# 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 $\mathbf{y}=\left(y_{1}, \ldots, y_{n}\right): M_{1}$ and $M_{2}$.
- Let $p_{i}\left(\mathbf{y} \mid \theta_{i}\right)$ denote the data density under model $M_{i}$.
- If know $\theta_{1}$ and $\theta_{2}$, the likelihood ratio is useful

$$
\frac{p_{1}\left(\mathbf{y} \mid \theta_{1}\right)}{p_{2}\left(\mathbf{y} \mid \theta_{2}\right)}
$$

- The likelihood ratio with ML estimates plugged in:

$$
\frac{p_{1}\left(\mathbf{y} \mid \hat{\theta}_{1}\right)}{p_{2}\left(\mathbf{y} \mid \hat{\theta}_{2}\right)}
$$

- 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 $p_{1}\left(\theta_{1}\right)$ och $p_{2}\left(\theta_{2}\right)$.
- The marginal likelihood for model $M_{k}$ with parameters $\theta_{k}$

$$
p_{k}(y)=\int p_{k}\left(y \mid \theta_{k}\right) p_{k}\left(\theta_{k}\right) d \theta_{k}
$$

- $\theta_{k}$ 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



## PRIORS MATTER



## Example: Geometric vs Poisson

- Model 1 - Geometric with Beta prior:
- $y_{1}, \ldots, y_{n} \mid \theta_{1} \sim \operatorname{Geo}\left(\theta_{1}\right)$
- $\theta_{1} \sim \operatorname{Beta}\left(\alpha_{1}, \beta_{1}\right)$
- Model 2 - Poisson with Gamma prior:
- $y_{1}, \ldots, y_{n} \mid \theta_{2} \sim \operatorname{Poisson}\left(\theta_{2}\right)$
- $\theta_{2} \sim \operatorname{Gamma}\left(\alpha_{2}, \beta_{2}\right)$
- Marginal likelihood for $M_{1}$

$$
\begin{aligned}
p_{1}\left(y_{1}, \ldots, y_{n}\right) & =\int p_{1}\left(y_{1}, \ldots, y_{n} \mid \theta_{1}\right) p\left(\theta_{1}\right) d \theta_{1} \\
& =\frac{\Gamma\left(\alpha_{1}+\beta_{1}\right)}{\Gamma\left(\alpha_{1}\right) \Gamma\left(\beta_{1}\right)} \frac{\Gamma\left(n+\alpha_{1}\right) \Gamma\left(n \bar{y}+\beta_{1}\right)}{\Gamma\left(n+n \bar{y}+\alpha_{1}+\beta_{1}\right)}
\end{aligned}
$$

- Marginal likelihood for $M_{2}$

$$
p_{2}\left(y_{1}, \ldots, y_{n}\right)=\frac{\Gamma\left(n \bar{y}+\alpha_{2}\right) \beta_{2}^{\alpha_{2}}}{\Gamma\left(\alpha_{2}\right)\left(n+\beta_{2}\right)^{n \bar{y}+\alpha_{2}}} \frac{1}{\prod_{i=1}^{n} y_{i}!}
$$

## Geometric and Poisson




## Geometric vs Poisson, CONT.

- Priors match prior predictive means:

$$
E\left(y_{i} \mid M_{1}\right)=E\left(y_{i} \mid M_{2}\right) \quad \Longleftrightarrow \quad \alpha_{1} \alpha_{2}=\beta_{1} \beta_{2}
$$

## Geometric vs Poisson, cont.

- Priors match prior predictive means:

$$
E\left(y_{i} \mid M_{1}\right)=E\left(y_{i} \mid M_{2}\right) \quad \Longleftrightarrow \quad \alpha_{1} \alpha_{2}=\beta_{1} \beta_{2}
$$

- Data: $y_{1}=0, y_{2}=0$.

|  | $\alpha_{1}=1, \beta_{1}=2$ | $\alpha_{1}=10, \beta_{1}=20$ | $\alpha_{1}=100, \beta_{1}=200$ |
| :---: | :---: | :---: | :---: |
|  | $\alpha_{2}=2, \beta_{2}=1$ | $\alpha_{2}=20, \beta_{2}=10$ | $\alpha_{2}=200, \beta_{2}=100$ |
| $B F_{12}$ | 1.5 | 4.54 | 5.87 |
| $\operatorname{Pr}\left(M_{1} \mid \mathbf{y}\right)$ | 0.6 | 0.82 | 0.85 |
| $\operatorname{Pr}\left(M_{2} \mid \mathbf{y}\right)$ | 0.4 | 0.18 | 0.15 |

## Geometric vs Poisson, CONT.

- Priors match prior predictive means:

$$
E\left(y_{i} \mid M_{1}\right)=E\left(y_{i} \mid M_{2}\right) \quad \Longleftrightarrow \quad \alpha_{1} \alpha_{2}=\beta_{1} \beta_{2}
$$

- Data: $y_{1}=0, y_{2}=0$.

