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

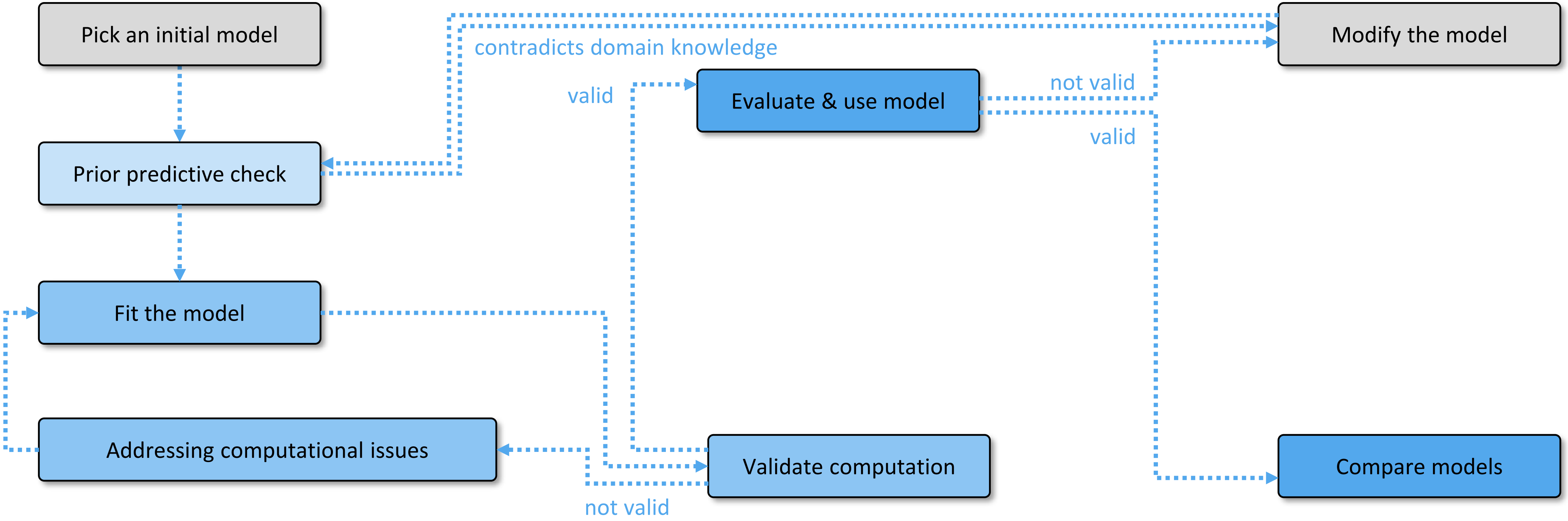


Figure reproduced from Gelman et al., 2020, *arXiv*

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

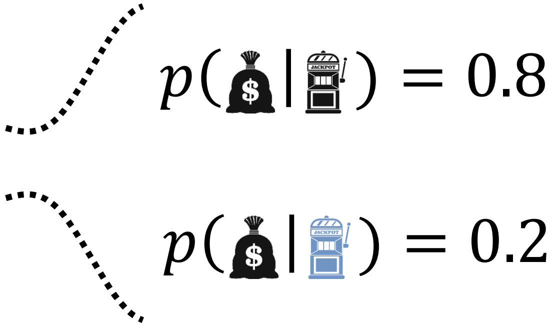
Define a range of *a priori* plausible parameter values

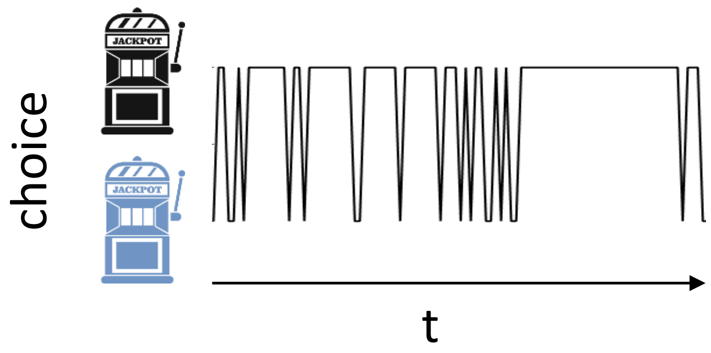
- Regularisation
- Informativeness
- Prior elicitation
  - Will depend on parametrisation
  - Previous literature
  - Expert knowledge (e.g. volume parameter in BOLD signal models)
  - Empirical priors (beware of double-dipping!)
  - …

