Fitting a model: Maximum likelihood

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Models for the multi-armed bandit

model 1
Random choice

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

$$0 \leq b \leq 1$$

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

model 2
Noisy win-stay-lose-switch

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

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

model 3
Rescorla Wagner

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

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

Wilson & Collins, 2019, *eLife*

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Maximum likelihood estimator

Maximum likelihood estimator (MLE)

Given: Data: $Y = \{y_1, \ldots, y_T\}$

Assume: Family / set of distributions : $\{p_\theta : \theta \in \Theta\}$ and $Y = \{y_1, \ldots, y_T\}$ is sample from p_θ iid

Goal: Estimate the θ that the data $Y = \{y_1, \ldots, y_T\}$ comes from

Likelihood

$$\boxed{\theta_{MLE} = \underset{\theta \in \Theta}{\operatorname{argmax}}\big(p(Y|\theta, m)\big)}$$

where: $$\boxed{p(Y|\theta, m) = p(y_{1..T}|\theta, m) = \prod_{t=1}^{T} p(y_t|\theta, m)}$$

Intuitively: *"Maximum likelihood estimation finds the θ for which the acquired data is most likely"*

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Notes:

- MLE might not be unique
- MLE might not exist

SPECIFYING THE LIKELIHOOD FUNCTION

model 1
Random choice

$p_t^1 = b$

$p_t^2 = 1 - b$

$0 \leq b \leq 1$

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

For single trial t: $p(y_t|\theta, m) = \theta^{y_t}(1-\theta)^{(1-y_t)}$

Bernoulli distribution

SPECIFYING THE LIKELIHOOD FUNCTION

model 1
Random choice

$p_t^1 = b$

$p_t^0 = 1 - b$

$0 \leq b \leq 1$

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

For single trial t: $\boxed{p(y_t|\theta, m) = \theta^{y_t}(1-\theta)^{(1-y_t)}}$

Bernoulli distribution

For all trials $1..T$: $p(Y|\theta, m) = p(y_{1..T}|\theta, m) = \prod_{t=1}^{T} \theta^{y_t}(1-\theta)^{(1-y_t)}$

$Y = \{y_1, \ldots, y_T\}$ iid

Maximizing the likelihood

$$p(Y|\theta, m) = \prod_{t=1}^{T} \theta^{y_t}(1-\theta)^{(1-y_t)}$$

Likelihood

Analytical solution

- If $p(Y|\theta, m)$ is differentiable, use the derivative test.
- i.e.: set first derivative to 0
- For simple cases, this yields an explicit (analytical) solution

Numerical solution

- Use numerical routines to find the maximum of $p(Y|\theta, m)$.
- E.g.: fminsearch (MATLAB)

Maximizing the Likelihood

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Analytical solution to MLE

model 1
Random choice

$$p(Y|\theta,m) = \prod_{t=1}^{T} \theta^{y_t}(1-\theta)^{(1-y_t)}$$

$$\log\big(p(Y|\theta,m)\big) = \log\left(\prod_{t=1}^{T} \theta^{y_t}(1-\theta)^{(1-y_t)}\right)$$

$$= \sum_{t=1}^{T} \log\big(\theta^{y_t}(1-\theta)^{(1-y_t)}\big)$$

$$= \sum_{t=1}^{T} \big(y_t \log(\theta) + (1-y_t)\log(1-\theta)\big)$$

$$\frac{d}{d\theta}\log\big(p(Y|\theta,m)\big) = \frac{d}{d\theta}\sum_{t=1}^{T} \big(y_t \log(\theta) + (1-y_t)\log(1-\theta)\big) \overset{!}{=} 0$$

ANALYTICAL SOLUTION TO MLE

model 1
Random choice

$$\frac{d}{d\theta}\sum_{t=1}^{T}(y_t\log(\theta)+(1-y_t)\log(1-\theta))=0$$

$$\left(\frac{d}{d\theta}\log(\theta)\right)\left(\sum_{t=1}^{T}y_t\right)+\left(\frac{d}{d\theta}\log(1-\theta)\right)\left(\sum_{t=1}^{T}(1-y_t)\right)=0$$

$$\frac{1}{\theta(1-\theta)}\left(\sum_{t=1}^{T}y_t-\theta\sum_{t=1}^{T}y_t-\theta T+\theta\sum_{t=1}^{T}y_t\right)=0$$

