

BAYESIAN STATISTICS - LECTURE 11

LECTURE 11: COMPUTATIONS. VARIABLE SELECTION.

MATTIAS VILLANI

DEPARTMENT OF STATISTICS

STOCKHOLM UNIVERSITY

AND

DEPARTMENT OF COMPUTER AND INFORMATION SCIENCE

LINKÖPING UNIVERSITY

- **Computing the marginal likelihood**
- **Bayesian variable selection**
- **Model averaging**

MARGINAL LIKELIHOOD IN CONJUGATE MODELS

- **Marginal likelihood:** $\int p(\mathbf{y}|\theta)p(\theta)d\theta$. Integration!
- Short cut for **conjugate models:**

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

- 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

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

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

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

Unstable when posterior is different from prior.

- **Importance sampling.** Let $\theta^{(1)}, \dots, \theta^{(N)}$ 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.

- To use $p(\mathbf{y}) = p(\mathbf{y}|\theta)p(\theta)/p(\theta|\mathbf{y})$ we need $p(\theta|\mathbf{y})$.
- 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's method** (1995, JASA). Great, but only applied to **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).

■ Taylor approximation of the log likelihood

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

so

$$\begin{aligned} p(\mathbf{y}|\theta)p(\theta) &\approx p(\mathbf{y}|\hat{\theta}) \exp \left[-\frac{1}{2} J_{\hat{\theta}, \mathbf{y}} (\theta - \hat{\theta})^2 \right] p(\hat{\theta}) \\ &= p(\mathbf{y}|\hat{\theta}) p(\hat{\theta}) (2\pi)^{p/2} \left| J_{\hat{\theta}, \mathbf{y}}^{-1} \right|^{1/2} \\ &= \underbrace{\times (2\pi)^{-p/2} \left| J_{\hat{\theta}, \mathbf{y}}^{-1} \right|^{-1/2} \exp \left[-\frac{1}{2} J_{\hat{\theta}, \mathbf{y}} (\theta - \hat{\theta})^2 \right]}_{\text{multivariate normal density}} \end{aligned}$$

■ The Laplace approximation:

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

where p is the number of unrestricted parameters.

■ **The Laplace approximation:**

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

- $\hat{\theta}$ and $J_{\hat{\theta}, \mathbf{y}}$ can be obtained with **numerical optimization**.
- The **BIC approximation** assumes that $J_{\hat{\theta}, \mathbf{y}}$ behaves like $n \cdot I_p$ in large samples and the small term $+\frac{p}{2} \ln(2\pi)$ is ignored

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

- Linear regression:

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \varepsilon.$$

- Which variables have **non-zero** coefficient?

$$H_0 : \beta_0 = \beta_1 = \dots = \beta_p = 0$$

$$H_1 : \beta_1 = 0$$

$$H_2 : \beta_1 = \beta_2 = 0$$

- Introduce **variable selection indicators** $\mathcal{I} = (I_1, \dots, I_p)$.

- Example: $\mathcal{I} = (1, 1, 0)$ means that $\beta_1 \neq 0$ and $\beta_2 \neq 0$, but $\beta_3 = 0$, so x_3 drops out of the model.

- Model inference, just crank the Bayesian machine:

$$p(\mathcal{I}|\mathbf{y}, \mathbf{X}) \propto p(\mathbf{y}|\mathbf{X}, \mathcal{I}) \cdot p(\mathcal{I})$$

- The prior $p(\mathcal{I})$ is typically taken to be

$$I_1, \dots, I_p | \theta \stackrel{iid}{\sim} \text{Bernoulli}(\theta)$$

- θ is the **prior inclusion probability**.
- Challenge: Computing the **marginal likelihood** for each model (\mathcal{I})

$$p(\mathbf{y}|\mathbf{X}, \mathcal{I}) = \int p(\mathbf{y}|\mathbf{X}, \mathcal{I}, \beta) p(\beta|\mathbf{X}, \mathcal{I}) d\beta$$

- Let $\beta_{\mathcal{I}}$ denote the **non-zero** coefficients under \mathcal{I} .
- Prior:

$$\begin{aligned}\beta_{\mathcal{I}}|\sigma^2 &\sim N\left(\mathbf{0}, \sigma^2 \Omega_{\mathcal{I},0}^{-1}\right) \\ \sigma^2 &\sim \text{Inv-}\chi^2\left(\nu_0, \sigma_0^2\right)\end{aligned}$$

■ Marginal likelihood

$$p(\mathbf{y}|\mathbf{X}, \mathcal{I}) \propto \left| \mathbf{X}'_{\mathcal{I}}\mathbf{X}_{\mathcal{I}} + \Omega_{\mathcal{I},0}^{-1} \right|^{-1/2} |\Omega_{\mathcal{I},0}|^{1/2} \left(\nu_0 \sigma_0^2 + \text{RSS}_{\mathcal{I}} \right)^{-(\nu_0+n-1)/2}$$

where $\mathbf{X}_{\mathcal{I}}$ is the covariate matrix for the subset selected by \mathcal{I} .