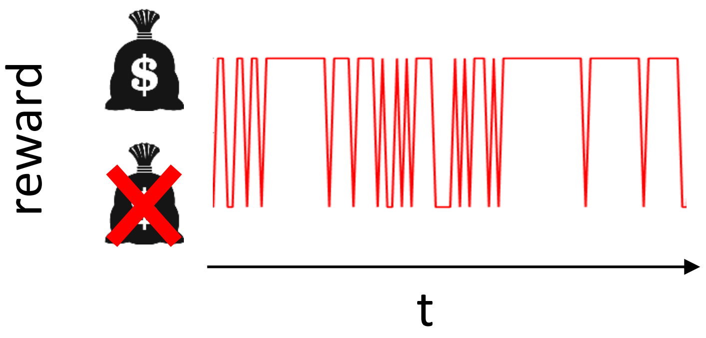
Useful resource: Prior Choice Wiki (https://github.com/stan-dev/stan/wiki/Prior-Choice-Recommendations)

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*

Pick initial model

model 1
Random choice

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

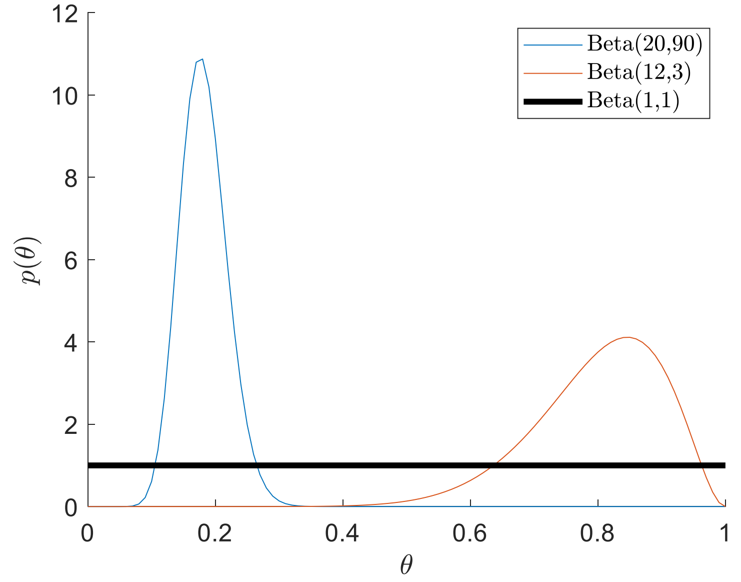
$$0 \le b \le 1$$

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

Prior elicitation

- Conjugacy: $\mathrm{Beta} \propto \mathrm{Binomial} * \mathrm{Beta}$
- No preference for specific values *a priori*

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



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

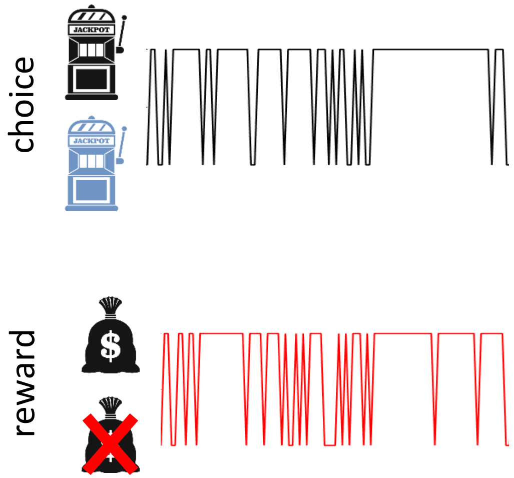
model 1

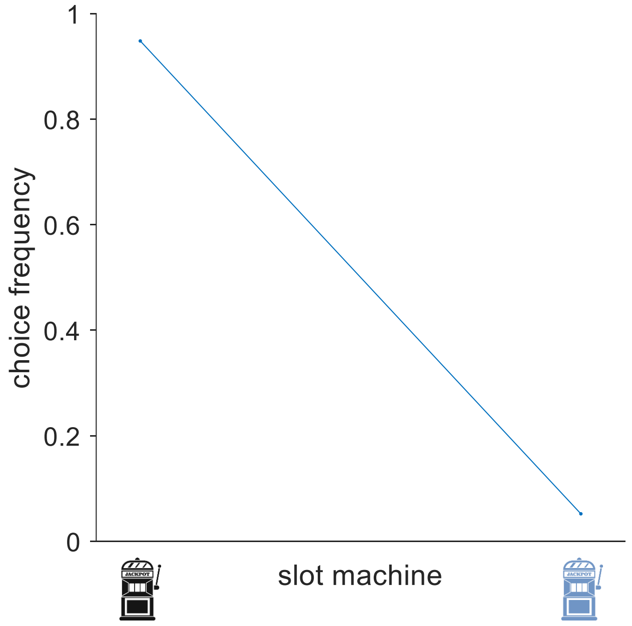
Random Choice

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

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

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





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Use simulations to refine model without using data multiple times

