

An introduction to Bayesian statistical inference

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JC(2)BIM, June 2018, Fréjus

Outline

Statistical inference: Bayesian point-of-view

- Statistical inference: frequentist / Bayesian
- Basics of Bayes inference
- Some typical uses of Bayesian inference

Evaluating the posterior distribution: Monte-Carlo

- Conjugate priors
- Monte Carlo integration
- Monte Carlo Markov chains (MCMC)

Extensions

- Sequential Monte-Carlo (SMC)
- Approximate Bayesian computation (ABC)

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An example

Example:

- ▶ n patients: $i = 1 \dots n$
- ▶ $Y_i = \text{status}$ (0 = healthy, 1 = sick) of patient i
- ▶ $\mathbf{x}_i = (x_{i1}, \dots, x_{ip}) = \text{vector of gene expression for patient } i \text{ (gene } j = 1 \dots p)$

Dataset: $n = 78$, $p = 15$

| | AB033066 | NM003056 | NM000903 | ... | Status |
|---|----------|----------|----------|-----|--------|
| 1 | 0.178 | 0.116 | 0.22 | | 0 |
| 2 | 0.065 | -0.073 | -0.014 | | 0 |
| 3 | -0.077 | 0.03 | 0.043 | | 0 |
| 4 | 0.176 | -0.041 | 0.362 | | 0 |
| 5 | -0.089 | -0.164 | -0.266 | | 0 |

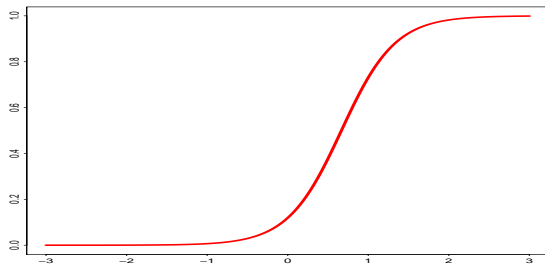
A statistical model

Logistic regression Logistic regression

- ▶ The patients are independent.
- ▶ The probability for patient i to be sick depends on \mathbf{x}_i :

$$\Pr\{Y_i = 1\} = \frac{e^{\mathbf{x}_i^\top \boldsymbol{\theta}}}{1 + e^{\mathbf{x}_i^\top \boldsymbol{\theta}}}, \quad \mathbf{x}_i^\top \boldsymbol{\theta} = \sum_{j=1}^p x_{ij} \theta_j$$

- ▶ $\boldsymbol{\theta} = (\theta_1, \dots, \theta_p)$: unknown parameter (regression coefficients, incl. intercept)



Frequentist inference

θ = fixed parameter:

- ▶ Statistical model:

$$\mathbf{Y} \sim p_{\theta}$$

- ▶ Inference: get a (point) estimate $\hat{\theta}$ e.g.

$$\hat{\theta} : \quad \log p_{\hat{\theta}}(\mathbf{Y}) = \max_{\theta} \log p_{\theta}(\mathbf{Y})$$

- ▶ The estimate $\hat{\theta}$ itself is random (depends on the data) → confidence interval, tests, ...

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Output: `GLM = glm(Y ~ X, family=binomial)`

| | Estimate | Std. Error | z value | Pr(> z) |
|-------------|------------|------------|------------|-------------|
| (Intercept) | -0.7212697 | 0.6512707 | -1.107481 | 0.2680861 |
| XAB033066 | 7.23375 | 2.505118 | 2.887589 | 0.003882068 |
| XNM003056 | -0.6116423 | 1.854695 | -0.3297806 | 0.7415658 |
| XNM000903 | 1.732625 | 1.199888 | 1.443988 | 0.1487423 |
| ... | | | | |

Bayesian inference

θ = random parameter:

- ▶ Statistical model:

$$\ell(\mathbf{Y} | \theta) := p(\mathbf{Y} | \theta) \quad (= \textit{likelihood})$$

- ▶ Inference: provide the conditional distribution of θ given the observed data \mathbf{Y} :

$$p(\theta | \mathbf{Y}) \quad (= \textit{posterior distribution})$$

→ credibility intervals

- ▶ Requires to define a marginal distribution:

$$\pi(\theta) := p(\theta) \quad (= \textit{prior distribution})$$

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Why 'Bayes'

Bayes formula:

$$P(A|B) = \frac{P(A, B)}{P(B)} = \frac{P(A)}{P(B)} P(B|A)$$

- ▶ $P(B)$ = marginal probability of B
- ▶ $P(A, B)$ = joint probability of A and B
- ▶ $P(A|B)$ = conditional probability of A given B [# 62]

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Be careful. Many methods, e.g.

Bayesian network, Naive Bayes, ...

- ▶ use conditional probabilities
- ▶ but have nothing to do with Bayesian inference (in the statistical sense)

Bayes formula for Bayesian inference (1/2)

Posterior distribution.

$$p(\boldsymbol{\theta} | \mathbf{Y}) = \frac{p(\mathbf{Y}, \boldsymbol{\theta})}{p(\mathbf{Y})} = \frac{\overbrace{\pi(\boldsymbol{\theta})}^{\text{prior}} \overbrace{\ell(\mathbf{Y} | \boldsymbol{\theta})}^{\text{likelihood}}}{p(\mathbf{Y})}$$

→ Requires to evaluate the *integrated likelihood* (i.e. marginal)

$$p(\mathbf{Y}) = \int \pi(\boldsymbol{\theta}) \ell(\mathbf{Y} | \boldsymbol{\theta}) d\boldsymbol{\theta},$$

which act as the normalizing constant of the posterior $p(\boldsymbol{\theta} | \mathbf{Y})$.

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Some remarks.

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1. $p(\cdot)$ is sometimes denoted $[\cdot]$:

$$p(\theta | \mathbf{Y}) = \frac{\pi(\theta) \ell(\mathbf{Y} | \theta)}{p(\mathbf{Y})} \quad \Leftrightarrow \quad [\theta | \mathbf{Y}] = \frac{[\theta] [\mathbf{Y} | \theta]}{[\mathbf{Y}]}$$

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2. Computing $p(\mathbf{Y})$ is generally (very) difficult: see Section 2

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2. Computing $p(\mathbf{Y})$ is generally (very) difficult: see Section 2

3. Obviously

$$p(\theta | \mathbf{Y}) \propto \pi(\theta) \ell(\mathbf{Y} | \theta),$$

→ $p(\theta | \mathbf{Y})$ and $p(\theta' | \mathbf{Y})$ can be compared, **without computing $p(\mathbf{Y})$**

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4. Obviously, the posterior $p(\theta | \mathbf{Y})$ depends on the prior $\pi(\theta)$ (see next slides).

The posterior depends on the prior

Data & Model:

- ▶ $Y_i = 1$ if sick, 0 otherwise
- ▶ $n = 10$ patients
- ▶ $\dot{\cdot}$: number sick / n

