Bayesian Learning

Lecture 7 - Monte Carlo and Gibbs sampling

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Lecture overview

- Monte Carlo simulation
- Gibbs sampling
- Data augmentation
  - Mixture models
  - Logistic regression
  - Probit regression
- Regularized regression

Monte Carlo sampling

- If $\theta^{(1)}, ..., \theta^{(N)}$ is an iid **sequence** from $p(\theta)$, then

$$\bar{\theta} = \frac{1}{N}\sum_{t=1}^{N}\theta^{(t)} \quad \rightarrow \quad E(\theta)$$

$$\overline{g\left(\theta\right)} = \frac{1}{N}\sum_{t=1}^{N}g(\theta^{(t)}) \quad \rightarrow \quad E[g(\theta)]$$

for some function $g(\theta)$ of interest.
- $\mathbb{V}\left(\overline{g\left(\theta\right)}\right) = \frac{c}{N}$ for some constant c.
- Easy to compute **tail probabilities** $\Pr(\theta \leq c)$ by letting

$$g(\theta) = I\left(\theta \leq c\right)$$

and

$$\frac{1}{N}\sum_{t=1}^{N}g(\theta^{(t)}) = \frac{\#\ \theta\text{-draws smaller than } c}{N}.$$

Direct sampling by the inverse CDF method

- Let $F(x)$ be the CDF of X. **Inverse CDF method**:
  1. Generate u from the uniform distribution on $[0, 1]$.
  2. Compute $x = F^{-1}(u)$.

- **Exponential distribution**:

$$u = F(x) = 1 - \exp(-\lambda x)$$

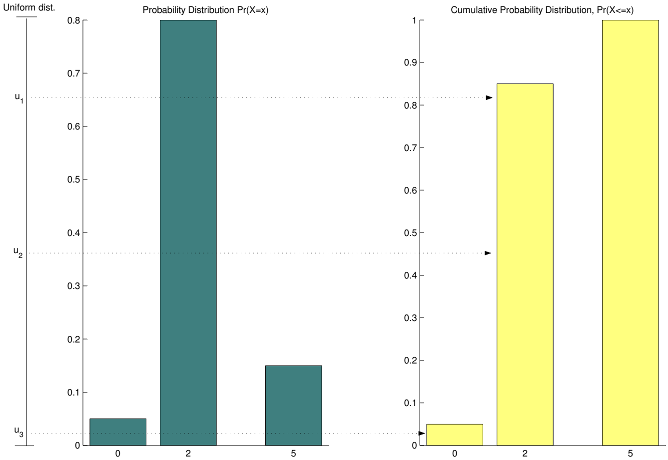
  Inverting gives

$$x = -\ln(1 - u)/\lambda$$

- So, if $u \sim U(0, 1)$ then

$$x = -\ln(1 - u)/\lambda \sim Expon(\lambda)$$

Inverse CDF method, discrete case



Direct sampling by the inverse CDF method

- **Cauchy distribution**:

$$\begin{aligned} f(x) &= \frac{1}{\pi}\frac{1}{1+x^2} \\ u &= F(x) = \frac{1}{2} + \frac{1}{\pi}\arctan(x) \end{aligned}$$

  Inverting ...

$$x = \tan[\pi(u - 1/2)].$$

- Can also use **relations**:

$$y, z \text{ are indep } N(0,1) \Rightarrow \frac{y}{z} \sim \text{Cauchy}(0,1)$$

- **Chi-square**. If $x_1, ..., x_v \overset{iid}{\sim} N(0,1)$, then $\sum_{i=1}^{v} x_i^2 \sim \chi_v^2$.