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

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

Examine characteristics of interest

N

model 1
Random Choice

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

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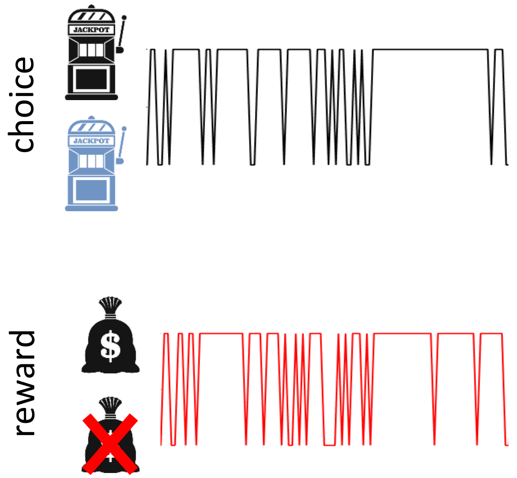

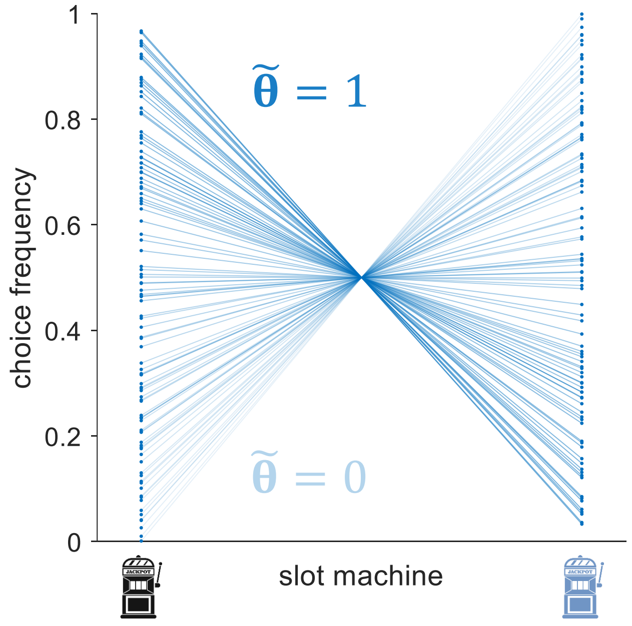

PRIOR PREDICTIVE CHECK

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

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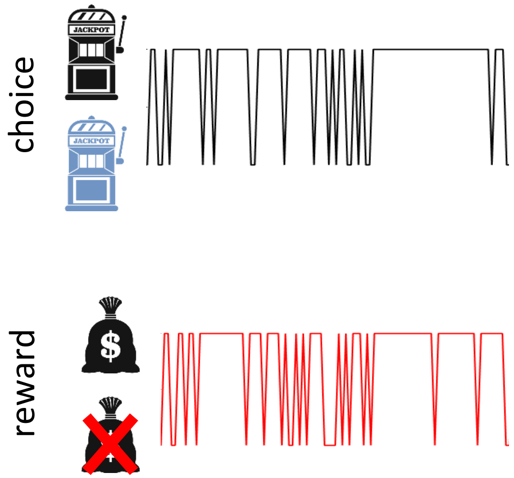