$$
B F_{12}
$$

$$
\operatorname{Pr}\left(M_{1} \mid \mathbf{y}\right)
$$

$$
\begin{array}{ccc}
\hline \alpha_{1}=1, \beta_{1}=2 & \alpha_{1}=10, \beta_{1}=20 & \alpha_{1}=100, \beta_{1}=200 \\
\alpha_{2}=2, \beta_{2}=1 & \alpha_{2}=20, \beta_{2}=10 & \alpha_{2}=200, \beta_{2}=100 \\
\hline 1.5 & 4.54 & 5.87 \\
0.6 & 0.82 & 0.85 \\
0.4 & 0.18 & 0.15
\end{array}
$$

$\operatorname{Pr}\left(M_{2} \mid \mathbf{y}\right)$

- Data: $y_{1}=3, y_{2}=3$.

$$
\operatorname{Pr}\left(M_{1} \mid \mathbf{y}\right)
$$

$$
\operatorname{Pr}\left(M_{2} \mid \mathbf{y}\right)
$$

$$
\begin{array}{ccc}
\hline \alpha_{1}=1, \beta_{1}=2 & \alpha_{1}=10, \beta_{1}=20 & \alpha_{1}=100, \beta_{1}=200 \\
\alpha_{2}=2, \beta_{2}=1 & \alpha_{2}=20, \beta_{2}=10 & \alpha_{2}=200, \beta_{2}=100 \\
\hline 0.26 & 0.29 & 0.30 \\
0.21 & 0.22 & 0.23 \\
0.79 & 0.78 & 0.77
\end{array}
$$

## Geometric vs Poisson for Pois(1) data

Convergence of posterior model probabilities


## Geometric vs Poisson for Pois(1) data

Convergence of posterior model probabilities


## Model Choice in multivariate time series

- Multivariate time series

$$
\mathbf{x}_{t}=\alpha \beta^{\prime} \mathbf{z}_{t}+\Phi_{1} \mathbf{x}_{t-1}+\ldots \Phi_{k} \mathbf{x}_{t-k}+\Psi_{1}+\Psi_{2} t+\Psi_{3} t^{2}+\varepsilon_{t}
$$

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

| The most probable $(\mathrm{k}, \mathrm{r}, \mathrm{s})$ | 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 |
| $p(k, r, s \mid y, x, z)$ | .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.

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

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

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


## BAYESIAN HYPOTHESIS TESTING

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

$$
\begin{gathered}
M_{0}: y_{1}, \ldots, y_{n} \stackrel{i i d}{\sim} \text { Bernoulli }\left(\theta_{0}\right) \\
M_{1}: y_{1}, \ldots, y_{n} \stackrel{i i d}{\sim} \operatorname{Bernoulli}(\theta), \theta \sim \operatorname{Beta}(\alpha, \beta) \\
p\left(y_{1}, \ldots, y_{n} \mid M_{0}\right)=\theta_{0}^{s}\left(1-\theta_{0}\right)^{f}, \\
p\left(y_{1}, \ldots, y_{n} \mid M_{1}\right) \\
=\int_{0}^{1} \theta^{s}(1-\theta)^{f} B(\alpha, \beta)^{-1} \theta^{\alpha-1}(1-\theta)^{\beta-1} d \theta \\
=B(\alpha+s, \beta+f) / B(\alpha, \beta) .
\end{gathered}
$$

- Posterior model probabilities

$$
\operatorname{Pr}\left(M_{k} \mid y_{1}, \ldots, y_{n}\right) \propto p\left(y_{1}, \ldots, y_{n} \mid M_{k}\right) \operatorname{Pr}\left(M_{k}\right), \text { for } k=0,1 .
$$

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

$$
p(\theta)=\pi l_{\theta_{0}}(\theta)+(1-\pi) \operatorname{Beta}(\alpha, \beta)
$$

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


## SPIKE-AND-SLAB PRIOR



## SpIKE-AND-SLAB PRIOR FOR VARIABLE SELECTION

Posterior summary of the one-component split- $t$ model. ${ }^{\text {a }}$

| Parameters | Mean | Stdev | Post.Incl. |
| :---: | :---: | :---: | :---: |
| Location $\mu$ |  |  |  |
| Const | 0.084 | 0.019 | - |
| Scale $\phi$ |  |  |  |
| 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 $\lambda$ |  |  |  |
| 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 $\mathcal{M}=\left\{M_{1}, \ldots, M_{K}\right\}$

$$
\operatorname{Pr}\left(M=M_{T R U E} \mid \mathbf{y}\right) \rightarrow 1 \quad \text { as } \quad n \rightarrow \infty
$$

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

$$
\operatorname{Pr}\left(M=M^{*} \mid \mathbf{y}\right) \rightarrow 1 \quad \text { as } \quad n \rightarrow \infty
$$

where $M^{*}$ is the model that minimizes Kullback-Leibler distance between $p_{M}(\mathbf{y})$ and $p_{\text {TRUE }}(\mathbf{y})$.