Gibbs sampling

- Easily implemented methods for **sampling from multivariate distributions**, $p(\theta_1, ..., \theta_k)$.
- Requirements: Easily sampled **full conditional distributions**:
  - $p(\theta_1 | \theta_2, \theta_3 ..., \theta_k)$
  - $p(\theta_2 | \theta_1, \theta_3, ..., \theta_k)$
  - $\vdots$
  - $p(\theta_k | \theta_1, \theta_2, ..., \theta_{k-1})$
- Gibbs sampling is a special case of **Metropolis-Hastings** (see Lecture 8).
- Metropolis-Hastings is a **Markov Chain Monte Carlo** (**MCMC**) algorithm.

The Gibbs sampling algorithm

- Choose initial values $\theta_2^{(0)}, \theta_3^{(0)}, ..., \theta_k^{(0)}$.
- Repeat for $j = 1, ..., N$:
  - Draw $\theta_1^{(j)}$ from $p(\theta_1 | \theta_2^{(j-1)}, \theta_3^{(j-1)}, ..., \theta_k^{(j-1)})$
  - Draw $\theta_2^{(j)}$ from $p(\theta_2 | \theta_1^{(j)}, \theta_3^{(j-1)}, ..., \theta_k^{(j-1)})$

    $\vdots$
  - Draw $\theta_k^{(j)}$ from $p(\theta_k | \theta_1^{(j)}, \theta_2^{(j)}, ..., \theta_{k-1}^{(j)})$
- Return draws: $\theta^{(1)}, ..., \theta^{(N)}$, where $\theta^{(j)} = (\theta_1^{(j)}, ..., \theta_k^{(j)})$.

Gibbs sampling, cont.

- Gibbs draws $\theta^{(1)}, ..., \theta^{(N)}$ are **dependent**, but

$$\bar{\theta} = \frac{1}{N}\sum_{t=1}^{N}\theta^{(t)} \quad \rightarrow \quad E(\theta)$$

$$\overline{g\left(\theta\right)} = \frac{1}{N}\sum_{t=1}^{N} g(\theta^{(t)}) \quad \rightarrow \quad E[g(\theta)]$$

- $\theta^{(1)}, ..., \theta^{(N)}$ **converges in distribution** to the target $p(\theta)$.
- $\theta_j^{(1)}, ..., \theta_j^{(N)}$ converges to the marginal distribution of θ_j.
- **Dependent draws** $\rightarrow$ **less efficient** than iid sampling.
- **IID samples**: $\theta^{(1)}, ..., \theta^{(N)}$: $\mathrm{Var}(\bar{\theta}) = \frac{\sigma^2}{N}$.
- **Autocorrelated samples**: $\mathrm{Var}(\bar{\theta}) = \frac{\sigma^2}{N}\left(1 + 2\sum_{k=1}^{\infty}\rho_k\right)$, where ρ_k is the autocorrelation at lag k.
- **Inefficiency Factor (IF)**: $1 + 2\sum_{k=1}^{\infty}\rho_k$.

Gibbs sampling bivariate normal

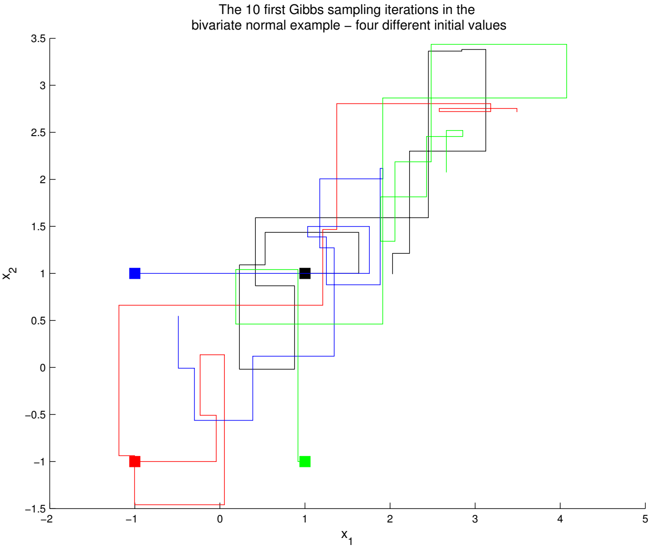
- **Joint distribution**

$$\begin{pmatrix} \theta_1 \\ \theta_2 \end{pmatrix} \sim N_2 \left[\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right]$$

