Bayesian model inference why, what and how? (and when not)

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Overview

- **Why** models?
- **What** is Bayesian model comparison?
- **How** are the actual computations done?
- **When not** to do Bayesian model comparison.

Me, Myself and I

- PhD in Statistics from Stockholm University (2000).
- Econometric research at Sveriges Riksbank in a previous life.
- Professor of Statistics at LiU (since 2011).
- Natural Born **Bayesian**.
- Current application areas:
  - Big data problems
  - Neuroimaging
  - Text analysis

Why models?

- A model can have many uses:
  - Abstraction to **aid in thinking** and **communication**.
  - **Prediction**.
  - **Compact description** of a complex phenomena.
- "All models are false, but some are useful"
- How to select a model from a set of models?
- Thou shalt not have more than one model? **Model averaging**.
- Models can be **derived** from assumptions of **exchangability** of observations (Bernardo and Smith, 1994).

USING LIKELIHOOD FOR MODEL COMPARISON

- Consider two models for the data $\mathbf{y} = (y_1, ..., y_n)$: M_1 and M_2.
- Let $p_i(\mathbf{y}|\theta_i)$ denote the data density under model M_i.
- If know θ_1 and θ_2, the **likelihood ratio** is useful

$$\frac{p_1(\mathbf{y}|\theta_1)}{p_2(\mathbf{y}|\theta_2)}.$$

- The **likelihood ratio** with ML estimates plugged in:

$$\frac{p_1(\mathbf{y}|\hat{\theta}_1)}{p_2(\mathbf{y}|\hat{\theta}_2)}.$$

- Bigger models always win in estimated likelihood ratio.
- **Hypothesis tests** are problematic for non-nested models. End results is not very useful for analysis.

Bayesian model comparison

- Just use your priors $p_1(\theta_1)$ och $p_2(\theta_2)$.
- The **marginal likelihood** for model M_k with parameters θ_k

$$p_k(y) = \int p_k(y|\theta_k)p_k(\theta_k)d\theta_k.$$

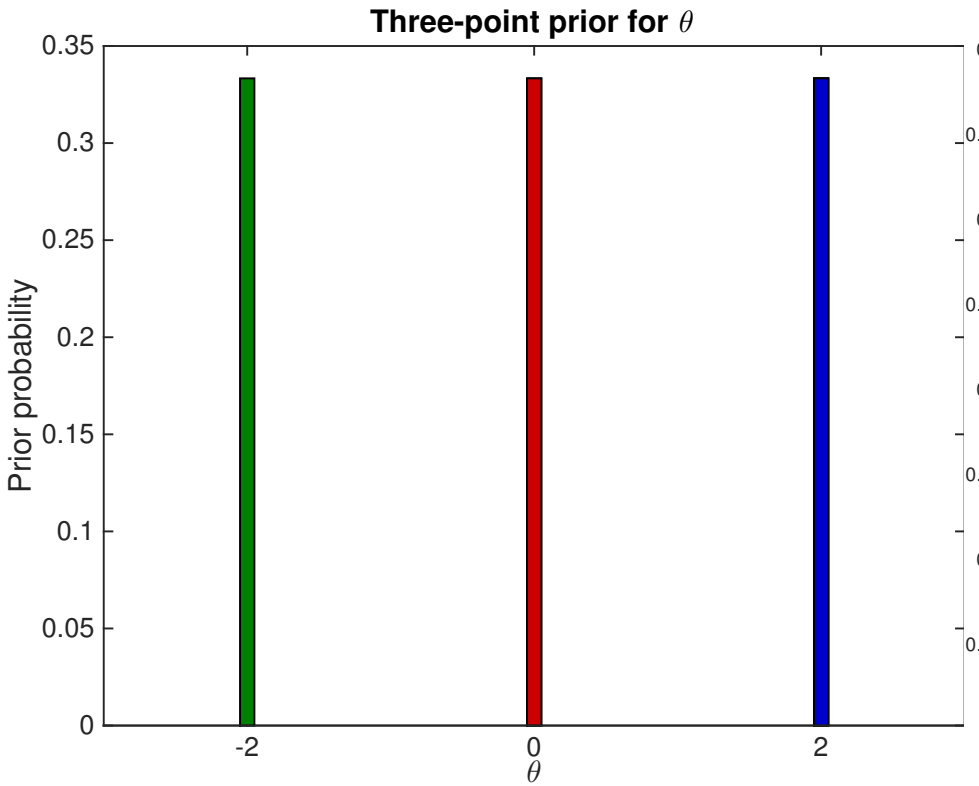
- θ_k is removed by the prior. **Not a magic bullet**. **Priors matter!**
- The **Bayes factor**

