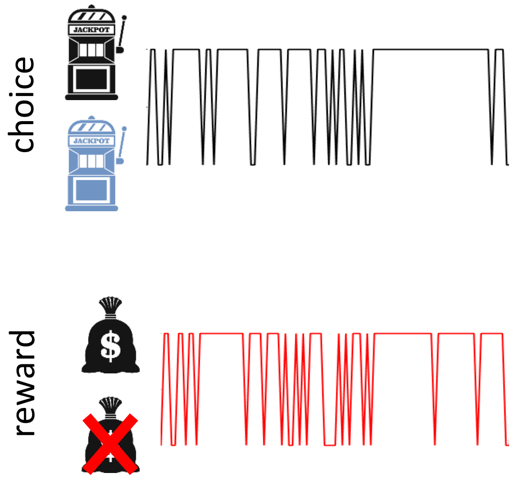
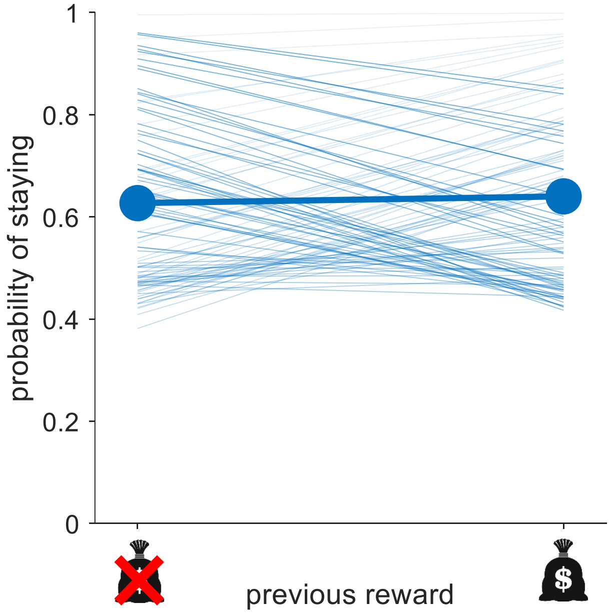