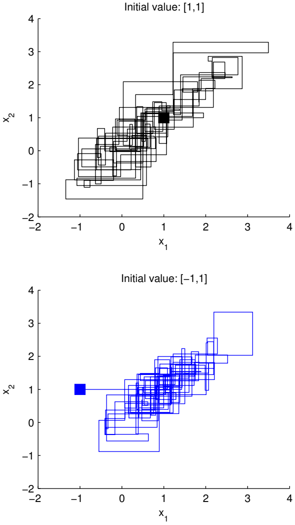
- **Full conditional posteriors**

$$\begin{aligned} \theta_1 | \theta_2 &\sim N[\mu_1 + \rho(\theta_2 - \mu_2), 1 - \rho^2] \\ \theta_2 | \theta_1 &\sim N[\mu_2 + \rho(\theta_1 - \mu_1), 1 - \rho^2] \end{aligned}$$

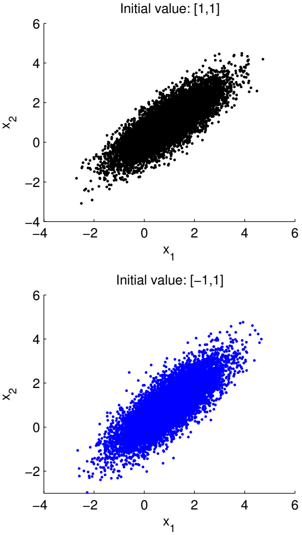
Gibbs sampling - Bivariate normal



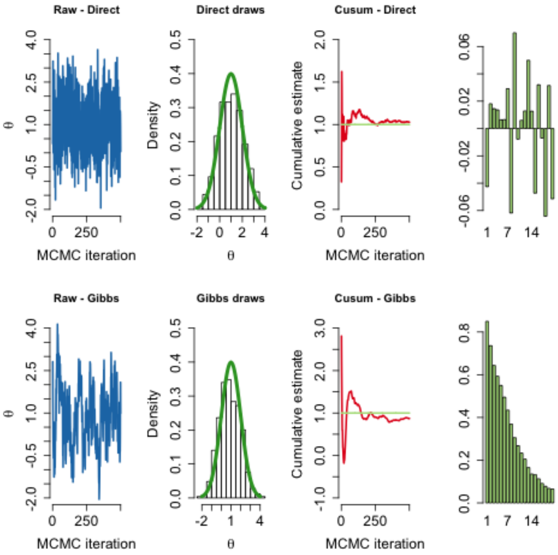
Gibbs sampling - Bivariate normal



Gibbs sampling - Bivariate normal



Direct sampling vs Gibbs sampling



Estimating $Pr(\theta_1 > 0, \theta_2 > 0)$

- Joint probability by counting:

$$Pr(\theta_1 > 0, \theta_2 > 0) \approx N^{-1} \sum_{i=1}^{N} 1(\theta_1^{(i)} > 0, \theta_2^{i)} > 0)$$

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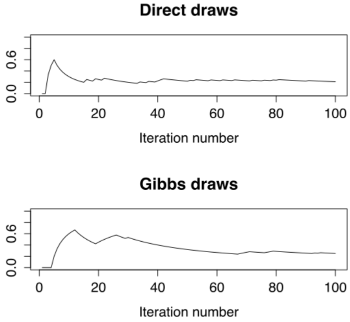


Normal model with conditionally conjugate prior

- **Normal model** with **conditionally conjugate prior**

$$\mu \sim N(\mu_0, \tau_o^2)$$
$$\sigma^2 \sim Inv - \chi^2(\nu_0, \sigma_0^2)$$

- **Full conditional posteriors**

$$\mu|\sigma^2, x \sim N\left(\mu_n, \tau_n^2\right)$$
$$\sigma^2|\mu, x \sim Inv - \chi^2\left(\nu_n, \frac{\nu_0\sigma_0^2 + \sum_{i=1}^n (x_i - \mu)^2}{n + \nu_0}\right)$$

with μ_n and τ_n^2 defined the same as when σ^2 is known.