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- ▶ — : prior $\pi(\theta)$

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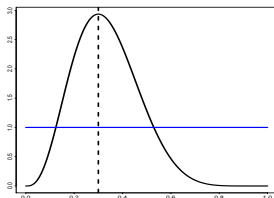
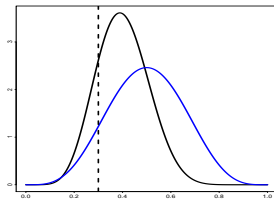
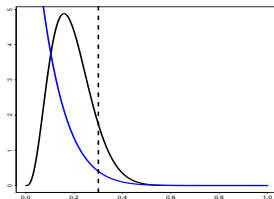
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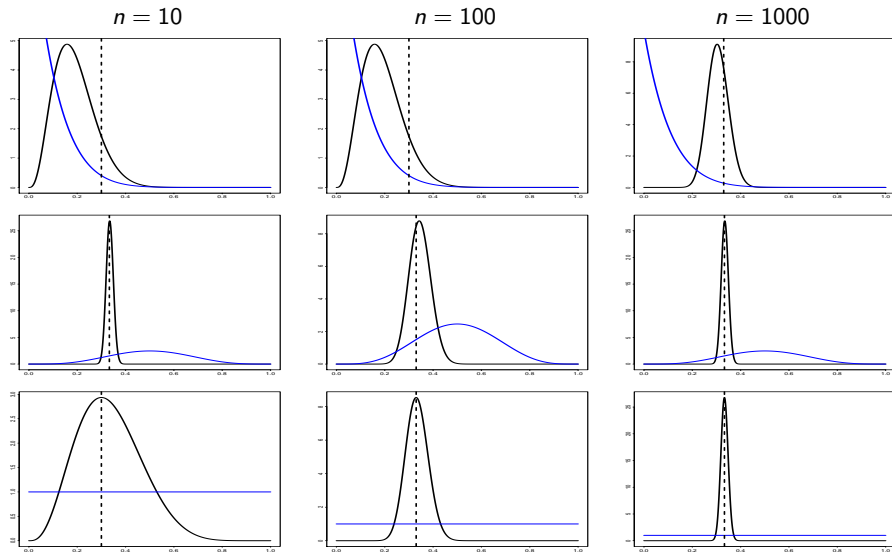
- ▶ θ = proba. sick
- ▶ — : prior $\pi(\theta)$

Output:

- ▶ — : posterior $p(\theta | \mathbf{Y})$



Dependency vanishes when n increases



Back to logistic regression

Model

- Prior: all coefficient θ_j independent:

$$\theta_j \sim \mathcal{N}(0, 100)$$

- Likelihood: all patients independent, *conditionally* on $\boldsymbol{\theta}$:

$$\Pr\{Y_i = 1 \mid \boldsymbol{\theta}\} = e^{\mathbf{x}_i^\top \boldsymbol{\theta}} / (1 + e^{\mathbf{x}_i^\top \boldsymbol{\theta}})$$

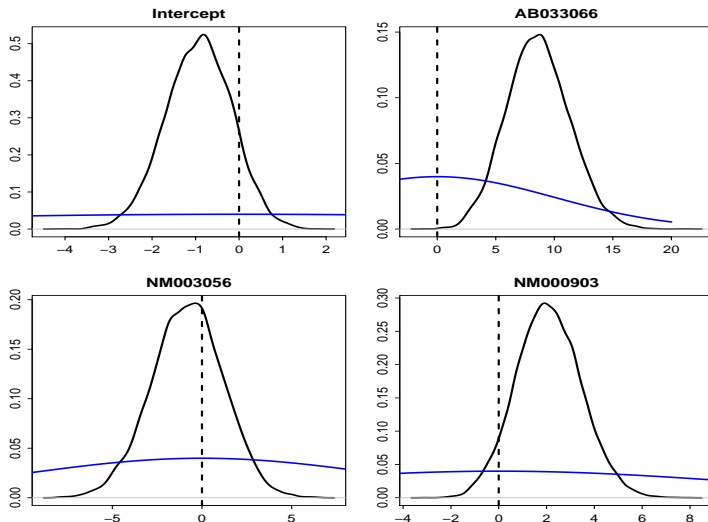
Inference:

$$\boldsymbol{\theta} \mid \mathbf{Y} \sim ?$$

(see later. For sure: $p(\boldsymbol{\theta} \mid \mathbf{Y}) \neq \mathcal{N}(\cdot, \cdot)$).

Bayesian inference

Output:



No test (and no estimator)

Frequentist hypothesis:

$$H_0 = \{\theta = 0\}$$

→ meaningless when θ is random: $P(H_0 | \mathbf{Y}) = 0$

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→ meaningless when θ is random: $P(H_0 | \mathbf{Y}) = 0$

Bayesian assessment:

$$Ch_{1-\alpha}(\theta | \mathbf{Y}) \ni 0 ?$$

Parameter estimate. For the same reason:

$\hat{\theta}$ can no be an estimate of θ

(because θ is random).

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Posterior distribution and confidence intervals

Parameter 'estimate'.

$$\text{posterior mean: } \hat{\theta}_j = \mathbb{E}(\theta_j \mid \mathbf{Y})$$

$$\text{posterior mode: } \hat{\theta}_j = \arg \max_{\theta_j} p(\theta_j \mid \mathbf{Y})$$

Credibility interval (CI). With level $1 - \alpha$ (e.g. 95%):

$$CI_{1-\alpha}(\theta_j \mid \mathbf{Y}) = [\theta_j^\ell; \theta_j^u] : \quad \Pr\{\theta_j^\ell < \theta_j < \theta_j^u \mid \mathbf{Y}\} = 1 - \alpha$$

Posterior distribution and confidence intervals

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Example. [# 4]

| | post.mean | post.mode | lower.CI | upper.CI |
|-----------|------------|------------|------------|-----------|
| Intercept | -0.9298079 | -0.8838218 | -2.457669 | 0.5376564 |
| AB033066 | 8.656539 | 8.497985 | 3.646142 | 13.98029 |
| NM003056 | -0.8669479 | -0.5323168 | -4.919099 | 3.084982 |
| NM000903 | 2.088584 | 1.852784 | -0.4736828 | 4.838164 |

Accounting for uncertainty

Question: What is the probability for patient 0 (with profile \mathbf{x}_0) to be sick?

Model answer:

$$\Pr\{Y_0 = 1 \mid \boldsymbol{\theta}\} = e^{\mathbf{x}_0^\top \boldsymbol{\theta}} / (1 + e^{\mathbf{x}_0^\top \boldsymbol{\theta}})$$

but $\boldsymbol{\theta}$ is unknown (and random).

Bayesian answer: *posterior predictive probability*

$$\Pr\{Y_0 = 1 \mid \mathbf{Y}\} = \int \Pr\{Y_0 = 1 \mid \boldsymbol{\theta}\} p(\boldsymbol{\theta} \mid \mathbf{Y}) d\boldsymbol{\theta}$$

Model comparison (1/2)

Problem. Which model fits the data better:

M_0 : none of the genes has an effect, i.e. $\boldsymbol{\theta} = (\theta_0, 0, \dots, 0)$

M_1 : only the first gene has an effect, i.e. $\boldsymbol{\theta} = (\theta_0, \theta_1, 0, \dots, 0)$

...

M_p : all genes have an effect, i.e. $\boldsymbol{\theta} = (\theta_0, \theta_1, \dots, \theta_p)$

Bayesian model comparison. For each model $M \in \mathcal{M} = \{M_0, \dots, M_p\}$, evaluate

$$p(M | \mathbf{Y})$$

Model comparison (2/2)

Ingredients:

- Prior on the models: $p(M)$, e.g.

$$p(M) = \text{cst} \quad (\text{uniform prior})$$

- Conditional prior on the parameters: $\pi(\boldsymbol{\theta} | M)$, e.g.

$$\theta_j | M_k \begin{cases} \sim \mathcal{N}(0, 100) & \text{if } j \leq k \\ = 0 & \text{otherwise} \end{cases}$$

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Recipe:

- Evaluate the marginal likelihood of the data for each model M :

$$p(\mathbf{Y} | M) = \int \ell(\mathbf{Y} | \boldsymbol{\theta}) \pi(\boldsymbol{\theta} | M) \, d\boldsymbol{\theta}$$

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Recipe:

- Evaluate the marginal likelihood of the data for each model M :

$$p(\mathbf{Y} | M) = \int \ell(\mathbf{Y} | \theta) \pi(\theta | M) d\theta$$

- Evaluate the $p(M_k | \mathbf{Y})$ using Bayes rule

$$p(M_k | \mathbf{Y}) = \frac{p(M_k)p(\mathbf{Y} | M_k)}{p(\mathbf{Y})} = \frac{p(M_k)p(\mathbf{Y} | M_k)}{\sum_{k'} p(M_{k'})p(\mathbf{Y} | M_{k'})}$$

Model averaging (uncertainty on models)

Question: Probability for patient 0 to be sick?

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Model selection.