Modify the model space

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

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

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

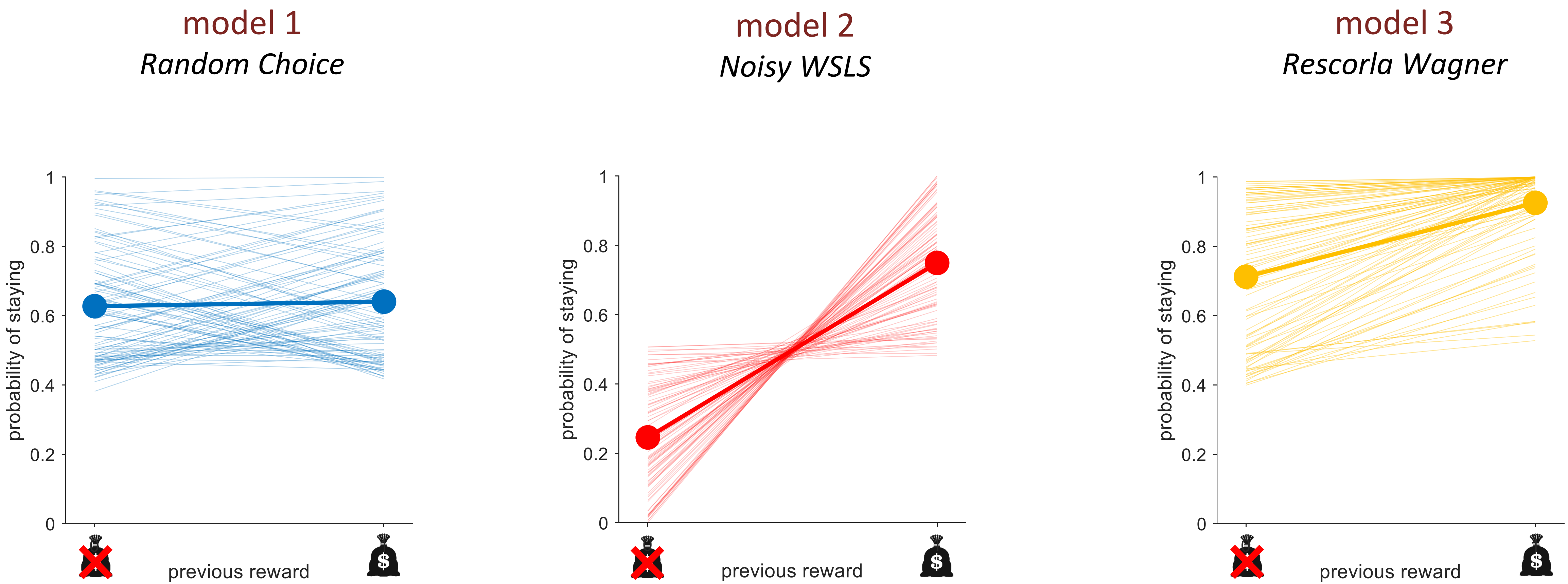
model 3
Rescorla Wagner

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

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