Gibbs sampling for AR processes

- **AR(p) process**

$$x_t = \mu + \phi_1(x_{t-1} - \mu) + \ldots + \phi_p(x_{t-p} - \mu) + \varepsilon_t, \quad \varepsilon_t \overset{iid}{\sim} N(0, \sigma^2).$$

- Let $\phi = (\phi_1, \ldots, \phi_p)'$.
- **Prior**:
  - $\mu \sim$Normal
  - $\phi \sim$Multivariate Normal
  - $\sigma^2 \sim$Scaled Inverse χ^2.
- The **posterior** can be simulated by **Gibbs sampling**[1]:
  - $\mu|\phi, \sigma^2, x \sim$ Normal
  - $\phi|\mu, \sigma^2, x \sim$ Multivariate Normal
  - $\sigma^2|\mu, \phi, x \sim$ Scaled Inverse χ^2

[1] Villani (2009). Steady State Priors for Vector Autoregressions. *Journal of Applied Econometrics*.

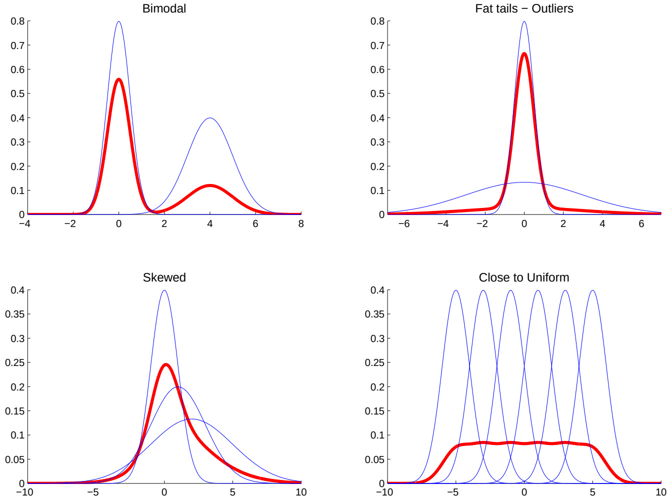
Data augmentation - Mixture distributions

- Let $\phi(x|\mu,\sigma^2)$ denote the **PDF** of $x \sim N(\mu,\sigma^2)$.
- Two-component **mixture of normals** [MN(2)]

$$p(x) = \pi \cdot \phi(x|\mu_1,\sigma_1^2) + (1-\pi)\cdot \phi(x|\mu_2,\sigma_2^2)$$

- **Simulate** from a MN(2):
  - Simulate a **membership indicator** $I \in \{1,2\}$: $I \sim Bern(\pi)$.
  - If $I = 1$, simulate x from $N(\mu_1,\sigma_1^2)$
  - If $I = 2$, simulate x from $N(\mu_2,\sigma_2^2)$.

Illustration of mixture distributions



Mixture distributions, cont.

- The **likelihood** is a product of sums. **Messy** to work with.
- **Assume** that we know where each observation comes from

$$I_i = \begin{cases} 1 \text{ if } x_i \text{ came from Density 1} \\ 2 \text{ if } x_i \text{ came from Density 2} \end{cases}.$$

- Given $I_1, ..., I_n$ it is easy to estimate π, $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$ by separating the sample according to the I's.
- But we do **not** know $I_1, ..., I_n$!
- **Data augmentation**: add $I_1, ..., I_n$ as unknown parameters.
- **Gibbs sampling**:
  - Sample π, $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$ **given** $I_1, ..., I_n$
  - Sample $I_1, ..., I_n$ **given** π, $\mu_1, \sigma_1^2, \mu_2, \sigma_2^2$