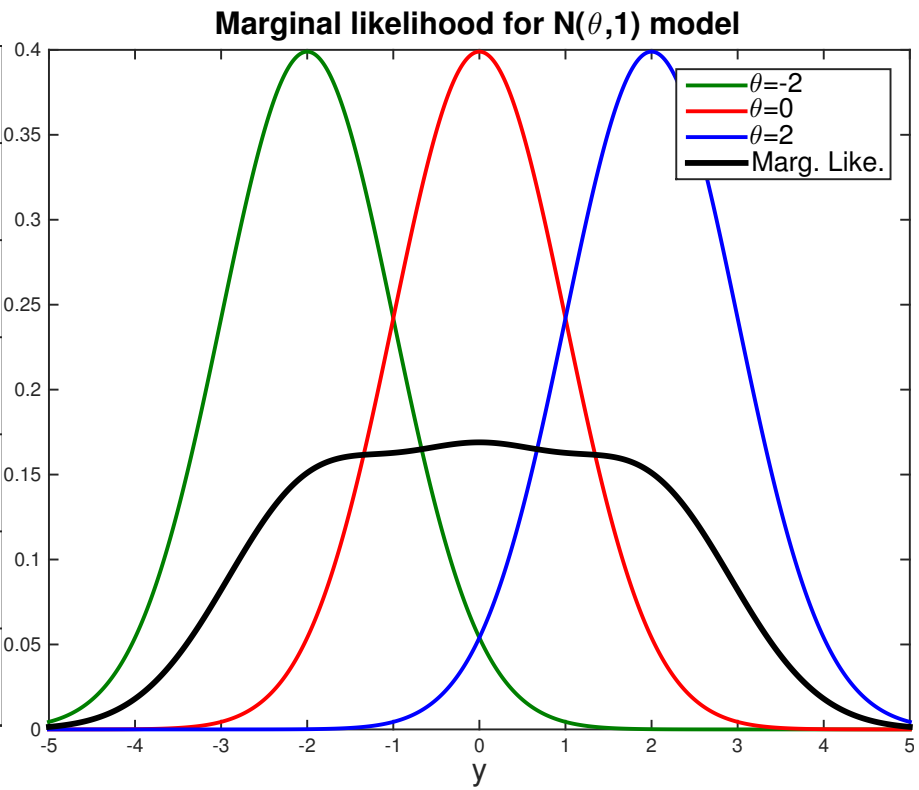
$$B_{12}(y) = \frac{p_1(y)}{p_2(y)}.$$

- **Posterior model probabilities**

$$\underbrace{\Pr(M_k|\mathbf{y})}_{\text{posterior model prob.}} \propto \underbrace{p(\mathbf{y}|M_k)}_{\text{marginal likelihood}} \cdot \underbrace{\Pr(M_k)}_{\text{prior model prob.}}$$

PRIORS MATTER





Example: Geometric vs Poisson

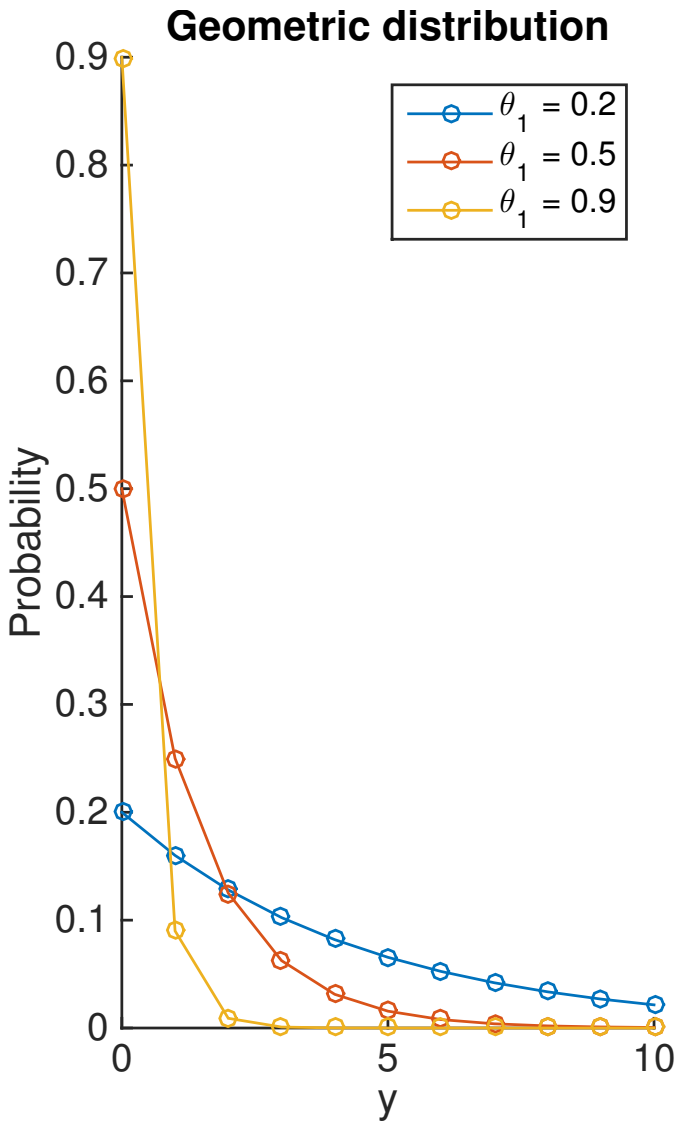
- Model 1 - **Geometric** with Beta prior:
  - $y_1, ..., y_n|\theta_1 \sim Geo(\theta_1)$
  - $\theta_1 \sim Beta(\alpha_1, \beta_1)$
- Model 2 - **Poisson** with Gamma prior:
  - $y_1, ..., y_n|\theta_2 \sim Poisson(\theta_2)$
  - $\theta_2 \sim Gamma(\alpha_2, \beta_2)$
- Marginal likelihood for M_1

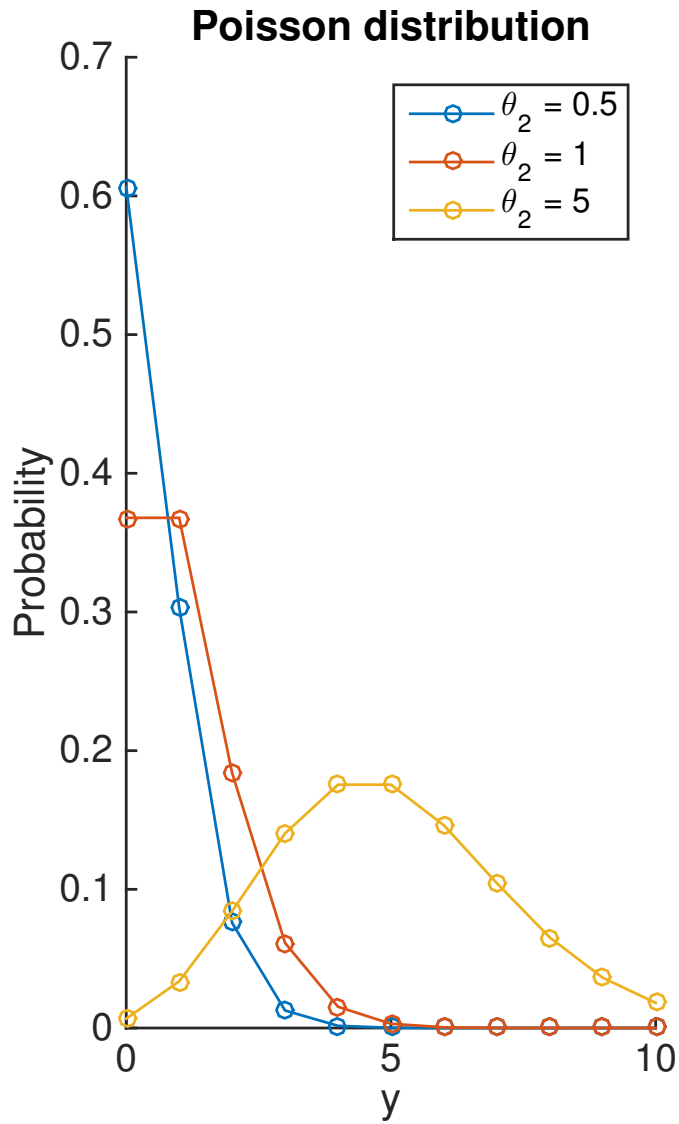
$$\begin{aligned} p_1(y_1, ..., y_n) &= \int p_1(y_1, ..., y_n|\theta_1)p(\theta_1)d\theta_1 \\ &= \frac{\Gamma(\alpha_1 + \beta_1)}{\Gamma(\alpha_1)\Gamma(\beta_1)} \frac{\Gamma(n + \alpha_1)\Gamma(n\bar{y} + \beta_1)}{\Gamma(n + n\bar{y} + \alpha_1 + \beta_1)} \end{aligned}$$