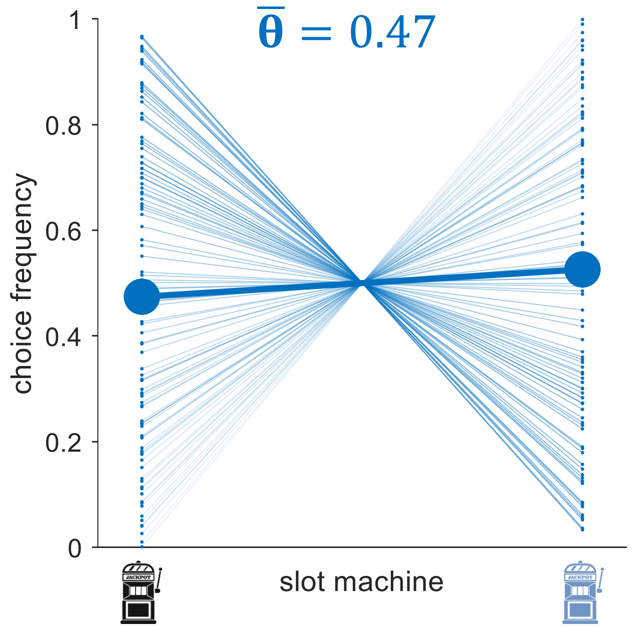

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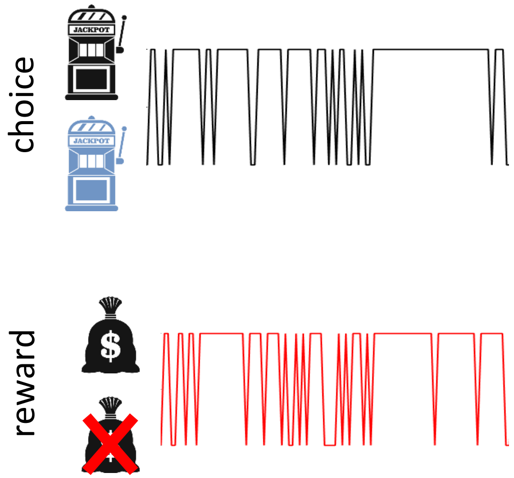
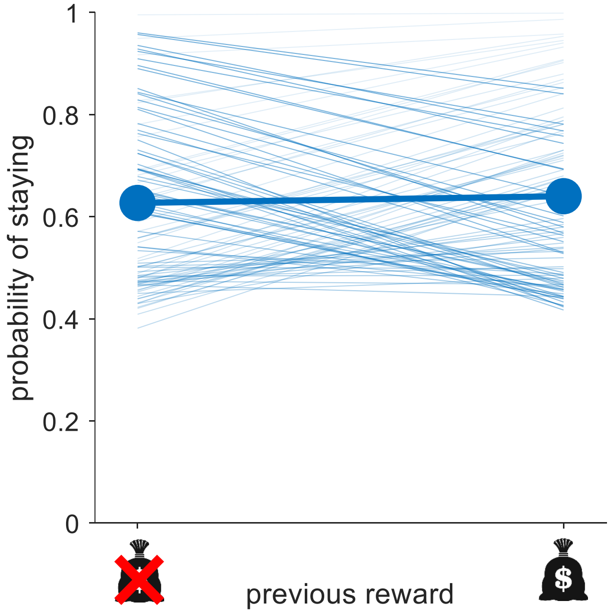




