# BAYESIAN MODEL INFERENCE WHY, WHAT AND HOW? (AND WHEN NOT)

### Mattias Villani

Division of Statistics and Machine Learning Department of Computer and Information Science Linköping University

MATTIAS VILLANI (STATISTICS, LIU)



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

MATTIAS VILLANI (STATISTICS, LIU)

# 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  $\theta_1$  and  $\theta_2$ , 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.

MATTIAS VILLANI (STATISTICS, LIU)

### 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  $\theta_k$

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

- $\theta_k$  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:
  - $y_1, ..., y_n | \theta_1 \sim Geo(\theta_1)$
  - $\theta_1 \sim Beta(\alpha_1, \beta_1)$
- 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<sub>1</sub>

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

► Marginal likelihood for *M*<sub>2</sub>

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

MATTIAS VILLANI (STATISTICS, LIU)

### GEOMETRIC AND POISSON



MATTIAS VILLANI (STATISTICS, LIU)

### GEOMETRIC VS POISSON, CONT.

Priors match prior predictive means:

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

MATTIAS VILLANI (STATISTICS, LIU)

### GEOMETRIC VS POISSON, CONT.

▶ Priors match prior predictive means:

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

<b>Data</b> : $y_1 = 0$ , $y_2 = 0$ .							
	$lpha_1=$ 1, $eta_1=$ 2	$lpha_1=$ 10, $eta_1=$ 20	$lpha_1=$ 100, $eta_1=$ 200				
	$lpha_2=$ 2, $eta_2=$ 1	$lpha_2=$ 20, $eta_2=$ 10	$lpha_2=$ 200, $eta_2=$ 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.

▶ Priors match prior predictive means:

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

<b>Data</b> : $y_1 = 0, y_2 = 0.$							
	$lpha_1=$ 1, $eta_1=$ 2	$lpha_1=$ 10, $eta_1=$ 20	$lpha_1=$ 100, $eta_1=$ 200				
	$lpha_2=$ 2, $eta_2=$ 1	$lpha_2=$ 20, $eta_2=$ 10	$lpha_2=$ 200, $eta_2=$ 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				
Data: $y_1 =$	3, $y_2 = 3$ .						
	$lpha_1=$ 1, $eta_1=$ 2	$lpha_1=$ 10, $eta_1=$ 20	$lpha_1=$ 100, $eta_1=$ 200				
	$lpha_2=$ 2, $eta_2=$ 1	$lpha_2=$ 20, $eta_2=$ 10	$lpha_2=200$ , $eta_2=100$				
$BF_{12}$	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				

MATTIAS VILLANI (STATISTICS, LIU)

## GEOMETRIC VS POISSON FOR POIS(1) DATA



# GEOMETRIC VS POISSON FOR POIS(1) DATA



### MODEL CHOICE IN MULTIVARIATE TIME SERIES

Multivariate time series

$$\mathbf{x}_{t} = \alpha \beta' \mathbf{z}_{t} + \Phi_{1} \mathbf{x}_{t-1} + \dots \Phi_{k} \mathbf{x}_{t-k} + \Psi_{1} + \Psi_{2} t + \Psi_{3} t^{2} + \varepsilon_{t}$$

- 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.



### BAYESIAN HYPOTHESIS TESTING

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

$$\begin{split} M_0 : & y_1, \dots, y_n \overset{iid}{\sim} Bernoulli(\theta_0) \\ M_1 : & y_1, \dots, y_n \overset{iid}{\sim} Bernoulli(\theta), \theta \sim Beta(\alpha, \beta) \\ & p(y_1, \dots, y_n | M_0) = \theta_0^s (1 - \theta_0)^f, \\ p(y_1, \dots, y_n | M_1) &= \int_0^1 \theta^s (1 - \theta)^f B(\alpha, \beta)^{-1} \theta^{\alpha - 1} (1 - \theta)^{\beta - 1} d\theta \\ &= B(\alpha + s, \beta + f) / B(\alpha, \beta). \end{split}$$

Posterior model probabilities

 $Pr(M_k|y_1, ..., y_n) \propto p(y_1, ..., y_n|M_k)Pr(M_k)$ , 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).

MATTIAS VILLANI (STATISTICS, LIU)

### Spike-and-slab prior



MATTIAS VILLANI (STATISTICS, LIU)

 $\pi$ 

### SPIKE-AND-SLAB PRIOR FOR VARIABLE SELECTION

#### ----- -

Posterior summary of the one-component split-t model.<sup>a</sup>

Parameters	Mean	Stdev	Post.Incl.				
location u							
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				

### MATTIAS VILLANI (STATISTICS, LIU)

PROPERTIES OF BAYESIAN MODEL COMPARISON

Coherence of pair-wise comparisons

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

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

$$\Pr\left(M = M_{TRUE} | \mathbf{y}\right) \rightarrow 1$$
 as  $n \rightarrow \infty$ 

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

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

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  $\theta$ :

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

- The prediction of y<sub>1</sub> is based on the prior of θ, and is therefore sensitive to the prior.
- The prediction of y<sub>n</sub> uses almost all the data to infer θ. Very little influenced by the prior when n is not small.

MATTIAS VILLANI (STATISTICS, LIU)

### NORMAL EXAMPLE

- Model:  $y_1, ..., y_n | \theta \sim N(\theta, \sigma^2)$  with  $\sigma^2$  known.
- **Prior**:  $\theta \sim N(0, \kappa^2 \sigma^2)$ .

• Intermediate posterior at time i-1

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

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:  $y_i|y_1, ..., y_{i-1} \stackrel{approx}{\sim} N\left(\bar{y}_{i-1}, \sigma^2\right)$ , 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  $\kappa$ .

MATTIAS VILLANI (STATISTICS, LIU)

### FIRST OBSERVATION IS SENSITIVE TO $\kappa$



MATTIAS VILLANI (STATISTICS, LIU)

### 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

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

- 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  $\gamma$  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  $\gamma$  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:

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

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

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

MATTIAS VILLANI (STATISTICS, LIU)

### 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(θ) = N(θ̃, Σ̃) · I<sub>c</sub>(θ), where θ̃ and Σ̃ is the posterior mean and covariance matrix estimated from an MCMC chain, and I<sub>c</sub>(θ) = 1 if (θ − θ̃)<sup>'</sup>Σ̃<sup>-1</sup>(θ − θ̃) ≤ c.

MATTIAS VILLANI (STATISTICS, LIU)

### 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  $\theta_0$ .
- 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

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

### The Laplace approximation:

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

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

- Note that \(\heta\) and \(J\_{\heta,y}\) can be obtained with numerical optimization with BFGS update of Hessian.
- ► The BIC approximation is obtained if J<sub>θ,y</sub> behaves like n · I<sub>p</sub> in large samples

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

MATTIAS VILLANI (STATISTICS, LIU)

## 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!



MATTIAS VILLANI (STATISTICS, LIU)