- Marginal likelihood for M_2

$$p_2(y_1, ..., y_n) = \frac{\Gamma(n\bar{y} + \alpha_2)\beta_2^{\alpha_2}}{\Gamma(\alpha_2)(n + \beta_2)^{n\bar{y}+\alpha_2}} \frac{1}{\prod_{i=1}^n y_i!}$$

Geometric and Poisson





Geometric vs Poisson, cont.

- Priors match prior predictive means:

$$E(y_i|M_1) = E(y_i|M_2) \quad \Longleftrightarrow \quad \alpha_1\alpha_2 = \beta_1\beta_2$$

Geometric vs Poisson, cont.

- Priors match prior predictive means:

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- **Data**: $y_1 = 0,\ y_2 = 0$.

	$\alpha_1 = 1, \beta_1 = 2$ $\alpha_2 = 2, \beta_2 = 1$	$\alpha_1 = 10, \beta_1 = 20$ $\alpha_2 = 20, \beta_2 = 10$	$\alpha_1 = 100, \beta_1 = 200$ $\alpha_2 = 200, \beta_2 = 100$
BF_{12}	1.5	4.54	5.87
$\Pr(M_1\|\mathbf{y})$	0.6	0.82	0.85
$\Pr(M_2\|\mathbf{y})$	0.4	0.18	0.15

Geometric vs Poisson, cont.