- ▶ Select the 'best' model \hat{M} , i.e. with largest posterior $p(M | \mathbf{Y})$
- ▶ Compute

$$\Pr\{Y_0 = 1 | \mathbf{Y}, \hat{M}\} = \int \Pr\{Y_0 = 1 | \boldsymbol{\theta}\} p(\boldsymbol{\theta} | \mathbf{Y}, \hat{M}) d\boldsymbol{\theta}$$

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Model averaging.

- ▶ Keep all models
- ▶ Compute

$$\Pr\{Y_0 = 1 | \mathbf{Y}\} = \sum_M \Pr\{Y_0 = 1 | \mathbf{Y}, M\} p(M | \mathbf{Y})$$

Model averaging: Illustration

Aim: Probability p_0 to be sick a patient with gene expression profile

$$\mathbf{x}_0 = (0.178, 0.116, \dots, 0.076, -0.231)$$

Results for models M_1, \dots, M_d :

| Model | $p(M \mathbf{Y})$ | $\mathbb{E}(p_0 \mathbf{Y}, M)$ | $\sqrt{\mathbb{V}}(p_0 \mathbf{Y}, M)$ |
|-----------|---------------------|-----------------------------------|--|
| M_1 | 1e-04 | 0.494 | 0.028 |
| M_2 | 7e-04 | 0.611 | 0.097 |
| M_3 | 5e-04 | 0.627 | 0.106 |
| ... | | | |
| M_{14} | 0.1436 | 0.242 | 0.18 |
| M_{15} | 0.2859 | 0.203 | 0.168 |
| M_{16} | 0.2726 | 0.195 | 0.168 |
| <hr/> | | | |
| Averaging | | $\mathbb{E}(p_0 \mathbf{Y})$ | $\sqrt{\mathbb{V}}(p_0 \mathbf{Y})$ |
| | | 0.249 | 0.198 |

Transfer of uncertainty from one experience to another

Combining samples. Consider two independent but similar datasets \mathbf{Y}_1 and \mathbf{Y}_2 .

Simple algebra gives:

$$p(\theta | \mathbf{Y}_1, \mathbf{Y}_2) = \frac{p(\theta | \mathbf{Y}_1)p(\mathbf{Y}_2 | \theta, \mathbf{Y}_1)}{p(\mathbf{Y}_2 | \mathbf{Y}_1)}$$

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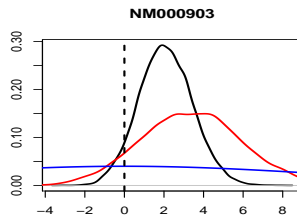
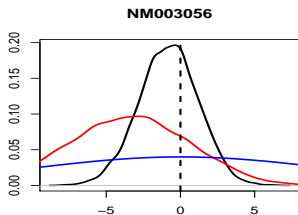
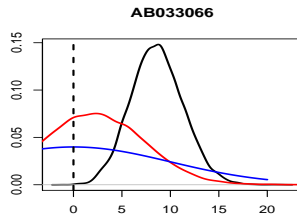
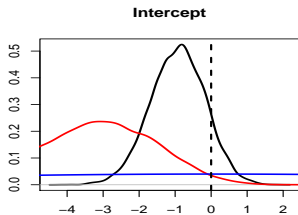
$$p(\theta | \mathbf{Y}_1, \mathbf{Y}_2) = \frac{p(\theta | \mathbf{Y}_1)p(\mathbf{Y}_2 | \theta, \mathbf{Y}_1)}{p(\mathbf{Y}_2 | \mathbf{Y}_1)}$$

In practice:

1. Perform inference using \mathbf{Y}_1 to get $p(\theta | \mathbf{Y}_1)$ from prior $\pi(\theta)$
2. Then perform inference using \mathbf{Y}_2 to get $p(\theta | \mathbf{Y}_1, \mathbf{Y}_2)$ using $p(\theta | \mathbf{Y}_1)$ as a prior

Combining experiments

Output: $n_1 = n_2 = 39$



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Posterior distribution

Aim: Evaluate

$$E[f(\boldsymbol{\theta})|\mathbf{Y}]$$

- ▶ Posterior mean: $f(\boldsymbol{\theta}) = \theta_j$
- ▶ Credibility interval: $f(\boldsymbol{\theta}) = \mathbb{I}\{\theta_j^\ell < \theta_j < \theta_j^u\}$
- ▶ Posterior variance: $f(\boldsymbol{\theta}) = \theta_j^2$ (+ posterior mean)

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Main problem: evaluate

$$p(\theta | \mathbf{Y}) = \frac{\pi(\theta)\ell(\mathbf{Y} | \theta)}{p(\mathbf{Y})}$$

which requires to evaluate

$$p(\mathbf{Y}) = \int \underbrace{\pi(\theta)}_{\text{prior}} \underbrace{\ell(\mathbf{Y} | \theta)}_{\text{likelihood}} d\theta$$

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Nice case: Conjugate priors

Example: Bernoulli¹

Prior: θ = probability to be sick.

$$\theta \sim \text{Beta}(a, b), \quad \pi(\theta) \propto \theta^{a-1}(1-\theta)^{b-1}$$

¹#13: from top to bottom, $(a, b) = (1, 10), (5, 5), (1, 1)$

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Likelihood: $Y_i = 1$ if sick, 0 otherwise. S = number of sick

$$Y_i | \theta \sim \mathcal{B}(\theta), \quad \ell(\mathbf{Y} | \theta) = \prod_i \theta^{Y_i} (1 - \theta)^{1 - Y_i} = \theta^S (1 - \theta)^{n - S}$$

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Posterior:

$$p(\theta | \mathbf{Y}) \propto \pi(\theta) \ell(\mathbf{Y} | \theta) = \theta^{a+S-1} (1-\theta)^{b+n-S-1}$$

which means that

$$\theta | \mathbf{Y} \sim \text{Beta}(a + S, b + n - S)$$

¹#13: from top to bottom, $(a, b) = (1, 10), (5, 5), (1, 1)$

Conjugate priors: Discrete distributions

| Likelihood | Model parameters | Conjugate prior distribution | Prior hyperparameters | Posterior hyperparameters | Interpretation of hyperparameters ^[note 1] | Posterior predictive ^[note 2] |
|---|---|------------------------------|-------------------------------------|---|---|---|
| Bernoulli | p (probability) | Beta | α, β | $\alpha + \sum_{i=1}^n x_i, \beta + n - \sum_{i=1}^n x_i$ | $\alpha - 1$ successes, $\beta - 1$ failures ^[note 1] | $p(\tilde{x} = 1) = \frac{\alpha'}{\alpha' + \beta'}$ |
| Binomial | p (probability) | Beta | α, β | $\alpha + \sum_{i=1}^n x_i, \beta + \sum_{i=1}^n N_i - \sum_{i=1}^n x_i$ | $\alpha - 1$ successes, $\beta - 1$ failures ^[note 1] | $\text{BetaBin}(\tilde{x} \alpha', \beta')$ (beta-binomial) |
| Negative Binomial with known failure number r | p (probability) | Beta | α, β | $\alpha + \sum_{i=1}^n x_i, \beta + rn$ | $\alpha - 1$ total successes, $\beta - 1$ failures ^[note 1] (i.e. $\frac{\beta-1}{r}$ experiments, assuming r stays fixed) | |
| Poisson | λ (rate) | Gamma | k, θ | $k + \sum_{i=1}^n x_i, \frac{\theta}{n\theta + 1}$ | k total occurrences in $1/\theta$ intervals | $\text{NB}(\tilde{x} k', \frac{\theta'}{1+\theta'})$ (negative binomial) |
| Poisson | λ (rate) | Gamma | α, β ^[note 3] | $\alpha + \sum_{i=1}^n x_i, \beta + n$ | α total occurrences in β intervals | $\text{NB}(\tilde{x} \alpha', \frac{1}{1+\beta'})$ (negative binomial) |
| Categorical | \mathbf{p} (probability vector), k (number of categories, i.e. size of \mathbf{p}) | Dirichlet | $\boldsymbol{\alpha}$ | $\boldsymbol{\alpha} + (c_1, \dots, c_k)$, where c_i is the number of observations in category i | $\alpha_i - 1$ occurrences of category i ^[note 1] | $p(\tilde{x} = i) = \frac{\alpha_i'}{\sum_i \alpha_i'}$ $= \frac{\alpha_i + c_i}{\sum_i \alpha_i + n}$ |
| Multinomial | \mathbf{p} (probability vector), k (number of categories, i.e. size of \mathbf{p}) | Dirichlet | $\boldsymbol{\alpha}$ | $\boldsymbol{\alpha} + \sum_{i=1}^n \mathbf{x}_i$ | $\alpha_i - 1$ occurrences of category i ^[note 1] | $\text{DirMult}(\tilde{\mathbf{x}} \boldsymbol{\alpha}')$ (Dirichlet-multinomial) |
| Hypergeometric with known total population size N | M (number of target members) | Beta-binomial ^[4] | $n = N, \alpha, \beta$ | $\alpha + \sum_{i=1}^n x_i, \beta + \sum_{i=1}^n N_i - \sum_{i=1}^n x_i$ | $\alpha - 1$ successes, $\beta - 1$ failures ^[note 1] | |
| Geometric | p_0 (probability) | Beta | α, β | $\alpha + n, \beta + \sum_{i=1}^n x_i$ | $\alpha - 1$ experiments, $\beta - 1$ total failures ^[note 1] | |