Gibbs sampling for mixture distributions

- Prior: $\pi \sim Beta(\alpha_1, \alpha_2)$. Conjugate prior for (μ_j, σ_j^2), see slide 16.
- Define: $n_1 = \sum_{i=1}^{n}(I_i = 1)$ and $n_2 = n - n_1$.
- **Gibbs sampling**:
  - $\pi \mid \mathrm{I}, \mathrm{x} \sim Beta(\alpha_1 + n_1, \alpha_2 + n_2)$
  - $\sigma_1^2 \mid \mathrm{I}, \mu_1, \mathrm{x} \sim Inv\text{-}\chi^2(\nu_{n_1}, \sigma_{n_1}^2)$ and $\mu_1 | \mathrm{I}, \sigma_1^2, \mathrm{x} \sim N\left(\mu_{n_1}, \tau_{n_1}^2\right)$
  - $\sigma_2^2 \mid \mathrm{I}, \mu_2, \mathrm{x} \sim Inv\text{-}\chi^2(\nu_{n_2}, \sigma_{n_2}^2)$ and $\mu_2 | \mathrm{I}, \sigma_2^2, \mathrm{x} \sim N\left(\mu_{n_2}, \tau_{n_2}^2\right)$
  - $I_i \mid \pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2, \mathrm{x} \sim Bern(\theta_i)$, $i = 1, ..., n$,

$$\theta_i = \frac{\pi\phi(x_i; \mu_1, \sigma_1^2)}{\pi\phi(x_i; \mu_1, \sigma_1^2) + (1-\pi)\phi(x_i; \mu_2, \sigma_2^2)}.$$

Gibbs sampling for mixture distributions

- K-component mixture of normals

$$p(x) = \sum_{k=1}^{K} \pi_k \phi(x; \mu_k, \sigma_k^2)$$

- **Multi-class indicators**: $I_i = k$ if x_i comes from component k.
- **Gibbs sampling**
  - $(\pi_1, ..., \pi_K) \mid \mathrm{I}, \mathrm{x} \sim \mathit{Dirichlet}(\alpha_1 + n_1, \alpha_2 + n_2, ..., \alpha_K + n_K)$
  - $\sigma_k^2 \mid \mathrm{I}, \mu_k, \mathrm{x} \sim \mathit{Inv}\text{-}\chi^2$ and $\mu_k | \mathrm{I}, \sigma_k^2, \mathrm{x} \sim \mathit{Normal}$, $k = 1, ..., K$,
  - $I_i \mid \pi, \mu, \sigma^2, \mathrm{x} \sim \mathit{Categorical}(\theta_{i1}, ..., \theta_{iK})$, *for* $i = 1, ..., n$,

$$\theta_{ik} = \frac{\pi_k \phi(x_i; \mu_k, \sigma_k^2)}{\sum_{j=1}^{K} \pi_j \phi(x_i; \mu_j, \sigma_j^2)}.$$

- Gibbs sampling is very powerful for **missing data** problems.

Data augmentation - Logistic regression

- **Logistic regression**:

$$\Pr(y_i = 1 \mid x_i, \beta) = \frac{\exp(x_i^T \beta)}{1 + \exp(x_i^T \beta)} = \Lambda\left(x_i^T \beta\right)$$

- The posterior distribution is not known. Augment the data with Polya-gamma latent variables[2] $\omega_i, i = 1, \ldots, n$:

$$\omega_i = \frac{1}{2\pi^2} \sum_{k=1}^{\infty} \frac{g_k}{\left(k - \frac{1}{2}\right)^2 + \frac{\left(x_i' \beta\right)^2}{4\pi^2}},$$

where g_k are independent draws from the exponential distribution with mean 1.