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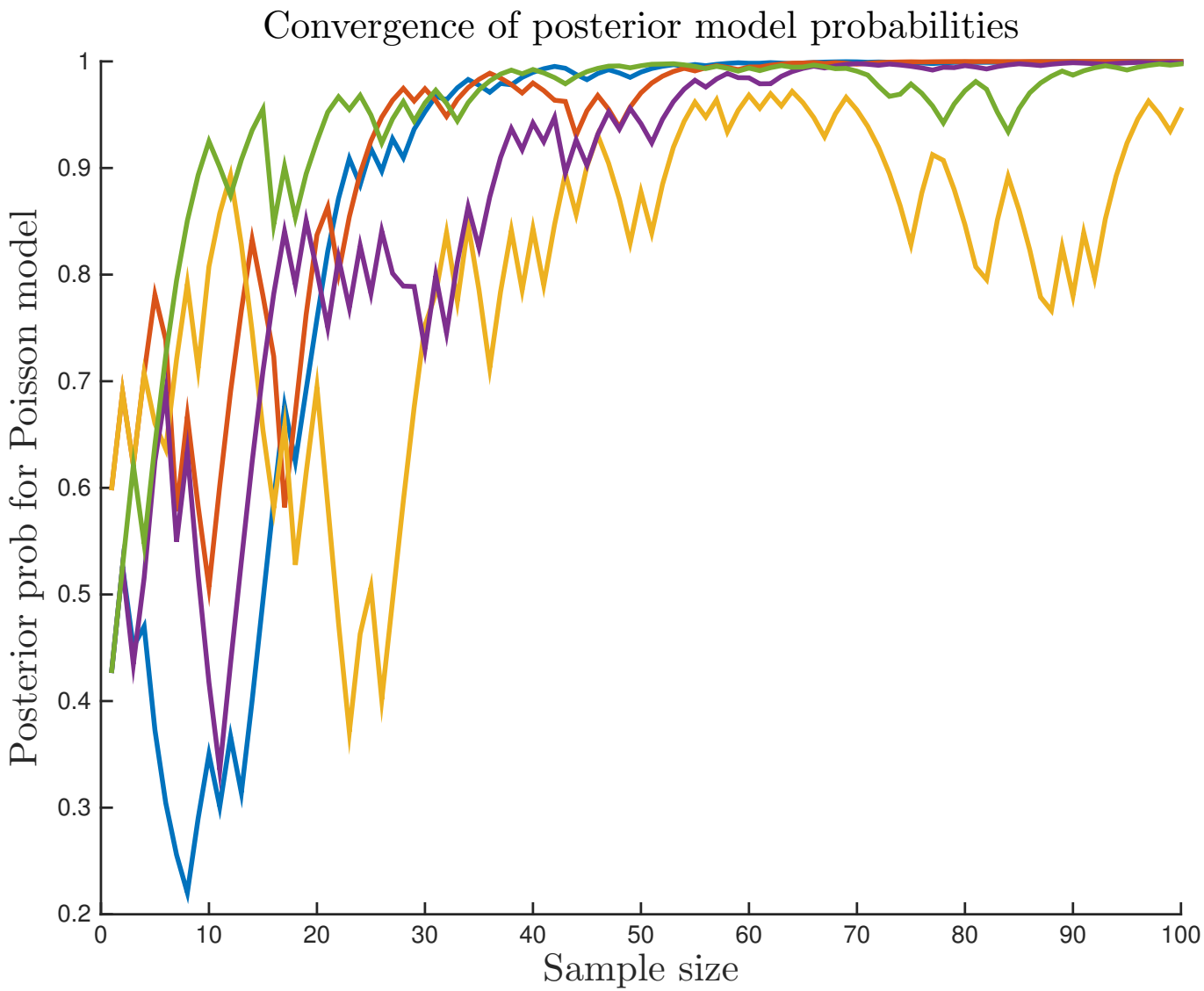
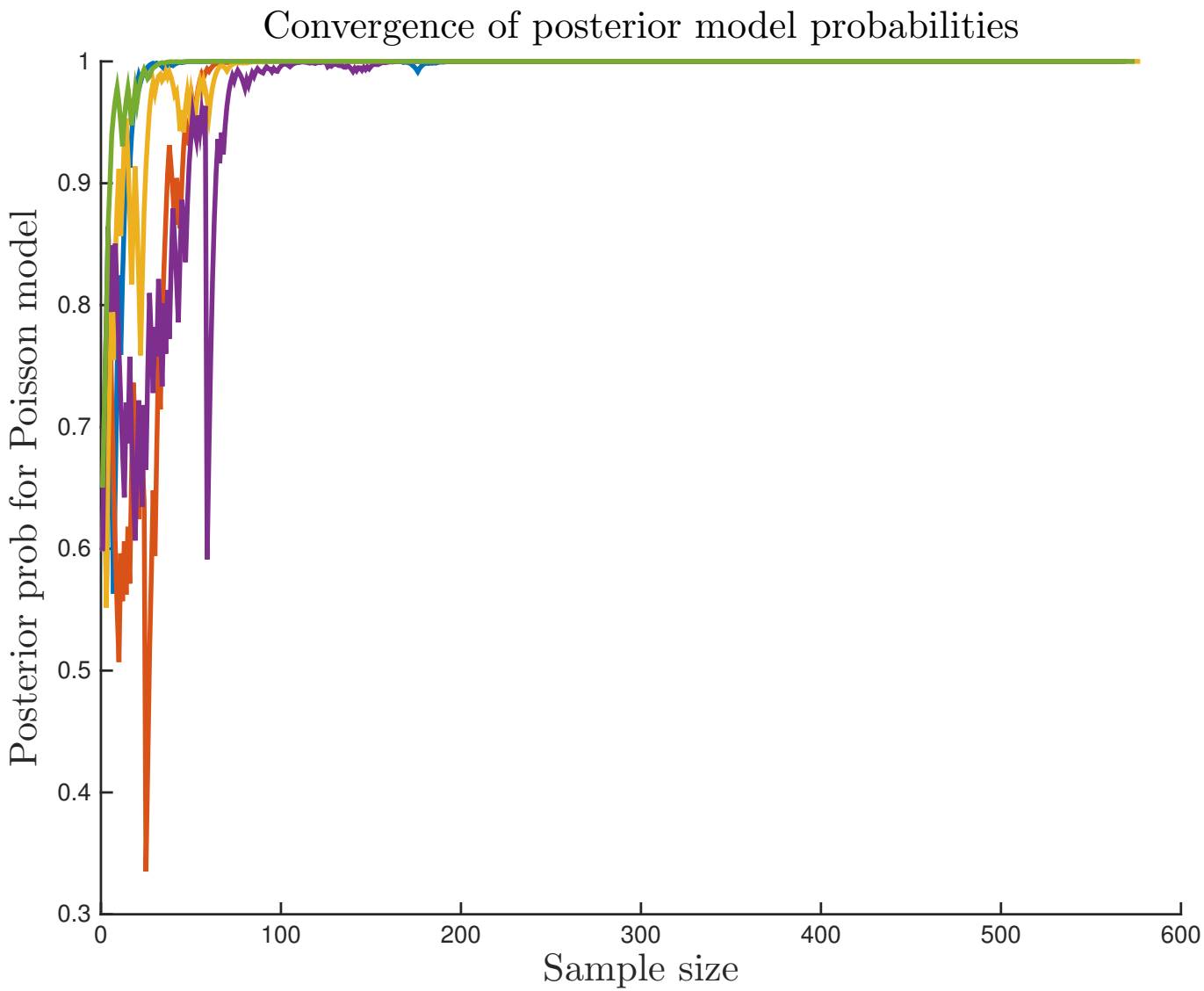
- **Data**: $y_1 = 3,\ y_2 = 3$.

	$\alpha_1 = 1, \beta_1 = 2$ $\alpha_2 = 2, \beta_2 = 1$	$\alpha_1 = 10, \beta_1 = 20$ $\alpha_2 = 20, \beta_2 = 10$	$\alpha_1 = 100, \beta_1 = 200$ $\alpha_2 = 200, \beta_2 = 100$
BF_{12}	0.26	0.29	0.30
$\Pr(M_1\|\mathbf{y})$	0.21	0.22	0.23
$\Pr(M_2\|\mathbf{y})$	0.79	0.78	0.77

Geometric vs Poisson for Pois(1) data



Geometric vs Poisson for Pois(1) data



Model choice in multivariate time series

- Multivariate time series

$$\mathbf{x}_t = \alpha\beta'\mathbf{z}_t + \Phi_1\mathbf{x}_{t-1} + ...\Phi_k\mathbf{x}_{t-k} + \Psi_1 + \Psi_2 t + \Psi_3 t^2 + \varepsilon_t$$

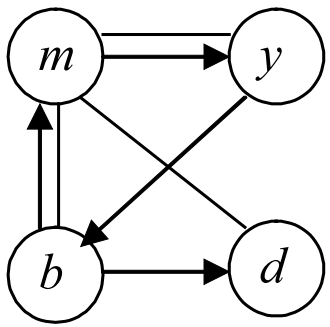
- Need to choose:
  - **Lag length**, $(k = 1, 2.., 4)$
  - **Trend model** $(s = 1, 2, ..., 5)$
  - **Long-run (cointegration) relations** $(r = 0, 1, 2, 3, 4)$.

The most probable (k, r, s) combinations in the Danish monetary data.