Modify the model space

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

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

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

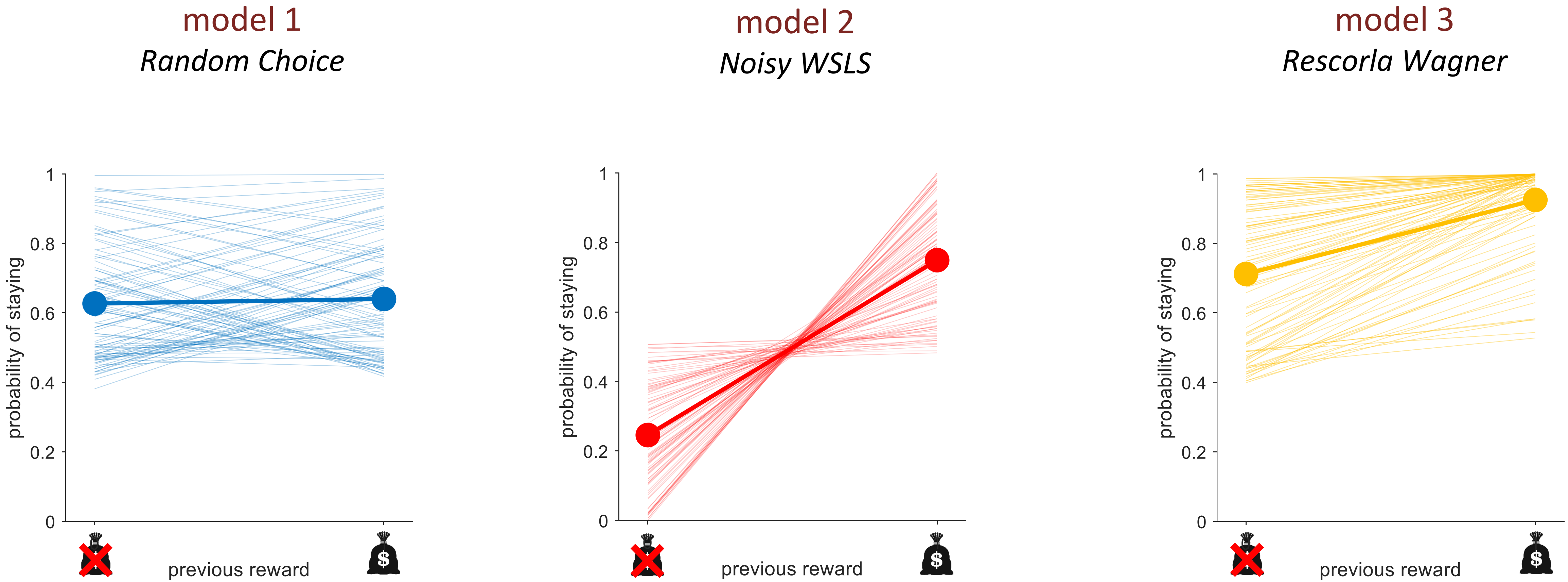
model 3
Rescorla Wagner

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

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

Wilson & Collins, 2019, *eLife*

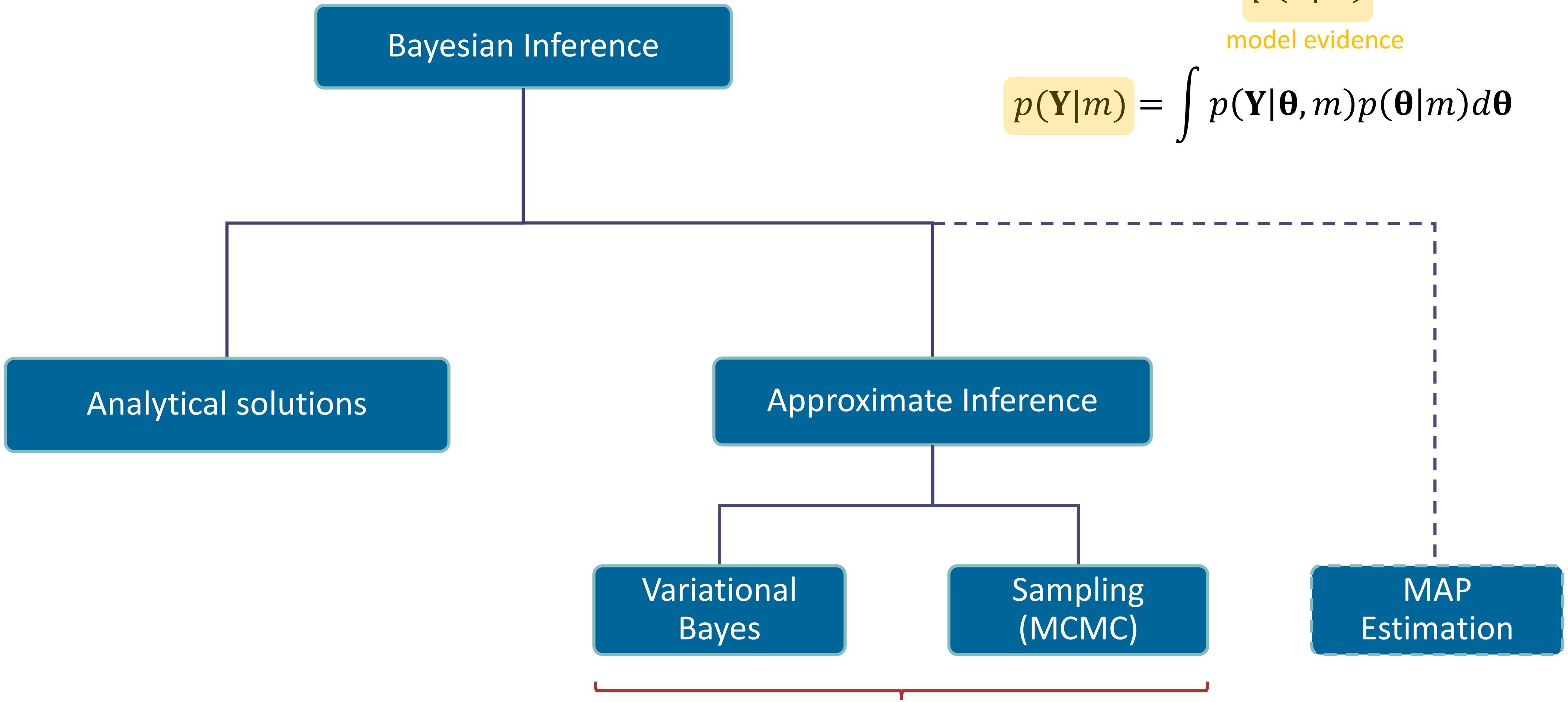