[2] Nicholas G. Polson , James G. Scott & Jesse Windle (2013) Bayesian Inference for Logistic Models Using Pólya–Gamma Latent Variables, Journal of the American Statistical Association

Gibbs sampling for the Logistic regression

- Given $\omega = (\omega_1, ..., \omega_n)$, the conditional posterior of β with prior $\beta \sim N(b, B)$ follows a multivariate normal distribution.
- ω is **not observed**. Gibbs sampling to the rescue!
- Simulate from the **joint posterior** $p(\omega, \beta | y)$ by iterating between
  - $\omega_i | \beta \sim \mathrm{PG}(1, x_i' \beta)$, $i = 1, ..., n$.
  - $\beta | y, \omega \sim N(m_\omega, V_\omega)$,

$$V_\omega = \left(X^T \Omega X + B^{-1} \right)^{-1}$$

$$m_\omega = V_\omega \left(X^T \kappa + B^{-1} b \right),$$

where $\kappa = (y_1 - 1/2, \ldots, y_n - 1/2)$, and Ω is the diagonal matrix of ω_i's.

- A Polya-gamma sampler, $\mathrm{PG}(1, x_i' \beta)$, is available in the R package ***BayesLogit***.

Data augmentation - Probit regression

- **Probit regression**:

$$\Pr(y_i = 1 \mid x_i) = \Phi(x_i^T \beta)$$

- **Random utility formulation**:

$$\begin{aligned} u_i &\sim N(x_i^T \beta, 1) \\ y_i &= \begin{cases} 1 & \text{if } u_i > 0 \\ 0 & \text{if } u_i \leq 0 \end{cases}. \end{aligned}$$

- Check: $\Pr(y_i = 1 \mid x_i) = \Pr(u_i > 0) = 1 - \Pr(u_i \leq 0) = 1 - \Pr(u_i - x_i^T \beta < -x_i^T \beta) = 1 - \Phi(-x_i^T \beta) = \Phi(x_i^T \beta)$.
- Given $u = (u_1, ..., u_n)$, β can be analyzed by linear regression.
- u is **not observed**. Gibbs sampling to the rescue![3]

[3] Albert and Chib (1993). Bayesian Analysis of Binary and Polychotomous Response Data. *JASA*.

Gibbs sampling for the Probit regression

- Simulate from **joint posterior** $p(u, \beta|y)$ by iterating between
  - $p(\beta|u, y)$ is multivariate normal (linear regression)
  - $p(u_i|\beta, y)$, $i = 1, ..., n$.
- The **full conditional** posterior distribution of u_i

$$p(u_i|\beta, y) \propto p(y_i|\beta, u_i)p(u_i|\beta)$$
$$= \begin{cases} N(u_i|x_i'\beta, 1) & \text{truncated to } u_i \in (-\infty, 0] \text{ if } y_i = 0 \\ N(u_i|x_i'\beta, 1) & \text{truncated to } u_i \in (0, \infty) \text{ if } y_i = 1 \end{cases}$$

- Histogram of β-draws approximates the marginal posterior of β

$$p(\beta|y) = \int p(u, \beta|y)du$$

Gibbs sampling for Regularized regression

- **Recap from lecture 5**: The joint posterior of β, σ^2 and λ is

$$
\begin{aligned}
\beta|\sigma^2, \lambda, \mathrm{y}, \mathrm{X} &\sim N\left(\mu_n, \sigma^2\Omega_n^{-1}\right) \\
\sigma^2|\lambda, \mathrm{y}, \mathrm{X} &\sim Inv-\chi^2\left(\nu_n, \sigma_n^2\right) \\
p(\lambda|\mathrm{y}, \mathrm{X}) &\propto \sqrt{\frac{|\Omega_0|}{|X'X+\Omega_0|}}\left(\frac{\nu_n\sigma_n^2}{2}\right)^{-\nu_n/2} \cdot p(\lambda)
\end{aligned}
$$

- This is the conditional-marginal decomposition

$$p(\beta, \sigma^2, \lambda|\mathrm{y}, \mathrm{X}) = p(\beta|\sigma^2, \lambda, \mathrm{y}, \mathrm{X})p(\sigma^2|\lambda, \mathrm{y}, \mathrm{X})p(\lambda|\mathrm{y}, \mathrm{X})$$

- Gibbs sampling can instead be used:
  - Sample $\beta|\sigma^2, \lambda, \mathrm{y}, \mathrm{X}$ from Normal
  - Sample $\sigma^2|\beta, \lambda, \mathrm{y}, \mathrm{X}$ from Inv-χ^2
  - Sample $\lambda|\beta, \sigma^2, \mathrm{y}, \mathrm{X}$ from Gamma
- λ is easy to simulate conditional on β and σ^2.