Wilson & Collins, 2019, *eLife*

Repeat prior predictive check

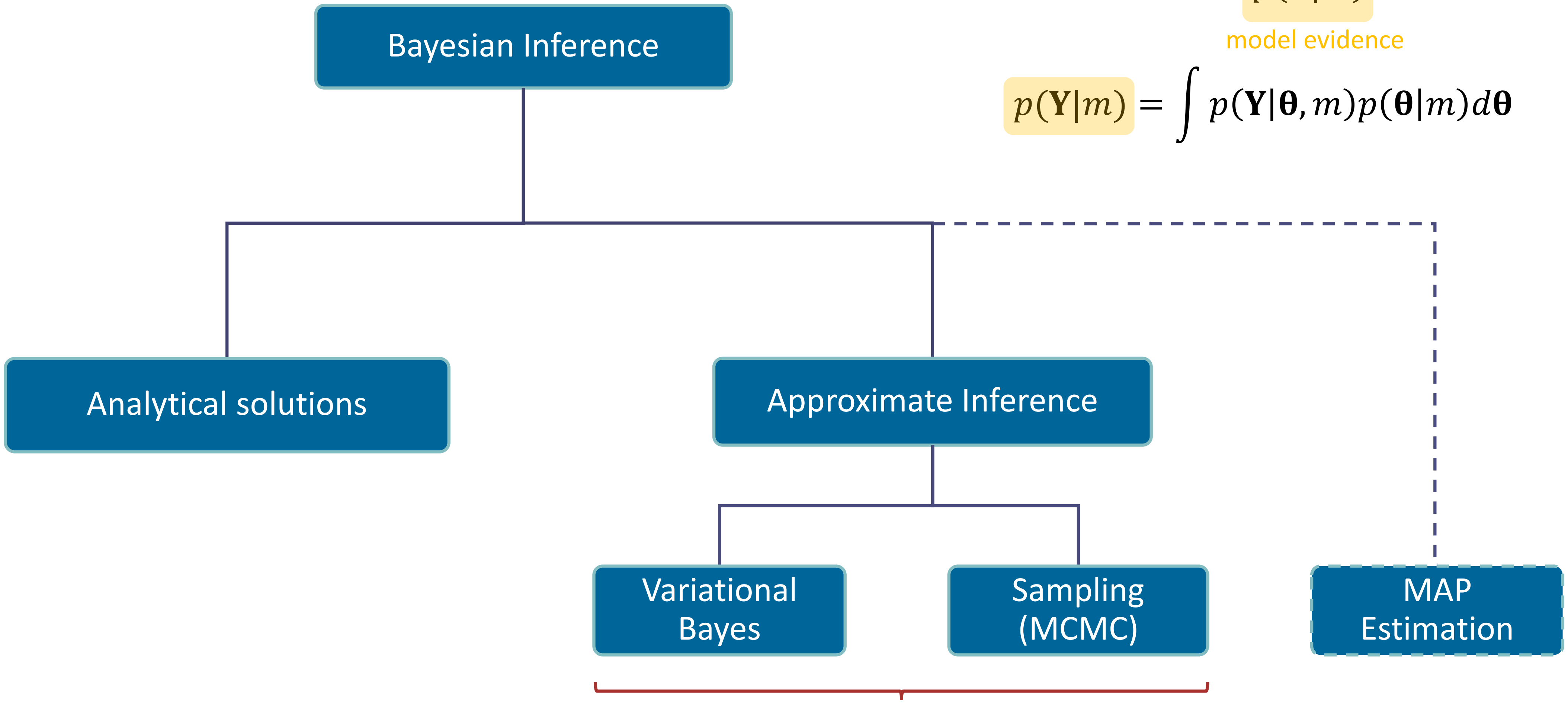


Inference on Model Parameters

posterior, likelihood, prior, model evidence

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

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



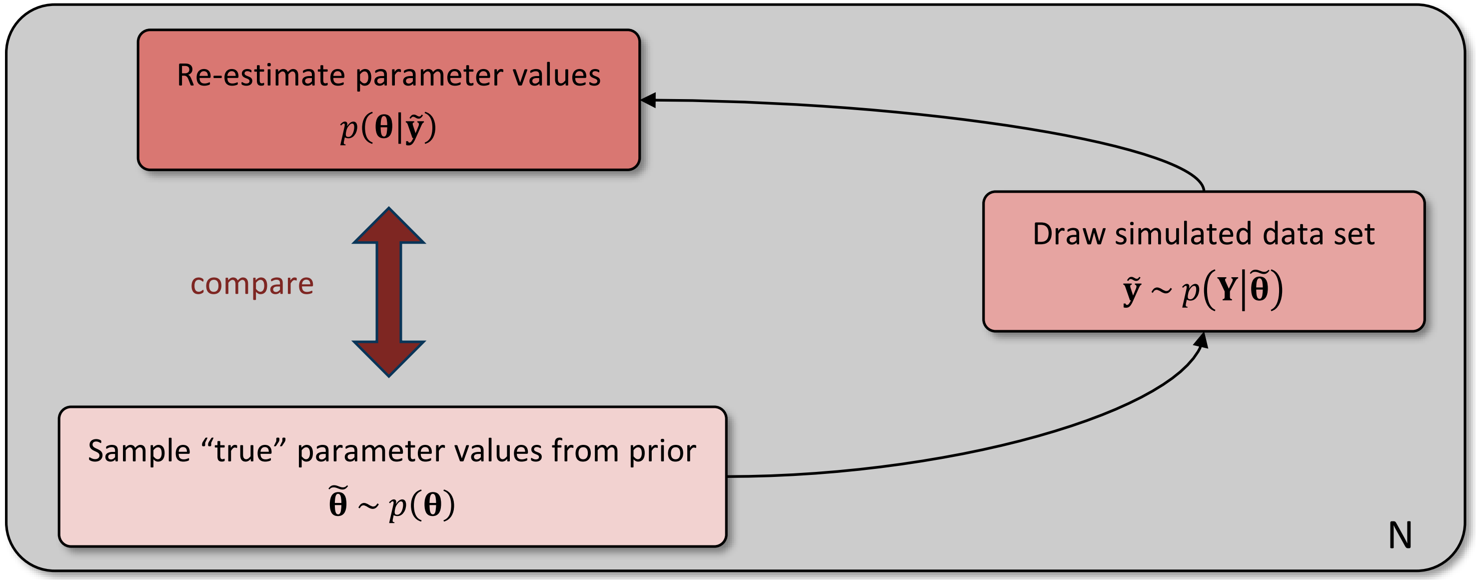
VB & MCMC: Lecture (*Today*)