Repeat prior predictive check



Inference on model parameters

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

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



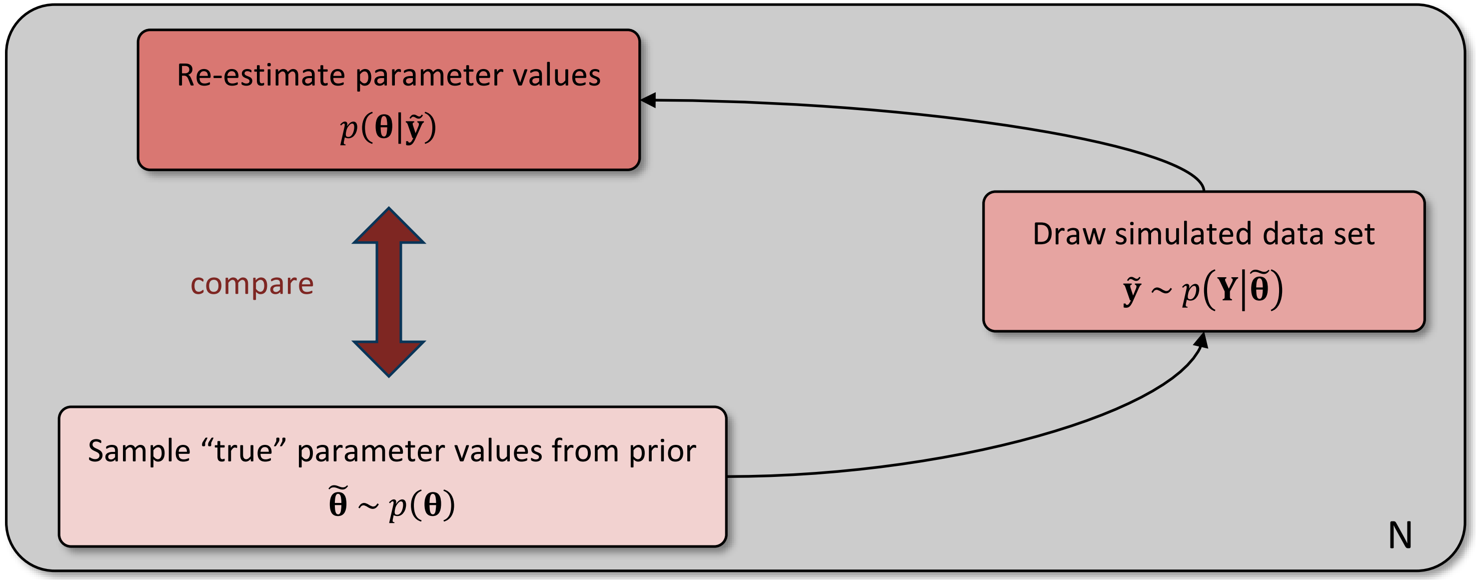
VB & MCMC: Lecture (*Today*)

Adapted from slide by Klaas Enno Stephan

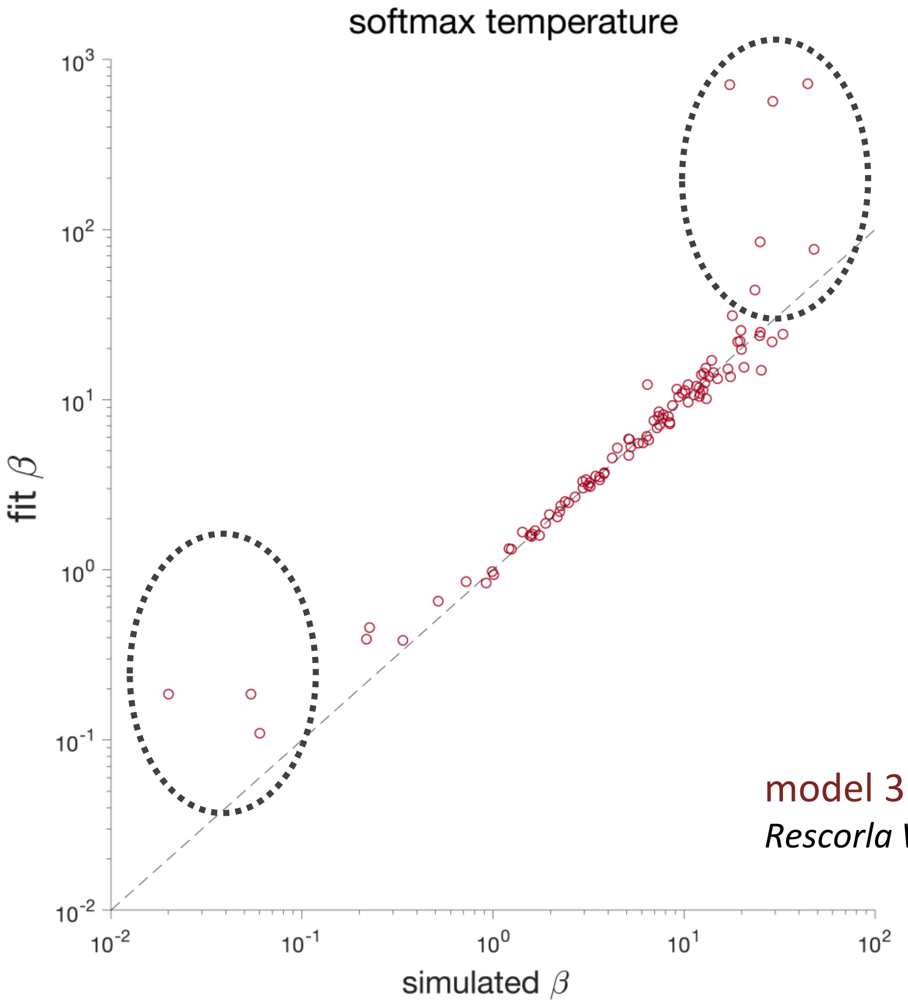
Validate computation

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 (formal and practical issues!)