Gibbs sampling for Regularized regression

- Assume a Gamma prior for λ (same as $\lambda^{-1} \sim \mathrm{Inv}-\chi^2$)

$$\lambda \sim \text{Gamma}\left(\frac{\eta_0}{2}, \frac{\eta_0}{2\lambda_0}\right).$$

- $\mathbb{E}(\lambda) = \frac{\eta_0/2}{\eta_0/(2\lambda_0)} = \lambda_0$ and $\mathbb{V}(\lambda) = \frac{\eta_0/2}{(\eta_0/(2\lambda_0))^2} = \frac{1}{2\eta_0\lambda_0^2}$.
- Using Bayes' theorem twice:

$$\begin{aligned} p\left(\lambda|\beta,\sigma^2,\mathrm{y}\right) &\propto p\left(\mathrm{y}|\beta,\sigma^2,\lambda\right) p\left(\lambda|\beta,\sigma^2\right) \\ &\propto p\left(\beta|\sigma^2,\lambda\right) p\left(\lambda|\sigma^2\right) \\ &\propto p\left(\beta|\sigma^2,\lambda\right) p\left(\lambda\right) \end{aligned}$$

- Note:
  - likelihood $p\left(\mathrm{y}|\beta,\sigma^2,\lambda\right)$ does not depend on λ.
  - prior $p\left(\lambda|\sigma^2\right)$ is assumed to not depend on σ^2.

Gibbs sampling for Regularized regression

- Full conditional posterior

$$p\left(\lambda|\beta,\sigma^2,y\right) \propto p\left(\beta|\sigma^2,\lambda\right) p\left(\lambda\right)$$
$$\propto \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2/\lambda}} \exp\left(-\frac{\beta_i^2}{2\sigma^2/\lambda}\right) \cdot \lambda^{\eta_0/2-1} \exp\left(-\lambda\frac{\eta_0}{2\lambda_0}\right)$$
$$\propto \lambda^{m/2} \exp\left(-\frac{\lambda}{2\sigma^2}\sum_{i=1}^{m}\beta_i^2\right) \cdot \lambda^{\eta_0/2-1} \exp\left(-\lambda\frac{\eta_0}{2\lambda_0}\right)$$
$$\propto \lambda^{(m+\eta_0)/2-1} \exp\left(-\lambda\left(\frac{\sigma^{-2}\sum_{i=1}^{m}\beta_i^2+\eta_0/\lambda_0}{2}\right)\right)$$

- This shows that

$$\lambda|\beta,\sigma^2,y \sim \text{Gamma}\left(\frac{m+\eta_0}{2}, \frac{\sigma^{-2}\sum_{i=1}^{m}\beta_i^2+\eta_0/\lambda_0}{2}\right).$$

- $\mathbb{E}(\lambda|\beta,\sigma^2,y) = \frac{m+\eta_0}{\sigma^{-2}\sum_{i=1}^{m}\beta_i^2+\eta_0/\lambda_0}$, so λ is learned from variability of the β_i and the number of coefficients m.

Improving the efficiency of the Gibbs sampler

- **Efficient blocking**. Correlated parameters should ideally be included in the same updating block.

- **Reparametrization**. Convergence can improve dramatically in alternative parametrizations.

- **Data augmentation**.
  - Augment with latent variables to make **full conditional posteriors more easily sampled** (Logistic, Probit, Mixture models).
  - But typically **increases the autocorrelation** between draws.