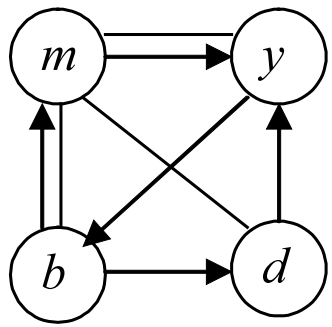
k	1	1	1	1	1	1	1	1	0	1
r	3	3	2	4	2	1	2	3	4	3
s	3	2	2	2	3	3	4	4	4	5
$p(k, r, s\|y, x, z)$	.106	.093	.091	.060	.059	.055	.054	.049	.040	.038

Graphical models for multivariate time series

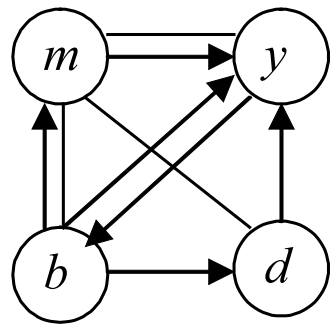
- **Graphical models** for multivariate time series.
- Zero-restrictions on the effect from time series i on time series j, for all lags. (**Granger Causality**).
- Zero-restrictions on the elements of the inverse covariance matrix of the errors.



$p(G|\mathbf{X}) = 0.0033$



$p(G|\mathbf{X}) = 0.0028$



$p(G|\mathbf{X}) = 0.0025$

Bayesian hypothesis testing

- **Hypothesis testing** is just a special case of model selection:

$$M_0 : y_1, ..., y_n \overset{iid}{\sim} Bernoulli(\theta_0)$$

$$M_1 : y_1, ..., y_n \overset{iid}{\sim} Bernoulli(\theta), \theta \sim Beta(\alpha, \beta)$$

$$p(y_1, ..., y_n | M_0) = \theta_0^s (1 - \theta_0)^f,$$

$$\begin{aligned} p(y_1, ..., y_n | M_1) &= \int_0^1 \theta^s (1-\theta)^f B(\alpha, \beta)^{-1} \theta^{\alpha - 1} (1-\theta)^{\beta - 1} d\theta \\ &= B(\alpha + s, \beta + f) / B(\alpha, \beta). \end{aligned}$$

- Posterior model probabilities

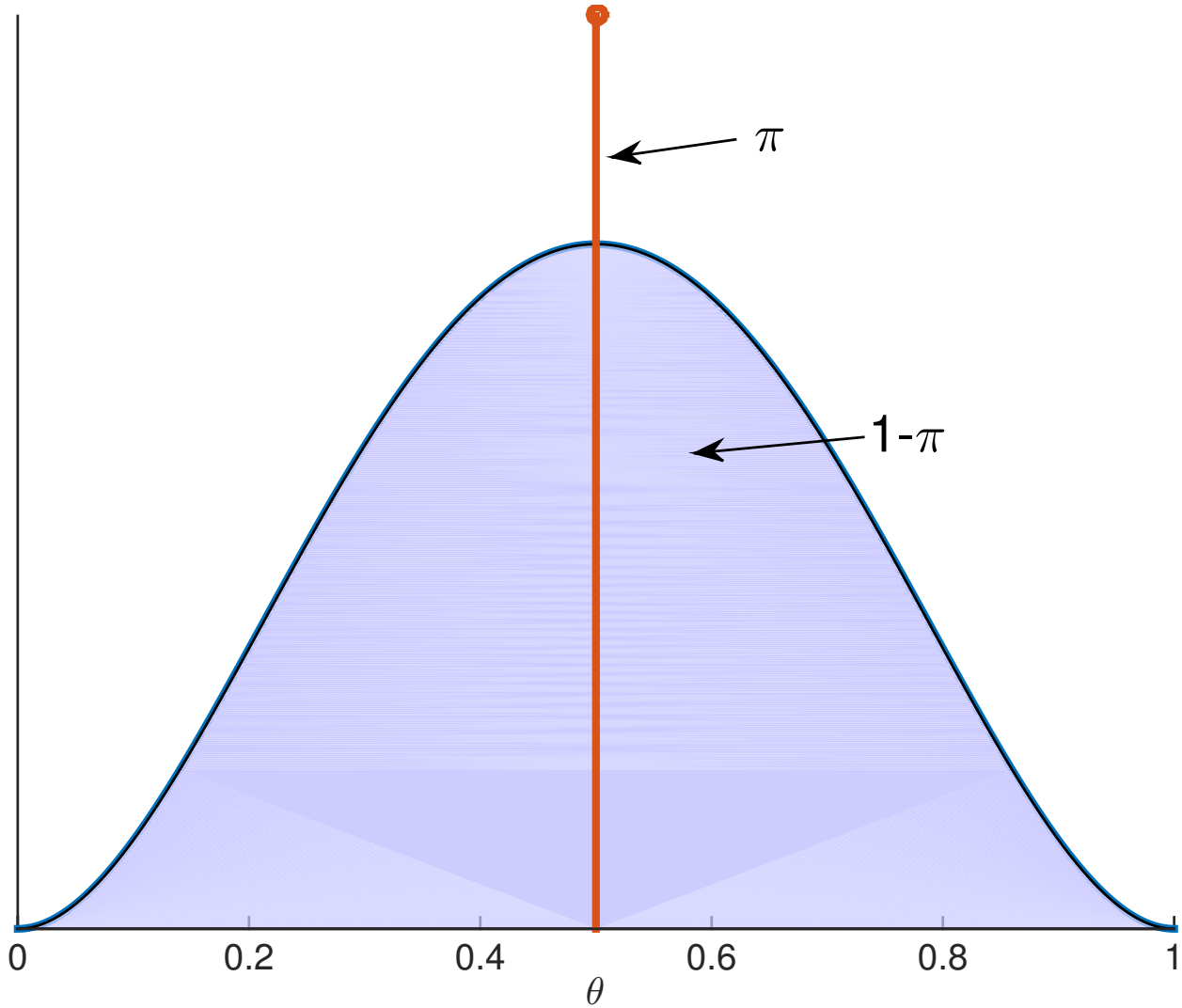
$$Pr(M_k | y_1, ..., y_n) \propto p(y_1, ..., y_n | M_k) Pr(M_k), \text{ for } k = 0, 1.$$

- Equivalent to using '**spike-and-slab**' prior:

$$p(\theta) = \pi I_{\theta_0}(\theta) + (1 - \pi) Beta(\alpha, \beta)$$

- Note: data can now *support* a null hypothesis (not only reject it).