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*

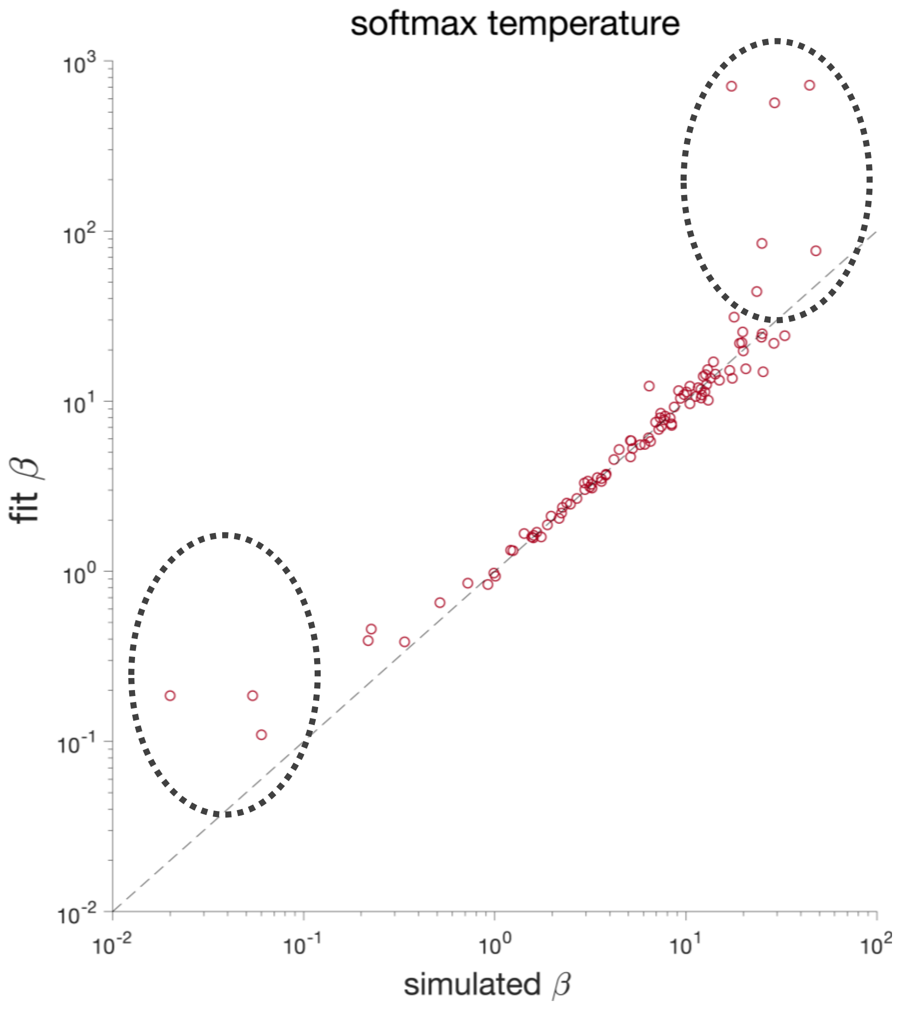
$$\underbrace{p(\boldsymbol{\theta})}_{\text{prior}} = \int \underbrace{p(\boldsymbol{\theta}|\tilde{\mathbf{y}})}_{\text{posterior}} \underbrace{p(\tilde{\mathbf{y}}|\tilde{\boldsymbol{\theta}})\, p(\tilde{\boldsymbol{\theta}})}_{\text{joint}} \, d\tilde{\boldsymbol{\theta}}\, d\tilde{\mathbf{y}}$$