en.wikipedia.org/wiki/Conjugate_prior

Conjugate priors: Continuous distributions

| Likelihood | Model parameters | Conjugate prior distribution | Prior hyperparameters | Posterior hyperparameters | Interpretation of hyperparameters | Posterior predictive ^[note 4] |
|---|--|------------------------------|-------------------------------------|--|---|---|
| Normal with known variance σ^2 | μ (mean) | Normal | μ_0, σ_0^2 | $\left(\frac{\mu_0}{\sigma_0^2} + \frac{\sum_{i=1}^n x_i}{\sigma^2} \right) / \left(\frac{1}{\sigma_0^2} + \frac{n}{\sigma^2} \right),$ $\left(\frac{1}{\sigma_0^2} + \frac{n}{\sigma^2} \right)^{-1}$ | mean was estimated from observations with total precision (sum of all individual precisions) $1/\sigma_0^2$ and with sample mean μ_0 | $\mathcal{N}(\tilde{x} \mu'_0, \sigma_0'^2 + \sigma^2)^{[5]}$ |
| Normal with known precision τ | μ (mean) | Normal | μ_0, τ_0 | $\left(\tau_0 \mu_0 + \tau \sum_{i=1}^n x_i \right) / (\tau_0 + n\tau), \tau_0 + n\tau$ | mean was estimated from observations with total precision (sum of all individual precisions) τ_0 and with sample mean μ_0 | $\mathcal{N}\left(\tilde{x} \mu'_0, \frac{1}{\tau_0} + \frac{1}{\tau}\right)^{[5]}$ |
| Normal with known mean μ | σ^2 (variance) | Inverse gamma | α, β ^[note 5] | $\alpha + \frac{n}{2}, \beta + \frac{\sum_{i=1}^n (x_i - \mu)^2}{2}$ | variance was estimated from 2α observations with sample variance β/α (i.e. with sum of squared deviations 2β , where deviations are from known mean μ) | $t_{2\alpha'}(\tilde{x} \mu, \sigma^2 = \beta'/\alpha')^{[5]}$ |
| Normal with known mean μ | σ^2 (variance) | Scaled inverse chi-squared | ν, σ_0^2 | $\nu + n, \frac{\nu\sigma_0^2 + \sum_{i=1}^n (x_i - \mu)^2}{\nu + n}$ | variance was estimated from ν observations with sample variance σ_0^2 | $t_{\nu'}(\tilde{x} \mu, \sigma_0'^2)^{[5]}$ |
| Normal with known mean μ | τ (precision) | Gamma | α, β ^[note 3] | $\alpha + \frac{n}{2}, \beta + \frac{\sum_{i=1}^n (x_i - \mu)^2}{2}$ | precision was estimated from 2α observations with sample variance β/α (i.e. with sum of squared deviations 2β , where deviations are from known mean μ) | $t_{2\alpha'}(\tilde{x} \mu, \sigma^2 = \beta'/\alpha')^{[5]}$ |
| Normal ^[note 6] | μ and σ^2 Assuming exchangeability | Normal-inverse gamma | $\mu_0, \nu, \alpha, \beta$ | $\frac{\nu\mu_0 + n\bar{x}}{\nu + n}, \nu + n, \alpha + \frac{n}{2},$ $\beta + \frac{1}{2} \sum_{i=1}^n (x_i - \bar{x})^2 + \frac{n\nu}{\nu + n} \frac{(\bar{x} - \mu_0)^2}{2}$ ▪ \bar{x} is the sample mean | mean was estimated from ν observations with sample mean μ_0 ; variance was estimated from 2α observations with sample mean μ_0 and sum of squared deviations 2β | $t_{2\alpha'}\left(\tilde{x} \mu', \frac{\beta'(\nu' + 1)}{\alpha'\nu'}\right)^{[5]}$ |
| Normal | μ and τ Assuming exchangeability | Normal-gamma | $\mu_0, \nu, \alpha, \beta$ | $\frac{\nu\mu_0 + n\bar{x}}{\nu + n}, \nu + n, \alpha + \frac{n}{2},$ $\beta + \frac{1}{2} \sum_{i=1}^n (x_i - \bar{x})^2 + \frac{n\nu}{\nu + n} \frac{(\bar{x} - \mu_0)^2}{2}$ ▪ \bar{x} is the sample mean | mean was estimated from ν observations with sample mean μ_0 , and precision was estimated from 2α observations with sample mean μ_0 and sum of squared deviations 2β | $t_{2\alpha'}\left(\tilde{x} \mu', \frac{\beta'(\nu' + 1)}{\alpha'\nu'}\right)^{[5]}$ |
| Multivariate normal with known covariance matrix Σ | $\boldsymbol{\mu}$ (mean vector) | Multivariate normal | $\boldsymbol{\mu}_0, \Sigma_0$ | $\left(\Sigma_0^{-1} + n\Sigma^{-1} \right)^{-1} \left(\Sigma_0^{-1} \boldsymbol{\mu}_0 + n\Sigma^{-1} \bar{\mathbf{x}} \right),$ $\left(\Sigma_0^{-1} + n\Sigma^{-1} \right)^{-1}$ ▪ $\bar{\mathbf{x}}$ is the sample mean | mean was estimated from observations with total precision (sum of all individual precisions) Σ_0^{-1} and with sample mean $\boldsymbol{\mu}_0$ | $\mathcal{N}(\bar{\mathbf{x}} \boldsymbol{\mu}', \Sigma_0' + \Sigma)^{[5]}$ |

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Outline

Statistical inference: Bayesian point-of-view

Statistical inference: frequentist / Bayesian

Basics of Bayes inference

Some typical uses of Bayesian inference

Evaluating the posterior distribution: Monte-Carlo

Conjugate priors

Monte Carlo integration

Monte Carlo Markov chains (MCMC)

Extensions

Sequential Monte-Carlo (SMC)

Approximate Bayesian computation (ABC)

Computing integrals

General case: $p(\boldsymbol{\theta} | \mathbf{Y})$ has no close form

Goal: compute

$$\mathbb{E}(f(\boldsymbol{\theta}) | \mathbf{Y}) = \int f(\boldsymbol{\theta}) p(\boldsymbol{\theta} | \mathbf{Y}) d\boldsymbol{\theta} = \int f(\boldsymbol{\theta}) \pi(\boldsymbol{\theta}) \ell(\mathbf{Y} | \boldsymbol{\theta}) d\boldsymbol{\theta} / p(\mathbf{Y})$$

where

$$p(\mathbf{Y}) = \int \pi(\boldsymbol{\theta}) \ell(\mathbf{Y} | \boldsymbol{\theta}) d\boldsymbol{\theta}$$