Spike-and-slab prior



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SPIKE-AND-SLAB PRIOR FOR VARIABLE SELECTION

Posterior summary of the one-component split-t model.[a]

Parameters	Mean	Stdev	Post.Incl.
Location μ			
Const	0.084	0.019	–
Scale ϕ			
Const	0.402	0.035	–
LastDay	−0.190	0.120	0.036
LastWeek	**−0.738**	**0.193**	**0.985**
LastMonth	**−0.444**	**0.086**	**0.999**
CloseAbs95	0.194	0.233	0.035
CloseSqr95	0.107	0.226	0.023
MaxMin95	**1.124**	**0.086**	**1.000**
CloseAbs80	0.097	0.153	0.013
CloseSqr80	0.143	0.143	0.021
MaxMin80	−0.022	0.200	0.017
Degrees of freedom v			
Const	2.482	0.238	–
LastDay	0.504	0.997	0.112
LastWeek	**−2.158**	**0.926**	**0.638**
LastMonth	0.307	0.833	0.089
CloseAbs95	0.718	1.437	0.229
CloseSqr95	1.350	1.280	0.279
MaxMin95	1.130	1.488	0.222
CloseAbs80	0.035	1.205	0.101
CloseSqr80	0.363	1.211	0.112
MaxMin80	−1.672	1.172	0.254
Skewness λ			
Const	−0.104	0.033	–
LastDay	−0.159	0.140	0.027
LastWeek	−0.341	0.170	0.135
LastMonth	−0.076	0.112	0.016
CloseAbs95	−0.021	0.096	0.008
CloseSqr95	−0.003	0.108	0.006
MaxMin95	0.016	0.075	0.008
CloseAbs80	0.060	0.115	0.009
CloseSqr80	0.059	0.111	0.010
MaxMin80	0.093	0.096	0.013

Properties of Bayesian model comparison

- Coherence of pair-wise comparisons

$$B_{12} = B_{13} \cdot B_{32}$$

- **Consistency** when true model is in $\mathcal{M} = \{M_1, ..., M_K\}$

$$\Pr(M = M_{TRUE}|\mathbf{y}) \to 1 \quad \text{as} \quad n \to \infty$$

- "KL-consistency" when $M_{TRUE} \notin \mathcal{M}$

$$\Pr(M = M^*|\mathbf{y}) \to 1 \quad \text{as} \quad n \to \infty$$

  where M^* is the model that minimizes Kullback-Leibler distance between $p_M(\mathbf{y})$ and $p_{TRUE}(\mathbf{y})$.
- Smaller models always win when priors are very vague.
- **Improper priors** cannot be used for model comparison.

Marginal likelihood measures out-of-sample predictive performance

- The marginal likelihood can be decomposed as

$$p(y_1, ..., y_n) = p(y_1)p(y_2|y_1) \cdots p(y_n|y_1, y_2, ..., y_{n-1})$$

- If we assume that y_i is independent of $y_1, ..., y_{i-1}$ conditional on θ:

$$p(y_i|y_1, ..., y_{i-1}) = \int p(y_i|\theta)p(\theta|y_1, ..., y_{i-1})d\theta$$

- The prediction of y_1 is based on the prior of θ, and is therefore sensitive to the prior.
- The prediction of y_n uses almost all the data to infer θ. Very little influenced by the prior when n is not small.

Normal example

- **Model**: $y_1, ..., y_n|\theta \sim N(\theta, \sigma^2)$ with σ^2 known.
- **Prior**: $\theta \sim N(0, \kappa^2\sigma^2)$.
- Intermediate posterior at time $i-1$

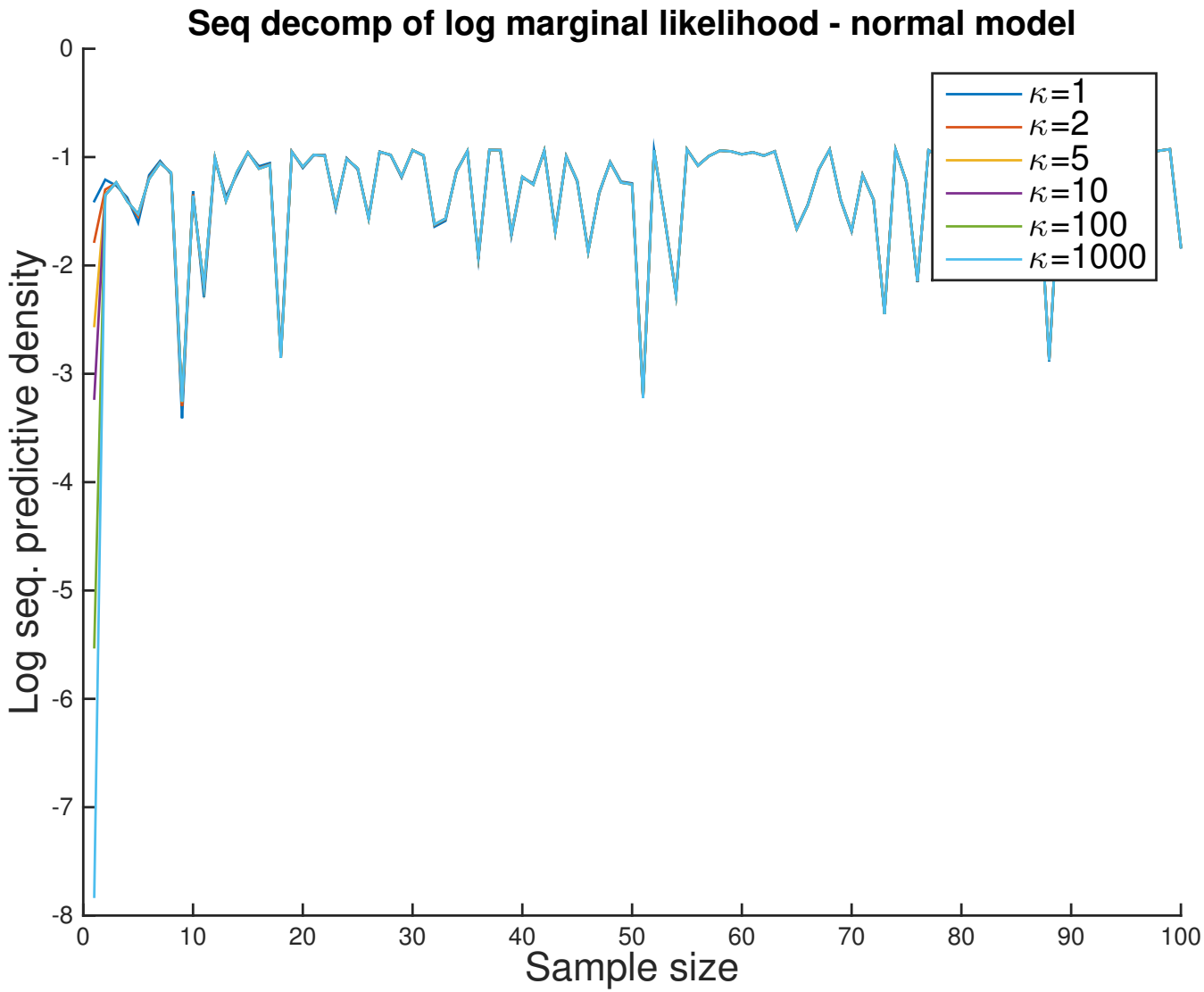
$$\theta|y_1, ..., y_{i-1} \sim N\left[w_i(\kappa) \cdot \bar{y}_{i-1}, \frac{\sigma^2}{i-1+\kappa^{-2}}\right]$$