- $\text{RSS}_{\mathcal{I}}$ is (almost) the residual sum of squares under model implied by \mathcal{I}

$$\text{RSS}_{\mathcal{I}} = \mathbf{y}'\mathbf{y} - \mathbf{y}'\mathbf{X}_{\mathcal{I}} \left(\mathbf{X}'_{\mathcal{I}}\mathbf{X}_{\mathcal{I}} + \Omega_{\mathcal{I},0} \right)^{-1} \mathbf{X}'_{\mathcal{I}}\mathbf{y}$$

- But there are 2^p model combinations to go through! *Ouch!*
- ... but most have essentially zero posterior probability. *Phew!*
- **Simulate** from the joint posterior distribution:

$$p(\beta, \sigma^2, \mathcal{I} | \mathbf{y}, \mathbf{X}) = p(\beta, \sigma^2 | \mathcal{I}, \mathbf{y}, \mathbf{X}) p(\mathcal{I} | \mathbf{y}, \mathbf{X}).$$

- Simulate from $p(\mathcal{I} | \mathbf{y}, \mathbf{X})$ using **Gibbs sampling**:
 - Draw $l_1 | \mathcal{I}_{-1}, \mathbf{y}, \mathbf{X}$
 - Draw $l_2 | \mathcal{I}_{-2}, \mathbf{y}, \mathbf{X}$
 - ...
 - Draw $l_p | \mathcal{I}_{-p}, \mathbf{y}, \mathbf{X}$
- Only need to compute $Pr(l_i = 0 | \mathcal{I}_{-i}, \mathbf{y}, \mathbf{X})$ and $Pr(l_i = 1 | \mathcal{I}_{-i}, \mathbf{y}, \mathbf{X})$.
- Automatic model averaging, all in one simulation run.
- If needed, simulate from $p(\beta, \sigma^2 | \mathcal{I}, \mathbf{y}, \mathbf{X})$ for each draw of \mathcal{I} .

PSEUDO CODE FOR BAYESIAN VARIABLE SELECTION

o Initialize $\mathcal{I}^{(0)} = (I_1^{(0)}, I_2^{(0)}, \dots, I_p^{(0)})$

1 Simulate σ^2 and β from $[\nu_n, \sigma_n^2, \mu_n, \Omega_n]$ all depend on $\mathcal{I}^{(0)}$

- $\sigma^2 | \mathcal{I}^{(0)}, \mathbf{y}, \mathbf{X} \sim \text{Inv} - \chi^2(\nu_n, \sigma_n^2)$
- $\beta | \sigma^2, \mathcal{I}^{(0)}, \mathbf{y}, \mathbf{X} \sim N[\mu_n, \sigma^2 \Omega_n^{-1}]$

2.1 Simulate $I_1 | \mathcal{I}_{-1}, \mathbf{y}, \mathbf{X}$ by [define $\mathcal{I}_{prop}^{(0)} = (1 - I_1^{(0)}, I_2^{(0)}, \dots, I_p^{(0)})$]

- compute marginal likelihoods: $p(\mathbf{y} | \mathbf{X}, \mathcal{I}^{(0)})$ and $p(\mathbf{y} | \mathbf{X}, \mathcal{I}_{prop}^{(0)})$
- Simulate $I_1^{(1)} \sim \text{Bernoulli}(\kappa)$ where

$$\kappa = \frac{p(\mathbf{y} | \mathbf{X}, \mathcal{I}^{(0)}) \cdot p(\mathcal{I}^{(0)})}{p(\mathbf{y} | \mathbf{X}, \mathcal{I}^{(0)}) \cdot p(\mathcal{I}^{(0)}) + p(\mathbf{y} | \mathbf{X}, \mathcal{I}_{prop}^{(0)}) \cdot p(\mathcal{I}_{prop}^{(0)})}$$

2.2 Simulate $I_2 | \mathcal{I}_{-2}, \mathbf{y}, \mathbf{X}$ as in Step 2.1, but $\mathcal{I}^{(0)} = (I_1^{(1)}, I_2^{(0)}, \dots, I_p^{(0)})$

\vdots

2.p Simulate $I_p | \mathcal{I}_{-p}, \mathbf{y}, \mathbf{X}$ as in Step 2.1, but $\mathcal{I}^{(0)} = (I_1^{(1)}, I_2^{(1)}, \dots, I_p^{(0)})$

3 Repeat Steps 1-2 many times.

SIMPLE GENERAL BAYESIAN VARIABLE SELECTION

- The previous algorithm only works when we can integrate out all the model parameters to obtain

$$p(\mathcal{I}|\mathbf{y}, \mathbf{X}) = \int p(\beta, \sigma^2, \mathcal{I}|\mathbf{y}, \mathbf{X}) d\beta d\sigma$$

- **MH** - **propose** β and \mathcal{I} jointly from the proposal distribution

$$q(\beta_p|\beta_c, \mathcal{I}_p)q(\mathcal{I}_p|\mathcal{I}_c)$$

- Main difficulty: how to propose the non-zero elements in β_p ?
- Simple approach:

- Approximate posterior with all variables in the model:
 $\beta|\mathbf{y}, \mathbf{X} \stackrel{approx}{\sim} N[\hat{\beta}, J_{\mathbf{y}}^{-1}(\hat{\beta})]$
- Propose β_p from $N[\hat{\beta}, J_{\mathbf{y}}^{-1}(\hat{\beta})]$, conditional on the zero restrictions implied by \mathcal{I}_p . Formulas are available.

VARIABLE SELECTION IN MORE COMPLEX MODELS

Table 1
Posterior summary of the one-component split- t model.^a

Parameters	Mean	Stdev	Post.Incl.
<i>Location μ</i>			
Const	0.084	0.019	–
<i>Scale ϕ</i>			
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
<i>Degrees of freedom ν</i>			
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
<i>Skewness λ</i>			
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

- Let γ be a quantity with an interpretation which stays the same across the two models.
- Example: Prediction $\gamma = (y_{T+1}, \dots, y_{T+h})'$.
- 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)