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where

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We need to evaluate integrals of the form

$$\int [\cdots] \pi(\boldsymbol{\theta}) \ell(\mathbf{Y} | \boldsymbol{\theta}) d\boldsymbol{\theta}$$

Monte Carlo

Principle. To evaluate

$$\mathbb{E}_q[f(\boldsymbol{\theta})] = \int f(\boldsymbol{\theta})q(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta}$$

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► Works fine to evaluate $\mathbb{E}[f(\boldsymbol{\theta})]$, taking $q(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta})$

$$\widehat{\mathbb{E}}_{\mathcal{N}(0,10)} \left[e^{\theta} \right] = \text{mean}(\exp(\text{rnorm}(B, \text{mean}=0, \text{sd}=\text{sqrt}(10))))$$

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$$\widehat{\mathbb{E}}_{\mathcal{N}(0,10)} \left[e^{\theta} \right] = \text{mean}(\exp(\text{rnorm}(B, \text{mean}=0, \text{sd}=\text{sqrt}(10))))$$

► Useless to evaluate $\mathbb{E}[f(\boldsymbol{\theta})|\mathbf{Y}]$ as we do not know how to sample from $q(\boldsymbol{\theta}) = p(\boldsymbol{\theta} | \mathbf{Y})$

Importance Sampling (IS)

Main trick = weighting particles.

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$$\hat{\mathbb{E}}[f(\theta)] = \frac{1}{B} \sum_b W(\theta^b)f(\theta^b)$$

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for some **proposal** $q' \gg q$, from which you *know how to sample*, then

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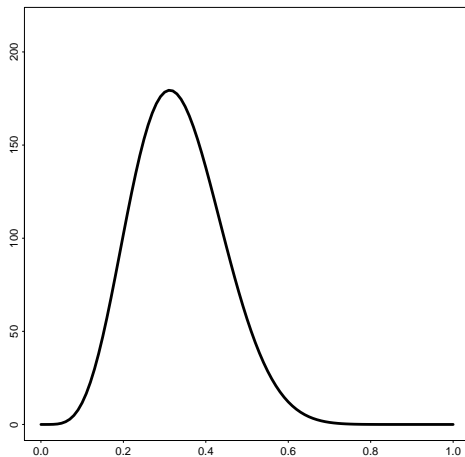
$$W(\boldsymbol{\theta}^b) = q(\boldsymbol{\theta}^b)/q'(\boldsymbol{\theta}^b),$$

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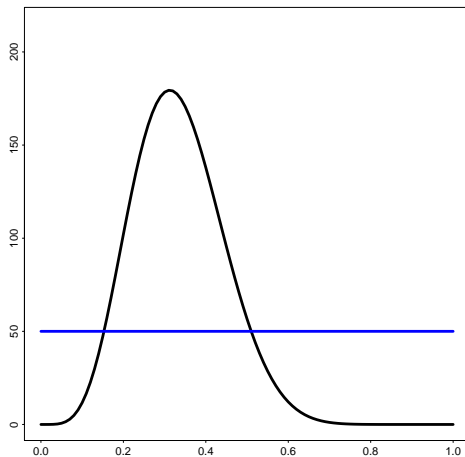
$$\widehat{\mathbb{E}}[f(\boldsymbol{\theta})] = \frac{1}{B} \sum_b W(\boldsymbol{\theta}^b) f(\boldsymbol{\theta}^b)$$

→ unbiased estimate of $\mathbb{E}[f(\boldsymbol{\theta})]$ with variance $\propto \sum_b W(\boldsymbol{\theta}^b)^2 / B$.

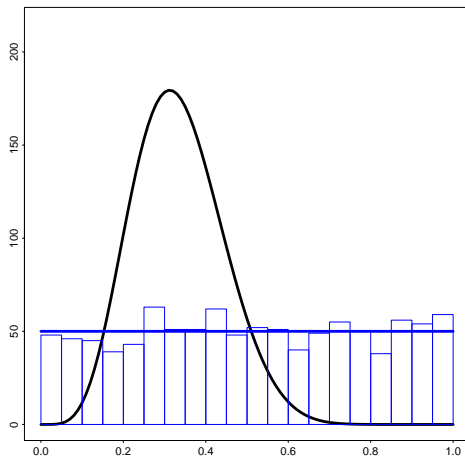
Importance Sampling (a picture)



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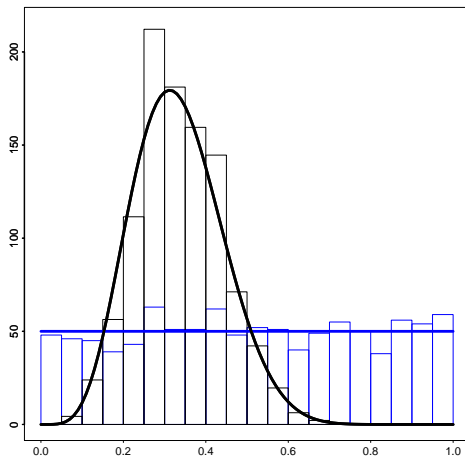
Importance Sampling (a picture)

Efficiency of sampling:

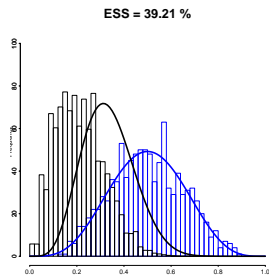
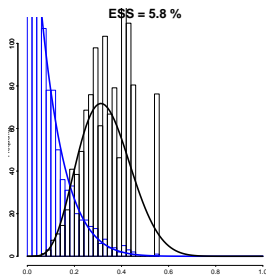
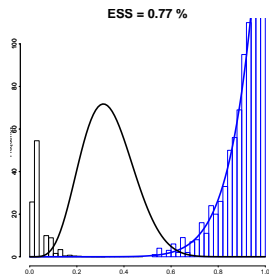
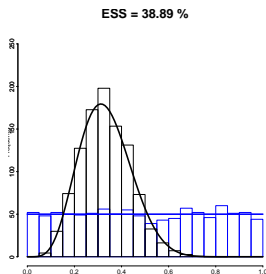
$$ESS = \overline{W}^2 / \overline{W^2}$$

$$q' = q$$

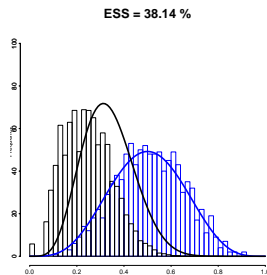
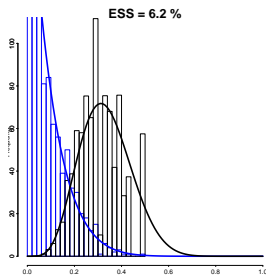
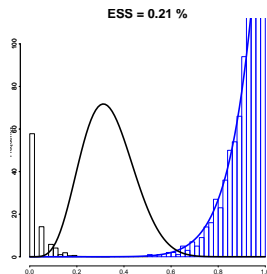
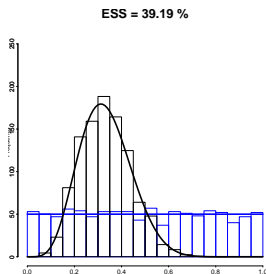
$$\Rightarrow ESS = 1$$



Importance Sampling: Importance of the proposal



Importance of the proposal: another draw



IS for posterior sampling

To evaluate $\mathbb{E}[f(\boldsymbol{\theta})|\mathbf{Y}]$, write it as

$$\begin{aligned}\mathbb{E}[f(\boldsymbol{\theta})|\mathbf{Y}] &= \int f(\boldsymbol{\theta})p(\boldsymbol{\theta}, \mathbf{Y}) \, d\boldsymbol{\theta} \Big/ p(\mathbf{Y}) = \dots \\ &= \int f(\boldsymbol{\theta}) \frac{\pi(\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{Y})}{q(\boldsymbol{\theta})} q(\boldsymbol{\theta}) \, d\boldsymbol{\theta} \Big/ \int \frac{\pi(\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathbf{Y})}{q(\boldsymbol{\theta})} q(\boldsymbol{\theta}) \, d\boldsymbol{\theta}\end{aligned}$$

1. sample

$$(\boldsymbol{\theta}^1, \dots, \boldsymbol{\theta}^B) \text{ iid } \sim q$$

2. compute the weights

$$W(\boldsymbol{\theta}^b) = \pi(\boldsymbol{\theta}^b)p(\boldsymbol{\theta}^b|\mathbf{Y}) \Big/ q(\boldsymbol{\theta}^b)$$

3. get

$$\widehat{\mathbb{E}}[f(\boldsymbol{\theta})|\mathbf{Y}] = \sum_b W(\boldsymbol{\theta}^b) f(\boldsymbol{\theta}^b) \Big/ \sum_b W(\boldsymbol{\theta}^b)$$

(slightly **biased**).