Adapted from slide by Klaas Enno Stephan

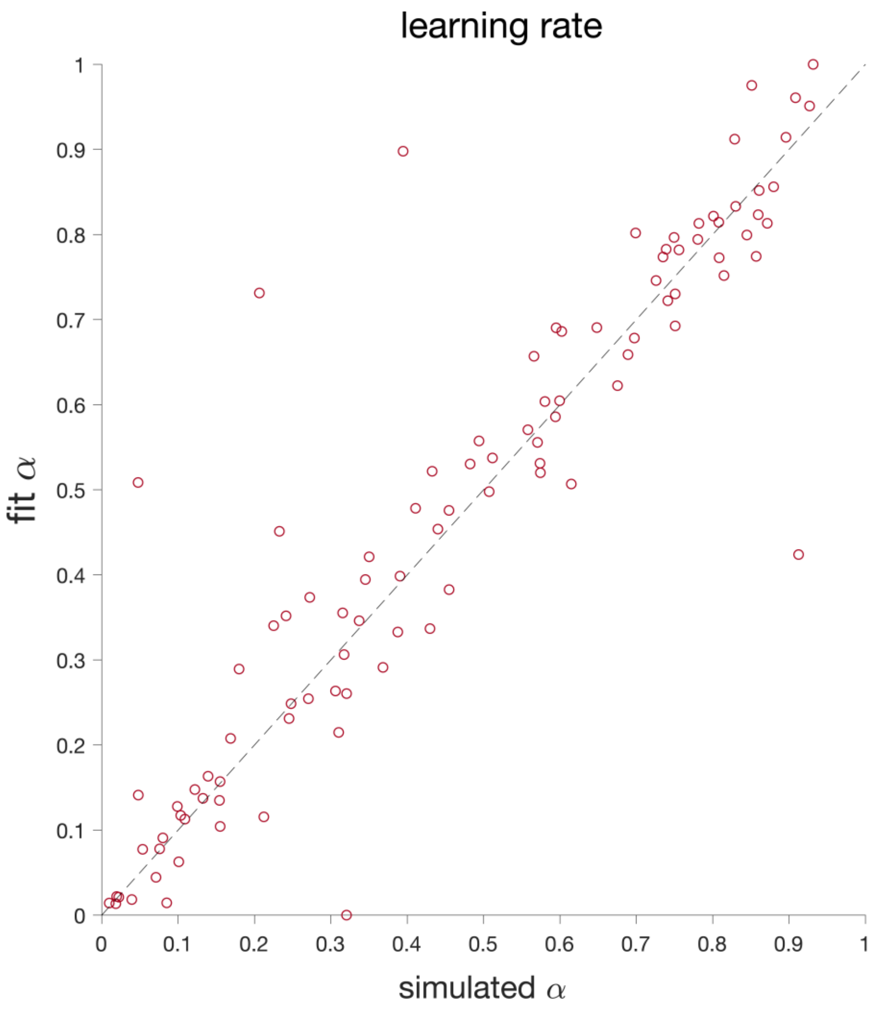
Validate computation

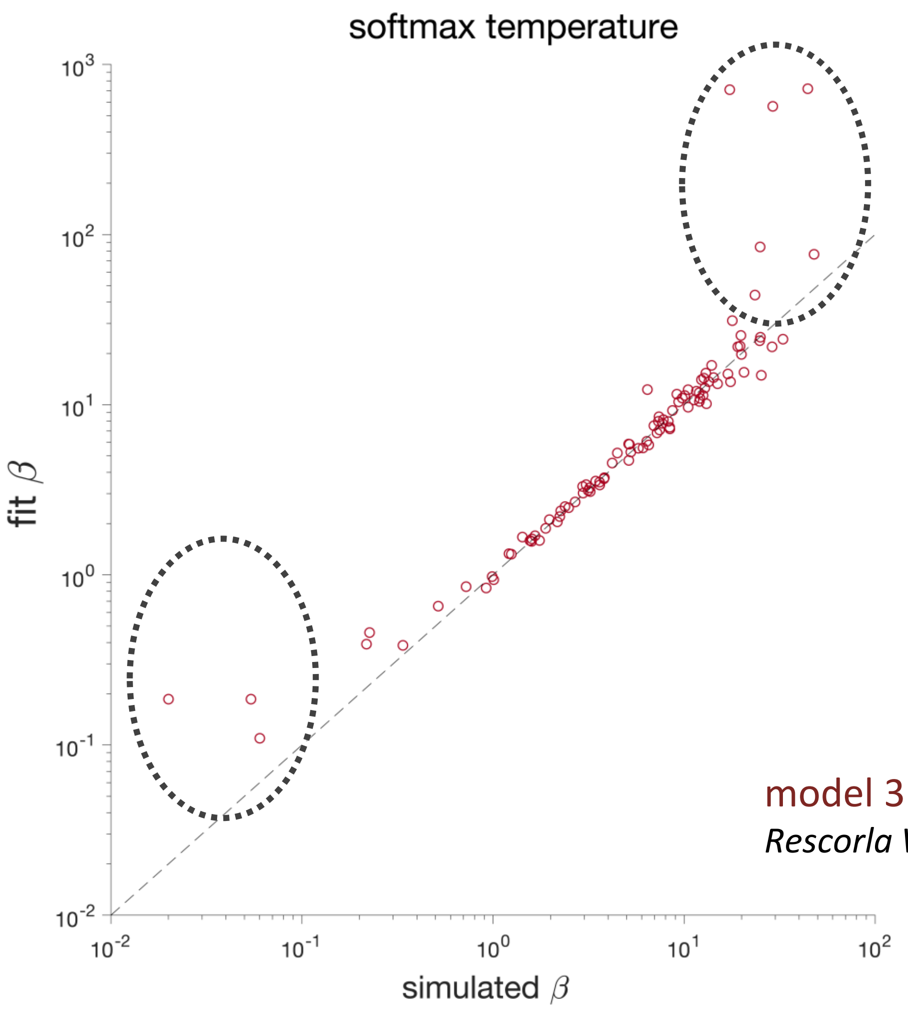
Ensure that the inference on latent variables is reliable