- 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

$$
p\left(y_{1}, \ldots, y_{n}\right)=p\left(y_{1}\right) p\left(y_{2} \mid y_{1}\right) \cdots p\left(y_{n} \mid y_{1}, y_{2}, \ldots, y_{n-1}\right)
$$

- If we assume that $y_{i}$ is independent of $y_{1}, \ldots, y_{i-1}$ conditional on $\theta$ :

$$
p\left(y_{i} \mid y_{1}, \ldots, y_{i-1}\right)=\int p\left(y_{i} \mid \theta\right) p\left(\theta \mid y_{1}, \ldots, y_{i-1}\right) d \theta
$$

- The prediction of $y_{1}$ is based on the prior of $\theta$, and is therefore sensitive to the prior.
- The prediction of $y_{n}$ uses almost all the data to infer $\theta$. Very little influenced by the prior when $n$ is not small.


## Normal example

- Model: $y_{1}, \ldots, y_{n} \mid \theta \sim N\left(\theta, \sigma^{2}\right)$ with $\sigma^{2}$ known.
- Prior: $\theta \sim N\left(0, \kappa^{2} \sigma^{2}\right)$.
- Intermediate posterior at time $i-1$

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

where $w_{i}(\kappa)=\frac{i-1}{i-1+\kappa^{-2}}$.

- Predictive density at time $i-1$

$$
y_{i} \mid y_{1}, \ldots, y_{i-1} \sim N\left[w_{i}(\kappa) \cdot \bar{y}_{i-1}, \sigma^{2}\left(1+\frac{1}{i-1+\kappa^{-2}}\right)\right]
$$

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


## First observation is sensitive To $\kappa$

Seq decomp of log marginal likelihood - normal model


## First observation is sensitive To $\kappa$



## 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

$$
P S\left(n^{*}\right)=p\left(y_{n^{*}+1} \mid y_{1}, \ldots, y_{n^{*}}\right) \cdots p\left(y_{n} \mid y_{1}, \ldots, y_{n-1}\right)
$$

- 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 $\gamma$ be a quanitity with an interpretation which stays the same across the two models.
- Example: Prediction $\gamma=\left(y_{T+1}, \ldots, y_{T+h}\right)^{\prime}$.
- The marginal posterior distribution of $\gamma$ reads

$$
p(\gamma \mid \mathbf{y})=p\left(M_{1} \mid \mathbf{y}\right) p_{1}(\gamma \mid \mathbf{y})+p\left(M_{2} \mid \mathbf{y}\right) p_{2}(\gamma \mid \mathbf{y})
$$

where $p_{k}(\gamma \mid \mathbf{y})$ is the marginal posterior of $\gamma$ conditional on model $k$.

- Predictive distribution includes three sources of uncertainty:
- Future errors/disturbances (e.g. the $\varepsilon$ '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. $\theta$.
- Short cut for conjugate models by rearragement of Bayes' theorem:

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

- Bernoulli model example

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

- 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

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

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

$$
\hat{p}(\mathbf{y})=\frac{1}{N} \sum_{i=1}^{N} p\left(\mathbf{y} \mid \theta^{(i)}\right)
$$

Unstable if the posterior is somewhat different from the prior.

- Importance sampling. Let $\theta^{(1)}, \ldots, \theta^{(N)}$ be iid draws from $g(\theta)$.

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

- 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 $(\theta-\tilde{\theta})^{\prime} \tilde{\Sigma}^{-1}(\theta-\tilde{\theta}) \leq c$.


## COMPUTING THE MARGINAL LIKELIHOOD, CONT.

- Rearrangement of Bayes' theorem: $p(\mathbf{y})=p(\mathbf{y} \mid \theta) p(\theta) / p(\theta \mid \mathbf{y})$.
- We must know the posterior, including the normalization constant.
- But we only need to know $p(\theta \mid \mathbf{y})$ in a single point $\theta_{0}$.
- Kernel density estimator to approximate $p\left(\theta_{0} \mid \mathbf{y}\right)$. 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 $\operatorname{Pr}\left(M_{k} \mid \mathbf{y}\right)$.
- Usually hard to find efficient proposals. Sloooow convergence.
- Bayesian nonparametrics (e.g. Dirichlet process priors).


## Approximate marginal Likelihoods

- Taylor approximation of the log posterior

$$
\begin{aligned}
\ln p(\mathbf{y} \mid \theta) p(\theta) & \approx \ln p(\mathbf{y} \mid \hat{\theta})+\ln p(\hat{\theta})-\frac{1}{2} J_{\hat{\theta}, \mathbf{y}}(\theta-\hat{\theta})^{2} \\
p(\mathbf{y} \mid \theta) p(\theta) & \approx p(\mathbf{y} \mid \hat{\theta}) p(\hat{\theta}) \exp \left[-\frac{1}{2} J_{\hat{\theta}, \mathbf{y}}(\theta-\hat{\theta})^{2}\right]
\end{aligned}
$$

- The Laplace approximation:

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

where $p$ is the number of unrestricted parameters in the model.

- Note that $\hat{\theta}$ and $J_{\hat{\theta}, \mathrm{y}}$ 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

$$
\ln \hat{p}(\mathbf{y})=\ln _{\text {BAYES@LUND2015 }} p(\mathbf{y} \mid \hat{\theta})+\ln p(\hat{\theta})-\frac{p}{2} \ln n
$$

## 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!