Good proposals

Choosing q is critical

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Typical choices

- Prior

$$q(\boldsymbol{\theta}) = \pi(\boldsymbol{\theta})$$

→ far from the target $p(\boldsymbol{\theta} | \mathbf{Y})$: small *ESS*

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$$q(\boldsymbol{\theta}) = \mathcal{N}(\hat{\boldsymbol{\theta}}_{MLE}, \mathbb{V}_{\infty}(\hat{\boldsymbol{\theta}}_{MLE}))$$

→ fine, as long as MLE is available

Good proposals

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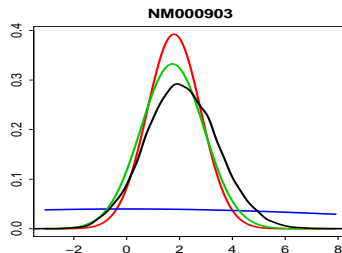
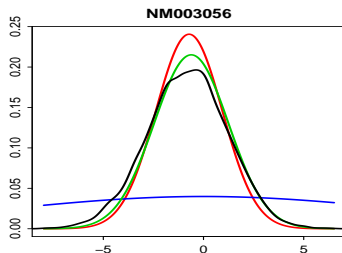
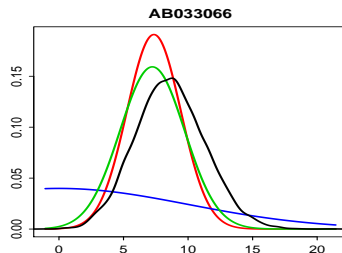
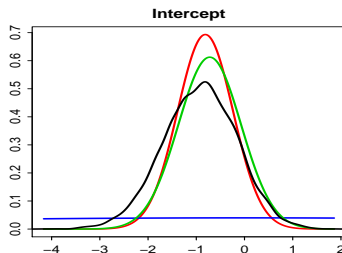
- Variational Bayes, expectation propagation, ...:

$$q(\boldsymbol{\theta}) = \arg \min_{q \in \mathcal{Q}} KL[q(\boldsymbol{\theta}) || p(\boldsymbol{\theta} | \mathbf{Y})]$$

→ fast and reasonably accurate

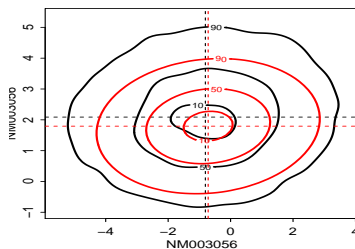
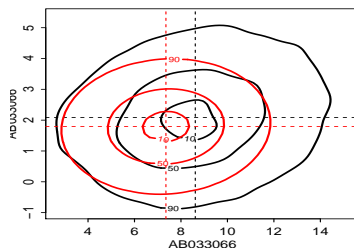
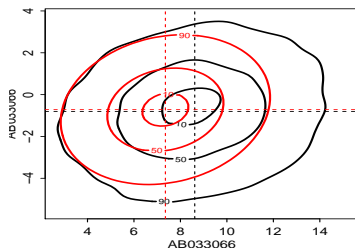
Variational Bayes & ML as a prior

— : prior, — : VB, — : MLE, — : posterior



Variational Bayes as a prior: joint distribution

— : VB, — : posterior



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Limit distribution of Markov chain

Property. If $\{\phi^b\}_{b \geq 0}$ is an ergodic Markov chain (irreducible, aperiodic, ...) with

- ▶ initial distribution $\phi^0 \sim \nu$,
- ▶ transition kernel $\phi^b | \phi^{b-1} \sim \kappa(\cdot | \phi^{b-1})$:

$$p(\{\phi^b\}) = \nu(\phi^0) \times \kappa(\phi^1 | \phi^0) \times \kappa(\phi^2 | \phi^1) \times \kappa(\phi^3 | \phi^2) \times \dots$$

then

- ▶ it admits a **unique stationary distribution** μ :

$$\phi^{b-1} \sim \mu \quad \Rightarrow \quad \phi^b \sim \mu$$

- ▶ ϕ^b converges towards μ in distribution

$$\phi^b \xrightarrow[b \rightarrow \infty]{\Delta} \mu$$

for **any initial distribution** ν

Use for Bayesian inference

Aim. Sample from

$$p(\boldsymbol{\theta} | \mathbf{Y})$$

Idea.

- ▶ Construct an ergodic Markov chain $\{\boldsymbol{\theta}^b\}_{b \geq 0}$ with stationary distribution

$$\mu(\boldsymbol{\theta}) = p(\boldsymbol{\theta} | \mathbf{Y})$$

- ▶ Choose 'any' initial ν and simulate $\{\boldsymbol{\theta}^b\}_{b \geq 0}$
- ▶ Until it 'reaches' its stationary distribution

Metropolis-Hastings

Algorithm. Define a shift kernel $\lambda(\cdot | \theta)$

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- ▶ At step b ,
 1. sample $\boldsymbol{\theta}' \sim \lambda(\cdot | \boldsymbol{\theta}^{b-1})$;
 2. compute the Metropolis-Hastings ratio (acceptance probability)

$$\alpha(\boldsymbol{\theta}', \boldsymbol{\theta}^{b-1}) = \frac{\lambda(\boldsymbol{\theta}^{b-1} | \boldsymbol{\theta}')}{\lambda(\boldsymbol{\theta}' | \boldsymbol{\theta}^{b-1})} \frac{p(\boldsymbol{\theta}' | \mathbf{Y})}{p(\boldsymbol{\theta}^{b-1} | \mathbf{Y})}$$

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$$\alpha(\boldsymbol{\theta}', \boldsymbol{\theta}^{b-1}) = \frac{\lambda(\boldsymbol{\theta}^{b-1} | \boldsymbol{\theta}')}{\lambda(\boldsymbol{\theta}' | \boldsymbol{\theta}^{b-1})} \frac{p(\boldsymbol{\theta}' | \mathbf{Y})}{p(\boldsymbol{\theta}^{b-1} | \mathbf{Y})} = \frac{\lambda(\boldsymbol{\theta}^{b-1} | \boldsymbol{\theta}')}{\lambda(\boldsymbol{\theta}' | \boldsymbol{\theta}^{b-1})} \frac{\pi(\boldsymbol{\theta}') \ell(\mathbf{Y} | \boldsymbol{\theta}')}{\pi(\boldsymbol{\theta}^{b-1}) \ell(\mathbf{Y} | \boldsymbol{\theta}^{b-1})};$$

Metropolis-Hastings

Algorithm. Define a shift kernel $\lambda(\cdot | \boldsymbol{\theta})$

- ▶ Start with $\boldsymbol{\theta}^0$
- ▶ At step b ,
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3. set $\boldsymbol{\theta}^b = \begin{cases} \boldsymbol{\theta}' & \text{with probability } \max(1, \alpha(\boldsymbol{\theta}', \boldsymbol{\theta}^{b-1})), \\ \boldsymbol{\theta}^{b-1} & \text{otherwise.} \end{cases}$

Metropolis-Hastings

Algorithm. Define a shift kernel $\lambda(\cdot | \theta)$

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- ▶ At step b ,
 1. sample $\theta' \sim \lambda(\cdot | \theta^{b-1})$;
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$$\alpha(\theta', \theta^{b-1}) = \frac{\lambda(\theta^{b-1} | \theta')}{\lambda(\theta' | \theta^{b-1})} \frac{p(\theta' | \mathbf{Y})}{p(\theta^{b-1} | \mathbf{Y})} = \frac{\lambda(\theta^{b-1} | \theta')}{\lambda(\theta' | \theta^{b-1})} \frac{\pi(\theta') \ell(\mathbf{Y} | \theta')}{\pi(\theta^{b-1}) \ell(\mathbf{Y} | \theta^{b-1})};$$

3. set $\theta^b = \begin{cases} \theta' & \text{with probability } \max(1, \alpha(\theta', \theta^{b-1})), \\ \theta^{b-1} & \text{otherwise.} \end{cases}$

Properties.