  - 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*

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

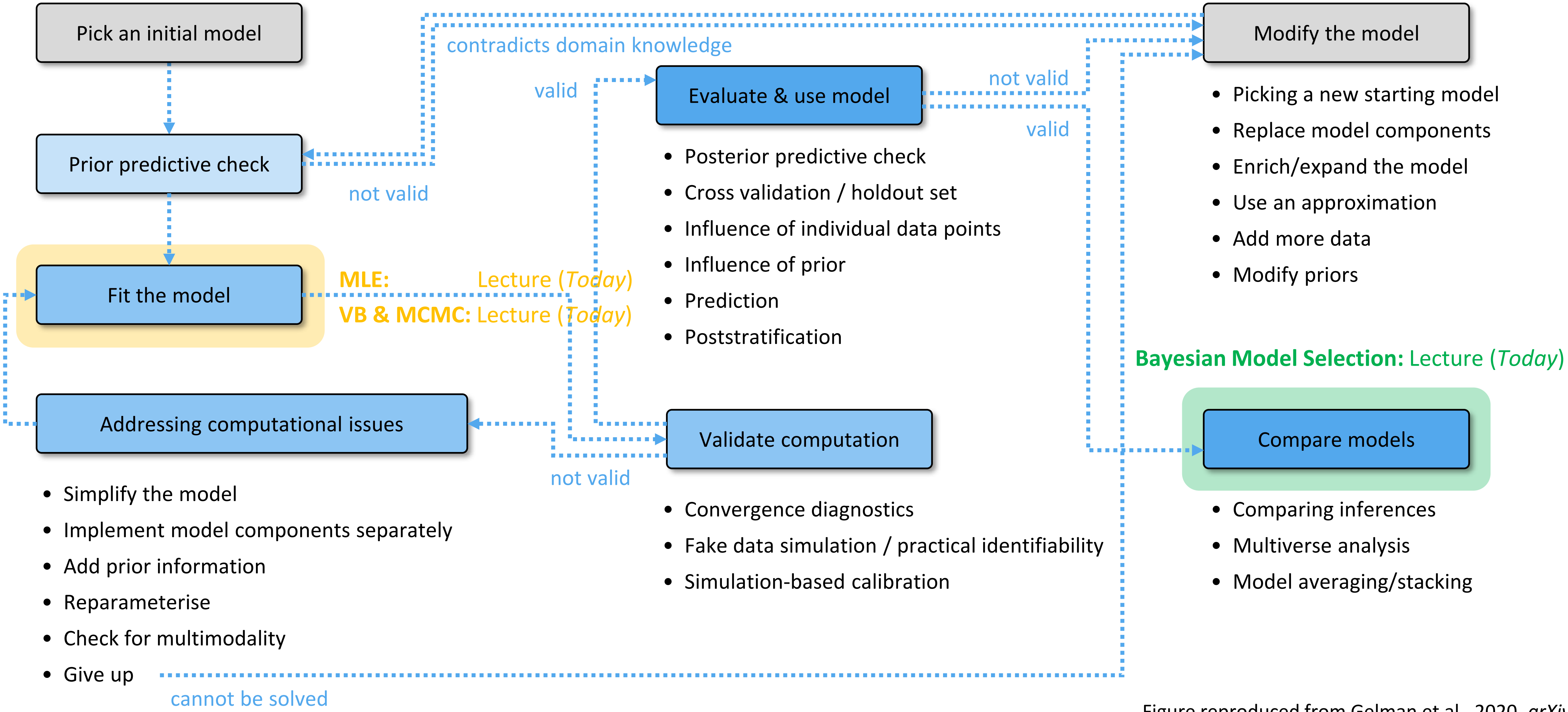


Figure reproduced from Gelman et al., 2020, *arXiv*

HAPPY SUBMITTING

nature
computational psychiatry

ARTICLES

How to get rich: our fancy model for maximizing wins at the slot machine

Your Name [1,2]

Casinos are an attractive alternative to third-party funding for starting your own research group or running projects you have in mind. We here present a fancy computational model that allows you to maximize the money you can get from playing the slot machine at your local casino. This will allow you to build your own group and run all the awesome experiments that you were planning for so long but never had the financial resources to do. You might even be able to invest in this awesome wide-screen monitor and the Italian coffee machine that you always wanted to have in your lab. Hence, this paper is of high practical relevance for the scientific community and should therefore be pu

Slide courtesy by Stefan Frässle

Further reading

OVERVIEW

Bayesian Workflow Gelman et al. 2020, *arXiv:2011.01808*

Bayesian Statistics and Modelling Etz et al. 2018, *Psychon B Rev*; van de Schoot et al. 2021, *Nat Rev Methods Primers*

Modelling Tutorial (non-Bayesian) Wilson & Collins 2019, *eLife*

Bayesian cognitive modelling Lee 2008, *Psychon B Rev*

COMPONENTS OF BAYESIAN WORKFLOW

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 Methods Vandekerckhove et al. 2015, *The Oxford Handbook of Computational and Mathematical Psychology*;

Universität Zürich[UZH] ETH zürich

Translational Neuromodeling Unit

Thank you!

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