$$\sum_{t=1}^{T}y_t-\theta T=0$$

Maximum likelihood estimator

$$\boxed{\theta_{MLE}=\frac{1}{T}\sum_{t=1}^{T}y_t}$$

Maximizing the likelihood

$$p(Y|\theta, m) = \prod_{t=1}^{T} \theta^{y_t}(1-\theta)^{(1-y_t)}$$

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Advantages of MLE

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- Easy to compute
- Interpretable
- Desirable asymptotic properties
  - Consistent: $\theta_{MLE} \xrightarrow{p} \theta_0$
  - Normal: $\sqrt{n} \cdot (\theta_{MLE} - \theta_0) \xrightarrow{d} \mathcal{N}(0, I^{-1})$
  - Statistically efficient: MLE reaches Cramér-Rao bound
- Invariant to reparameterization: if θ_{MLE} is a MLE for θ, then $g(\theta_{MLE})$ is a MLE for $g(\theta)$

Limitations of MLE

Limitations of MLE:

- Existence & uniqueness of MLE is not guaranteed
- MLE is a point estimate and therefore has no representation of uncertainty

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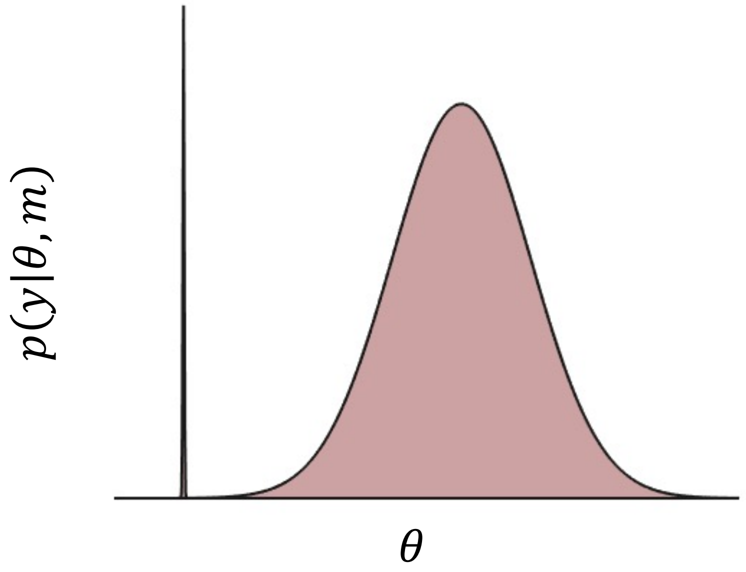

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- MLE might not be representative of the likelihood function
- Overfitting

black swan paradox

"Maximum likelihood estimation finds the θ for which the acquired data is most likely"

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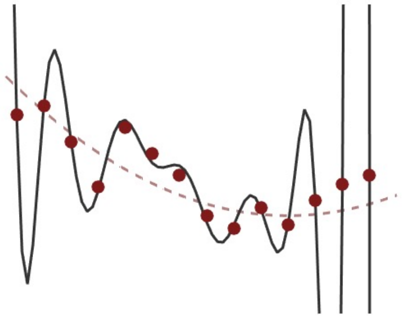

linear regression

Limitations of MLE

Limitations of MLE:

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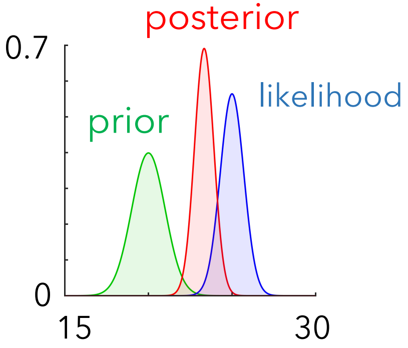
- MLE might not be representative of the likelihood function
- Overfitting
- …

ALTERNATIVES

Reverend Thomas Bayes
(1702-1761)