1. λ and α define a Markov chain with stationary distribution $\mu(\theta) = p(\theta | \mathbf{Y})$.
2. If $\lambda(\cdot | \theta)$ is symmetric, α reduce to $\pi(\theta') \ell(\mathbf{Y} | \theta') / [\pi(\theta^{b-1}) \ell(\mathbf{Y} | \theta^{b-1})]$

Metropolis-Hastings for logistic regression

Model.

$$\begin{aligned}\boldsymbol{\theta} &\sim \pi(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}_p, 100 \mathbf{I}_p) \\ \mathbf{Y} \mid \boldsymbol{\theta} &\sim \ell(\mathbf{Y} \mid \boldsymbol{\theta}) = \prod_i \left(\frac{e^{\mathbf{x}_i^\top \boldsymbol{\theta}}}{1 + e^{\mathbf{x}_i^\top \boldsymbol{\theta}}} \right)^{y_i} \left(\frac{1}{1 + e^{\mathbf{x}_i^\top \boldsymbol{\theta}}} \right)^{1-y_i}\end{aligned}$$

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Algorithm settings.

$$\begin{aligned}\boldsymbol{\theta}^0 &= \mathbf{0}_p \\ \lambda(\cdot \mid \boldsymbol{\theta}) &= \mathcal{N}(\mathbf{0}_p, .5 \mathbf{I}_p)\end{aligned}$$