- 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 issues!)
- 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: $\hat{R}$ statistic Gelman and Rubin 1992 *Stat Sci*

Bayesian workflow

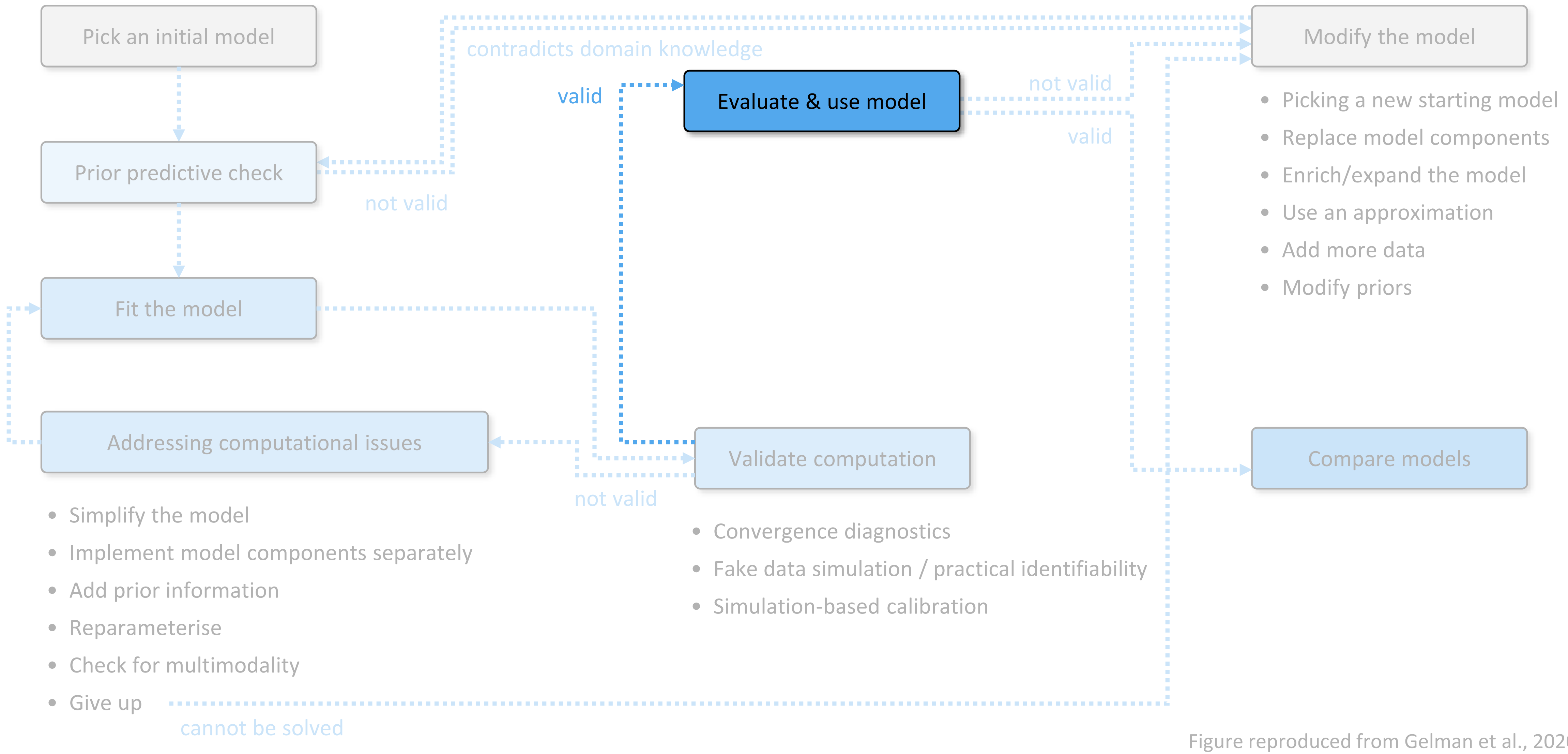
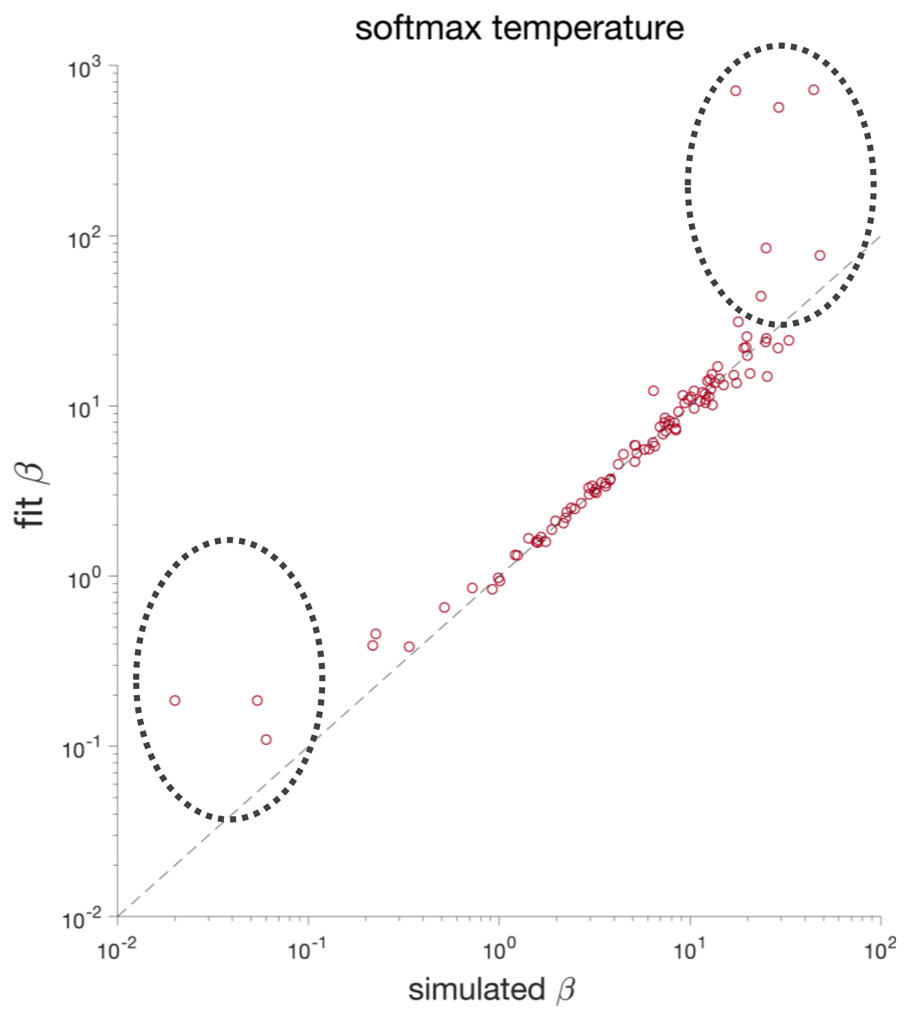