- Alternatives: Bayesian statistics

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

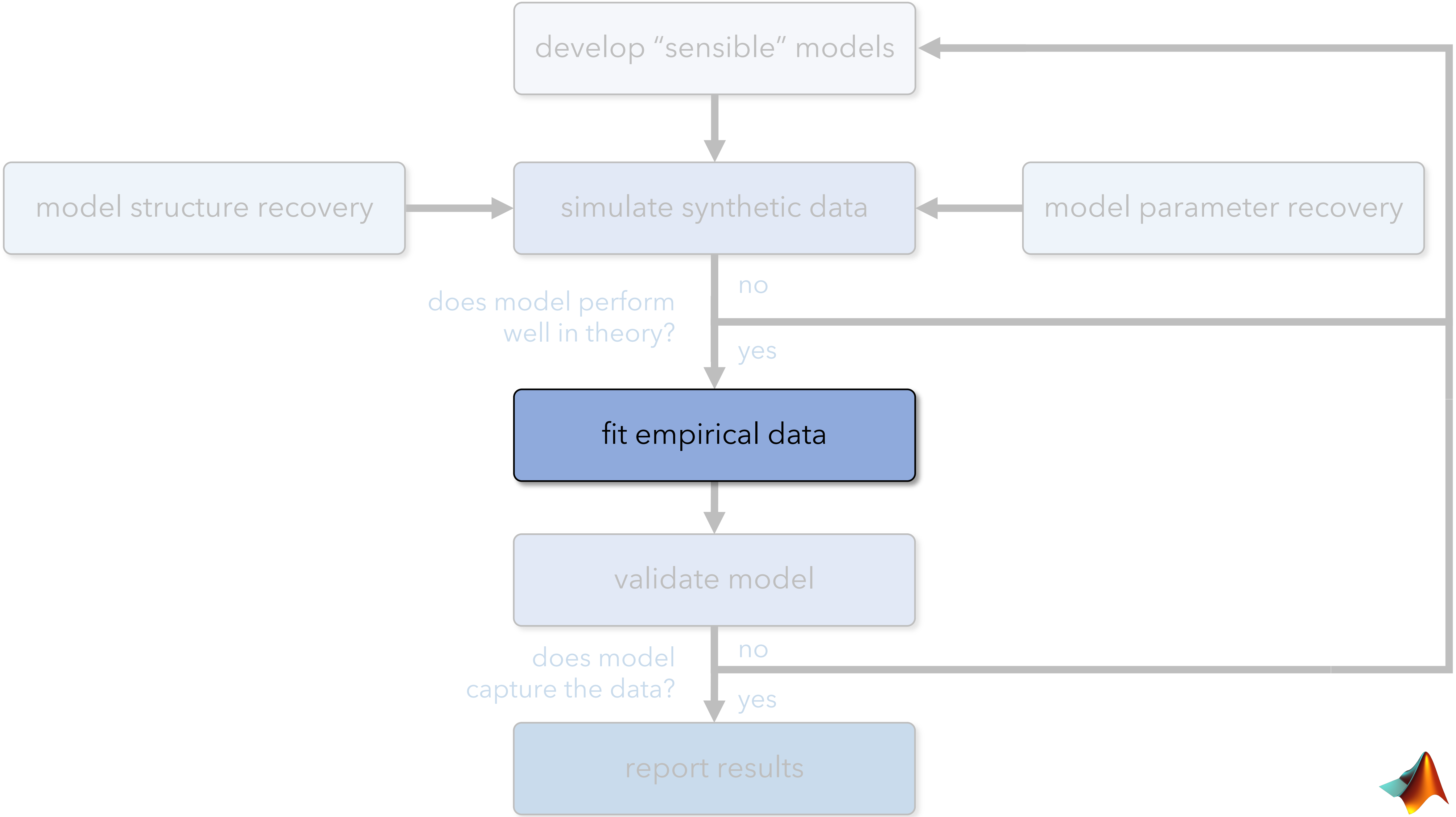


- Point estimates of the posterior can be obtained using maximum-a-posteriori (MAP) estimation

- Note: Under a flat prior, the MAP becomes equal to the MLE

- To obtain full posterior densities, one can resort to Variational Bayesian (VB) or sampling-based (Markov Chain Monte Carlo) techniques

Model inversion: Lecture (*Today, next talk*)



develop "sensible" models
model structure recovery
simulate synthetic data
model parameter recovery
does model perform well in theory?
no
yes
fit empirical data
validate model
does model capture the data?
no
yes
report results

THANK YOU FOR YOUR ATTENTION !

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