M-H for logistic regression: R code

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```
mu.prior = rep(0, p); Sigma.prior = 100*diag(p); Sigma.shift = .5*diag(p)
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logprior.cur = dmvnorm(theta.cur, mean=mu.prior, sigma=Sigma.prior, log=T)
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loglik.cur = sum(dbinom(Y, 1, prob.cur, log=T))
for (b in 2:B){
  theta.tmp = rmvnorm(1, mean=theta.sample[b-1, ], sigma=Sigma.shift)[1, ]
```

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  if(runif(1) < alpha){
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Sanity checks

Setting. Sample $1.2 \cdot 10^6$ θ , remove first $2 \cdot 10^5$, extract every 10 $\rightarrow B = 10^5$.

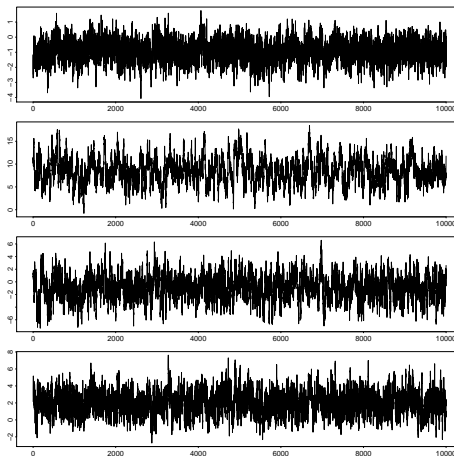
► Acceptance rate

| variance shift | 0.1 | 0.5 | 1 |
|-----------------|-------|-------|-------|
| acceptance rate | 0.035 | 0.011 | 0.004 |

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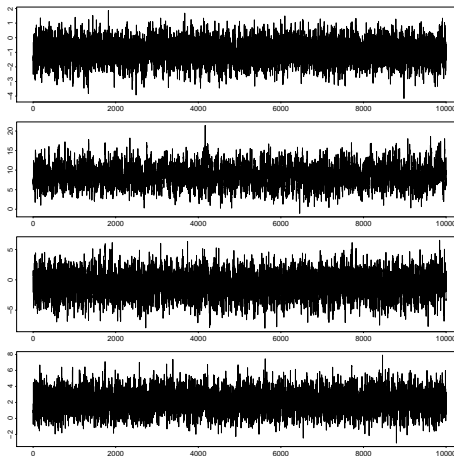
- Acceptance rate
- Stationarity:
var. shift = .1



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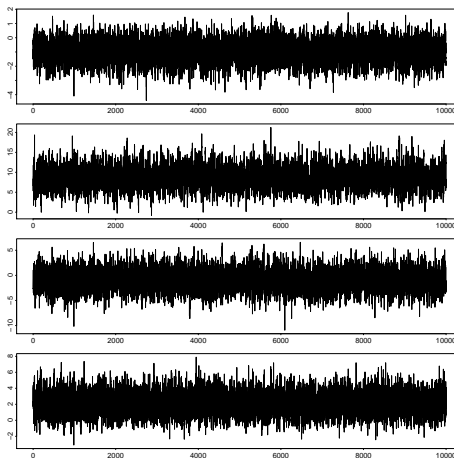
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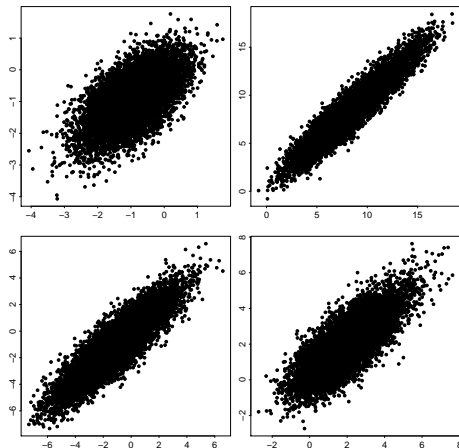
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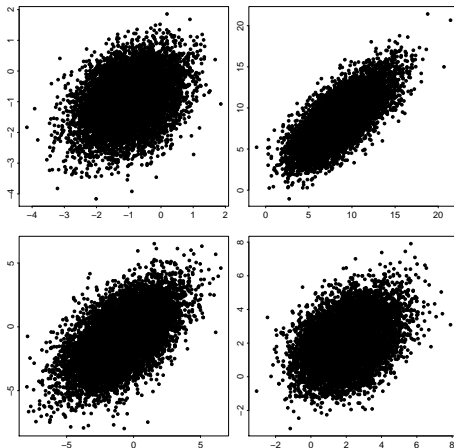
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 $\text{Cor}(\theta_j^{b-1}, \theta_j^b)$:
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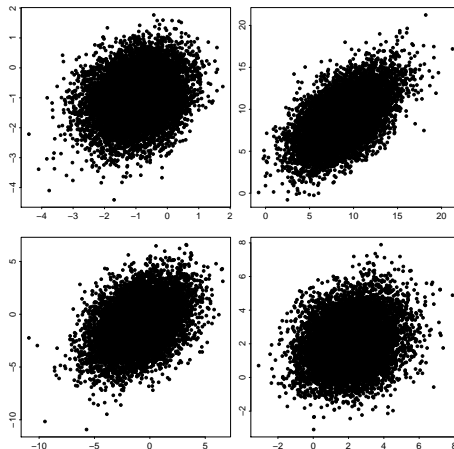
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Gibbs

Framework. We do not know how to sample the whole vector θ :

$$p(\theta \mid \mathbf{Y})$$

but we may know how to sample each coordinate (conditional on the others):

$$p(\theta_j \mid \mathbf{Y}, \theta_{-j})$$

$$\theta_{-j} = (\theta_1, \dots, \theta_{j-1}, \theta_{j+1}, \dots, \theta_p).$$

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Sampling a genotype.

- ▶ Hard to sample a whole genotype (accounting for linkage disequilibrium)
- ▶ Easy to sample the genotype at one locus, conditional on the rest of the genotype

Gibbs sampling for Bayesian inference

Algorithm. Sample $\{\boldsymbol{\theta}^b\}_{b=0,\dots,B}$ as follows.

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- ▶ At step b , for $j = 1, \dots, p$, sample θ_j^b :

$$\theta_j^b \mid \mathbf{Y}, \theta_1^b, \dots, \theta_{j-1}^b, \theta_{j+1}^{b-1}, \dots, \theta_{j+1}^{b-1}$$

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Property.

- ▶ Obviously, $p(\boldsymbol{\theta} \mid \mathbf{Y})$ is a stationary distribution.
- ▶ Does not suffices to prove ergodicity.

Outline

Statistical inference: Bayesian point-of-view

- Statistical inference: frequentist / Bayesian
- Basics of Bayes inference
- Some typical uses of Bayesian inference

Evaluating the posterior distribution: Monte-Carlo

- Conjugate priors
- Monte Carlo integration
- Monte Carlo Markov chains (MCMC)

Extensions

- Sequential Monte-Carlo (SMC)
- Approximate Bayesian computation (ABC)

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Sequential Monte-Carlo

Example: Hidden Markov models

- ▶ $\mathbf{Z} = (Z_t)_{t \leq t}$ hidden Markov chain
- ▶ $\mathbf{Y} =$ observed sequence
- ▶ $\boldsymbol{\theta} = (\Pi, \gamma)$: transition matrix and emission probabilities

Sequential Monte-Carlo

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Inference. Need to sample from

- ▶ $p(\theta | \mathbf{Y})$ (parameter inference)
- ▶ $p(\mathbf{Z} | \mathbf{Y})$ (classification)

Sequential Monte-Carlo

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Inference. Need to sample from

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Sequential Monte Carlo.

- ▶ Monte Carlo (stochastic) counterpart of the forward-backward recurrence
- ▶ Sequentially sample from $p(Z_t | \mathbf{Y}_1^t, \mathbf{Z}_1^{t-1})$.

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When the likelihood is intractable

Ex.: Population genetics. Complex demographic model for which

- ▶ we do not know how to compute the likelihood:

$$\ell(\mathbf{Y} | \boldsymbol{\theta}) \text{ intractable}$$

- ▶ but we know how to sample from it

$$\mathbf{Y}^b \sim \ell(\mathbf{Y} | \boldsymbol{\theta}).$$

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→ Importance sampling, Metropolis-Hastings, ... can not be implemented.

Principle. Get a sample $\{\theta^b\}$ such that

$$\mathbf{Y}^b \sim p(\mathbf{Y} | \theta^b) \text{ is 'similar' to } \mathbf{Y}_{\text{obs}}$$

Approximate Bayesian computation (ABC)

Ingredients.

- ▶ A set a *summary statistics* $\mathbf{s}(\mathbf{Y})$
- ▶ A 'distance' $d(\mathbf{s}, \mathbf{s}')$
- ▶ A threshold ε

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Algorithm.

- ▶ Compute $\mathbf{s}_{\text{obs}} = \mathbf{s}(\mathbf{Y}_{\text{obs}})$
- ▶ Until we get B realizations
 1. sample $\theta' \sim \pi(\theta)$ (from the prior)
 2. sample $\mathbf{Y}' \sim \ell(\mathbf{Y} | \theta')$ (from the model)
 3. compute $\mathbf{s}' = \mathbf{s}(\mathbf{Y}')$
 4. if $d(\mathbf{s}' - \mathbf{s}_{\text{obs}}) < \varepsilon$, keep θ' in the sample

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Rational. Do not sample from $p(\theta | \mathbf{Y})$ but from

$$p(\theta | d(\mathbf{s}(\mathbf{Y}) - \mathbf{s}(\mathbf{Y}_{\text{obs}})) < \varepsilon).$$

References

-  S. Jaakkola and M. I. Jordan. Bayesian parameter estimation via variational methods. *Statistics and Computing*, 10(1):25–37, 2000.
-  J.-M. Marin and Ch. P. Robert. *Bayesian Core: A Practical Approach to Computational Bayesian Statistics*. Springer-Verlag: New-York, 2007.

Outline

Appendix

Joint, Marginal, Conditional (1/2)

Reminder: 2 loci with 2 alleles each: (A, a) , (B, b)

- Joint distribution:

| | B | b | marginal |
|----------|-------------------------|-------------------------|---|
| A | f_{AB} | f_{Ab} | $p_A = f_{AB} + f_{Ab}$ |
| a | f_{aB} | f_{ab} | $p_a = f_{aB} + f_{ab}$ |
| marginal | $q_B = f_{AB} + f_{aB}$ | $q_b = f_{Ab} + f_{ab}$ | $f_{AB} + f_{Ab} + f_{aB} + f_{ab} = 1$ |

- Marginal distribution: 'integrate out' the allele of the other locus

$$\Pr\{B\} = q_B = f_{AB} + f_{aB}$$

- Conditional distribution: fix the allele of the other locus

$$\Pr\{A|b\} = \frac{\Pr\{A, b\}}{\Pr\{b\}} = \frac{f_{Ab}}{q_b} = \frac{f_{Ab}}{f_{Ab} + f_{ab}}$$

Joint, Marginal, Conditional (2/2)

Continuous case: 2 continuous random variables X and Y

- Joint distribution:

| | y | marginal |
|----------|---------------------------------|---------------------------------|
| x | $p_{XY}(x, y)$ | $p_X(x) = \int p_{XY}(x, y) dy$ |
| marginal | $p_Y(y) = \int p_{XY}(x, y) dx$ | $\int p_{XY}(x, y) dx dy = 1$ |

- Marginal distribution: 'integrate out' the other variable

$$p_X(x) = \int p_{XY}(x, y) dy$$

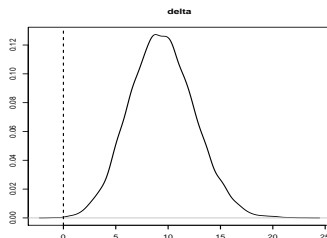
- Conditional distribution: fix the value of the other variable

$$p_{Y|X=x}(y) = \frac{p_{XY}(x, y)}{p_X(x)} = \frac{p_{XY}(x, y)}{\int p_{XY}(x, y) dy}$$

Posterior distribution and CI

The same holds for combination of parameters, e.g.

$$\delta = \theta_2 - \theta_3$$



| | post.mean | post.mode | lower.CI | upper.CI |
|-------|-----------|-----------|----------|----------|
| delta | 9.523487 | 9.45102 | 3.628611 | 15.78938 |

Monte Carlo: Illustration (1/3)

Example. $\pi(\theta) = \mathcal{N}(0, 10)$, $g(\theta) = e^\theta$:

- ▶ `theta.sample = rnorm(M, mean=0, sd=sqrt(10))`
- ▶ `mean(exp(theta.sample))`

Monte Carlo: Illustration (2/3)

Properties.

- Easy to implement

```
mean(exp(rnorm(M, mean=0, sd=sqrt(10))))
```

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- ▶ Precision proportional to $1/\sqrt{M}$

Monte Carlo: Illustration (2/3)

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- ▶ Unbiased: $\mathbb{E} \left[\widehat{\mathbb{E}}(g(\boldsymbol{\theta})) \right] = \mathbb{E}(g(\boldsymbol{\theta}))$
- ▶ Precision proportional to $1/\sqrt{M}$
- ▶ Still, very variant in practice (see next)

Monte Carlo: Illustration (3/3)

$$\theta \sim \mathcal{N}(0, 10), \quad g(\theta) = e^{\theta}$$

| | mean | sd |
|-------|--------|--------|
| 1000 | 194.67 | 338.96 |
| 10000 | 139.63 | 47.24 |
| 1e+05 | 155.65 | 86.93 |
| 1e+06 | 147.76 | 15.68 |
| truth | 148.41 | — |