  where $w_i(\kappa) = \frac{i-1}{i-1+\kappa^{-2}}$.
- Predictive density at time $i-1$

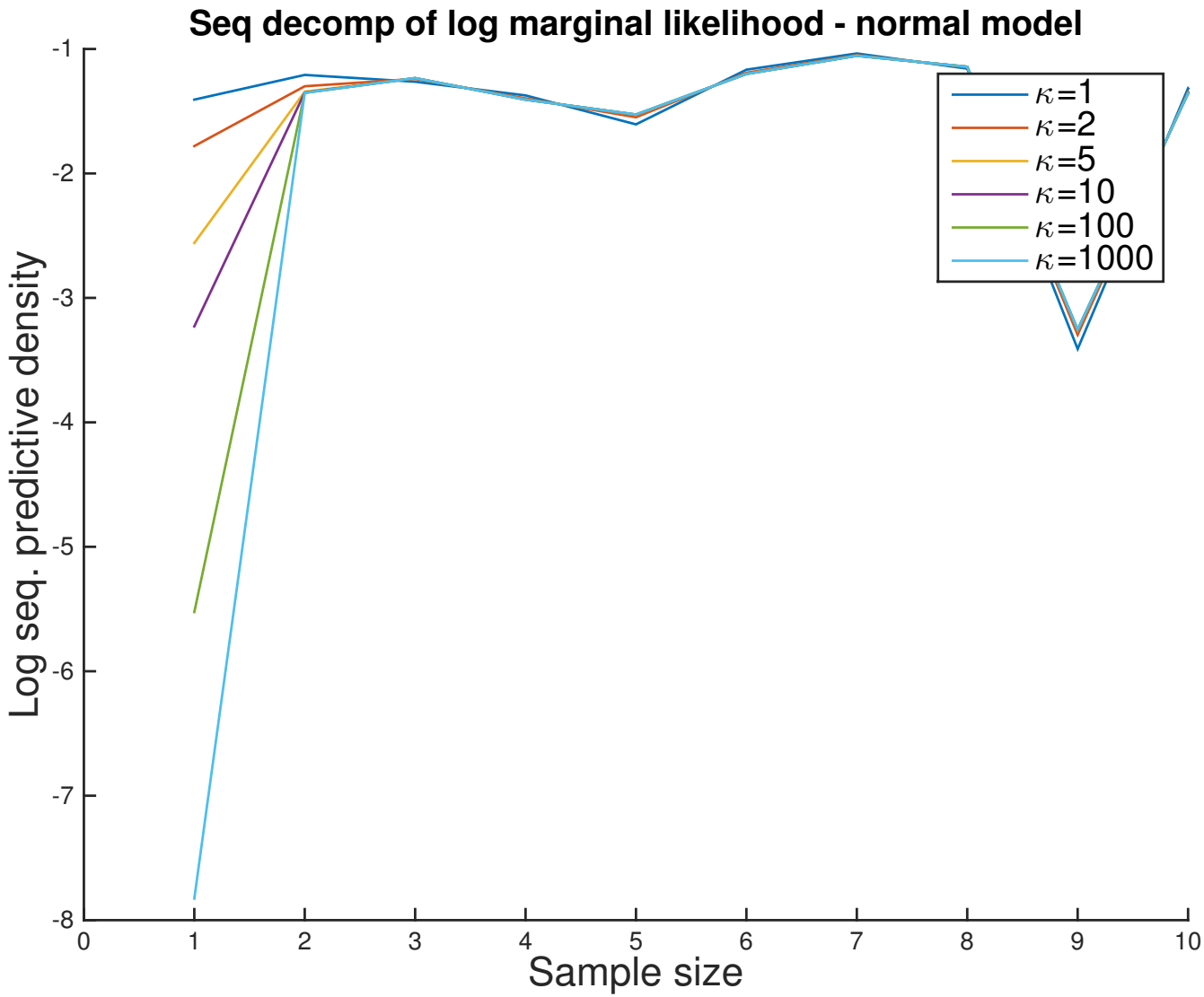
$$y_i|y_1, ..., y_{i-1} \sim N\left[w_i(\kappa) \cdot \bar{y}_{i-1}, \sigma^2\left(1 + \frac{1}{i-1+\kappa^{-2}}\right)\right]$$

- Terms with i large: $y_i|y_1, ..., y_{i-1} \overset{approx}{\sim} N\left(\bar{y}_{i-1}, \sigma^2\right)$, not sensitive to κ
- For $i = 1$, $y_1 \sim N\left[0, \sigma^2\left(1 + \frac{1}{\kappa^{-2}}\right)\right]$ can be very sensitive to κ.

First observation is sensitive to κ



First observation is sensitive to κ



Log Predictive Score - LPS

- To reduce sensitivity to the prior: sacrifice n^* observations to train the prior into a better posterior.
- Predictive density score: PS

$$PS(n^*) = p(y_{n^*+1}|y_1, ..., y_{n^*}) \cdots p(y_n|y_1, ..., y_{n-1})$$

- Usually report on log scale: **Log Predictive Score** (**LPS**).
- But which observations to train on (and which to test on)?
- Straightforward for time series.
- Cross-sectional data: **cross-validation**.