Figure reproduced from Gelman et al., 2020, *arXiv*

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



BAYESIAN WORKFLOW

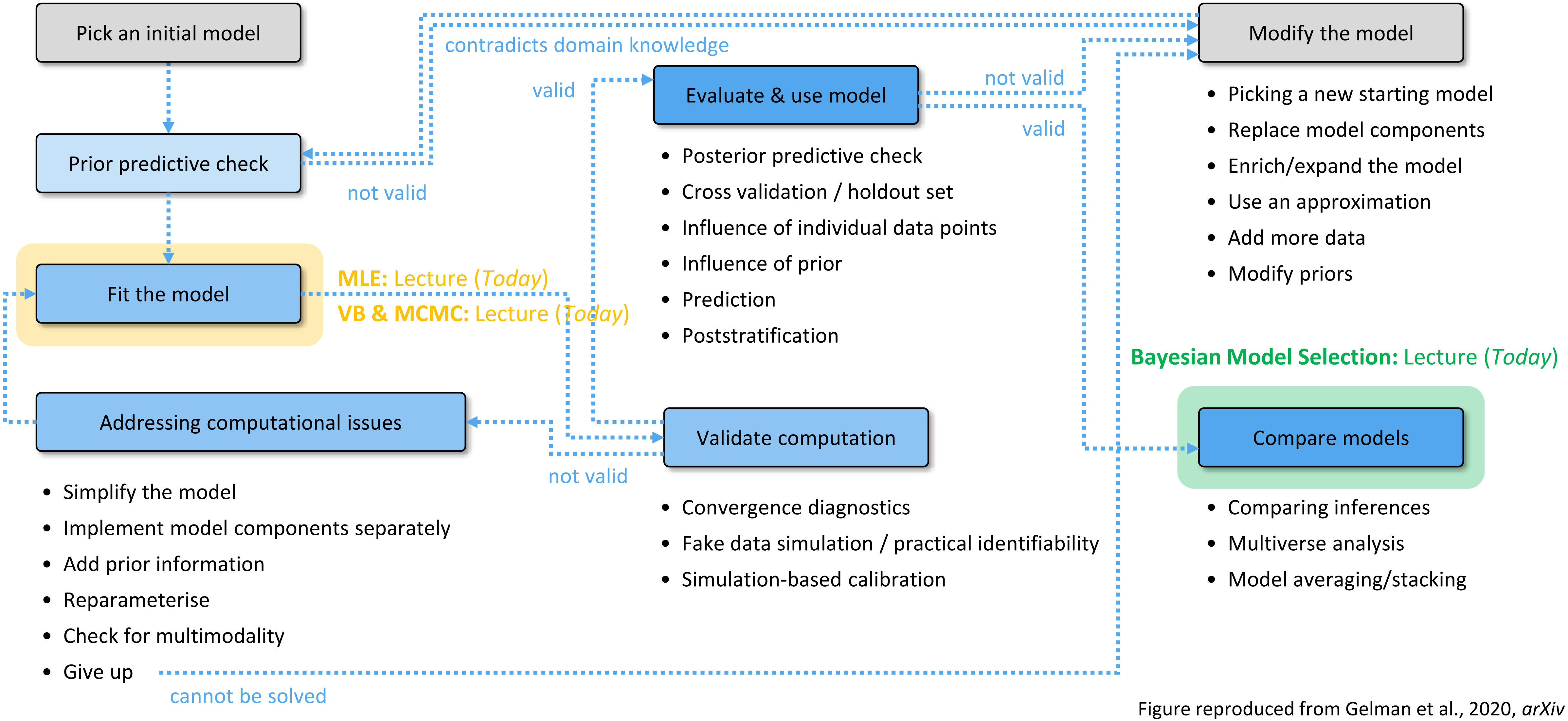


Figure reproduced from Gelman et al., 2020, *arXiv*

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Poster #3
(*Friday*)

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Bayesian Workflow for Generative Modeling in Computational Psychiatry

Alexander J. Hess, Sandra Iglesias, Laura Köchli, Stephanie Marino, Matthias Müller-Schrader, Lionel Rigoux, Christoph Mathys, Olivia K. Harrison, Jakob Heinzle, Stefan Frässle, Klaas Enno Stephan

doi: https://doi.org/10.1101/2024.02.19.581001

preprint

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. 2020, *bioRxiv*; …]

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* ; …]

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*; …]