Model averaging

- Let γ be a quanitity with an interpretation which stays the same across the two models.
- Example: Prediction $\gamma = (y_{T+1}, ..., y_{T+h})'$.
- The marginal posterior distribution of γ reads

$$p(\gamma|\mathbf{y}) = p(M_1|\mathbf{y})p_1(\gamma|\mathbf{y}) + p(M_2|\mathbf{y})p_2(\gamma|\mathbf{y}),$$

  where $p_k(\gamma|\mathbf{y})$ is the marginal posterior of γ conditional on model k.
- Predictive distribution includes three sources of uncertainty:
  - **Future errors**/disturbances (e.g. the ε's in a regression)
  - **Parameter uncertainty** (the predictive distribution has the parameters integrated out by their posteriors)
  - **Model uncertainty** (by model averaging)

Marginal likelihood in conjugate models

- Computing the marginal likelihood requires integration w.r.t. θ.
- Short cut for conjugate models by rearragement of Bayes' theorem:

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

- Bernoulli model example

$$p(\theta) = \frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}$$
$$p(y|\theta) = \theta^{s}(1-\theta)^{f}$$
$$p(\theta|y) = \frac{1}{B(\alpha+s,\beta+f)}\theta^{\alpha+s-1}(1-\theta)^{\beta+f-1}$$

- Marginal likelihood

$$p(y) = \frac{\theta^{s}(1-\theta)^{f}\frac{1}{B(\alpha,\beta)}\theta^{\alpha-1}(1-\theta)^{\beta-1}}{\frac{1}{B(\alpha+s,\beta+f)}\theta^{\alpha+s-1}(1-\theta)^{\beta+f-1}} = \frac{B(\alpha+s,\beta+f)}{B(\alpha,\beta)}$$

Computing the marginal likelihood

- Usually difficult to evaluate the integral

$$p(\mathbf{y}) = \int p(\mathbf{y}|\theta)p(\theta)d\theta = E_{p(\theta)}[p(\mathbf{y}|\theta)].$$

- Draw from the prior $\theta^{(1)}, ..., \theta^{(N)}$ and use the Monte Carlo estimate

$$\hat{p}(\mathbf{y}) = \frac{1}{N}\sum_{i=1}^{N} p(\mathbf{y}|\theta^{(i)}).$$

  Unstable if the posterior is somewhat different from the prior.
- **Importance sampling**. Let $\theta^{(1)}, ..., \theta^{(N)}$ be iid draws from $g(\theta)$.

$$\int p(\mathbf{y}|\theta)p(\theta)d\theta = \int \frac{p(\mathbf{y}|\theta)p(\theta)}{g(\theta)}g(\theta)d\theta \approx N^{-1}\sum_{i=1}^{N} \frac{p(\mathbf{y}|\theta^{(i)})p(\theta^{(i)})}{g(\theta^{(i)})}$$

- **Modified Harmonic mean**: $g(\theta) = N(\tilde{\theta}, \tilde{\Sigma}) \cdot I_c(\theta)$, where $\tilde{\theta}$ and $\tilde{\Sigma}$ is the posterior mean and covariance matrix estimated from an MCMC chain, and $I_c(\theta) = 1$ if $(\theta - \tilde{\theta})'\tilde{\Sigma}^{-1}(\theta - \tilde{\theta}) \leq c$.

Computing the marginal likelihood, cont.

- Rearrangement of Bayes' theorem: $p(\mathbf{y}) = p(\mathbf{y}|\theta)p(\theta)/p(\theta|\mathbf{y})$.
- We must know the posterior, **including** the normalization constant.
- But we only need to know $p(\theta|\mathbf{y})$ in a single point θ_0.
- **Kernel density estimator** to approximate $p(\theta_0|\mathbf{y})$. Unstable.
- Chib (1995, JASA) provide better solutions for **Gibbs sampling**.
- Chib-Jeliazkov (2001, JASA) generalizes to **MH algorithm** (good for IndepMH, terrible for RWM).
- **Reversible Jump MCMC** (RJMCMC) for model inference.
  - MCMC methods that moves in model space.
  - Proportion of iterations spent in model k estimates $\Pr(M_k|\mathbf{y})$.
  - Usually hard to find efficient proposals. Sloooow convergence.
- **Bayesian nonparametrics** (e.g. Dirichlet process priors).

Approximate marginal likelihoods

- Taylor approximation of the log posterior

$$\ln p(\mathbf{y}|\theta)p(\theta) \approx \ln p(\mathbf{y}|\hat{\theta}) + \ln p(\hat{\theta}) - \frac{1}{2} J_{\hat{\theta},\mathbf{y}} (\theta - \hat{\theta})^2,$$

$$p(\mathbf{y}|\theta)p(\theta) \approx p(\mathbf{y}|\hat{\theta})p(\hat{\theta}) \exp\left[-\frac{1}{2} J_{\hat{\theta},\mathbf{y}} (\theta - \hat{\theta})^2 \right]$$

- **The Laplace approximation**:

$$\ln \hat{p}(\mathbf{y}) = \ln p(\mathbf{y}|\hat{\theta}) + \ln p(\hat{\theta}) + \frac{1}{2} \ln \left| J^{-1}_{\hat{\theta},\mathbf{y}} \right| + \frac{p}{2} \ln(2\pi),$$

  where p is the number of unrestricted parameters in the model.
- Note that $\hat{\theta}$ and $J_{\hat{\theta},\mathbf{y}}$ can be obtained with **numerical optimization** with BFGS update of Hessian.
- The **BIC approximation** is obtained if $J_{\hat{\theta},\mathbf{y}}$ behaves like $n \cdot I_p$ in large samples

$$\ln \hat{p}(\mathbf{y}) = \ln p(\mathbf{y}|\hat{\theta}) + \ln p(\hat{\theta}) - \frac{p}{2} \ln n.$$

And hey! ... let's be careful out there.

- Be especially careful with Bayesian model comparison when
  - The compared models are
    - very different in structure
    - severly misspecified
    - very complicated (black boxes).
  - The priors for the parameters in the models are
    - not carefully elicited
    - only weakly informative
    - not matched across models.
  - The data
    - has outliers (in all models)
    - has a multivariate response.

Hasta La Victoria Siempre!