An introduction to Bayesian statistical inference

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Outline

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An example

Example:

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

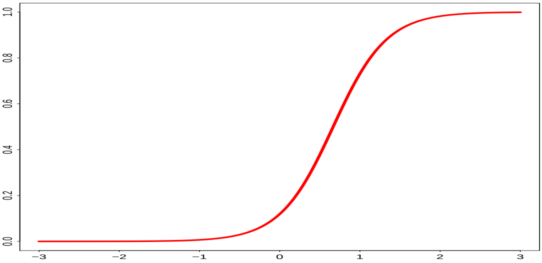
A statistical model

Logistic regression Logistic regression

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

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

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



Frequentist inference

$\boldsymbol{\theta}$ = fixed parameter:

- Statistical model:

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

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

$$\widehat{\boldsymbol{\theta}}: \qquad \log p_{\widehat{\boldsymbol{\theta}}}(\mathbf{Y}) = \max_{\boldsymbol{\theta}} \log p_{\boldsymbol{\theta}}(\mathbf{Y})$$

- The estimate $\widehat{\boldsymbol{\theta}}$ itself is random (depends on the data) $\rightarrow$ 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

$\boldsymbol{\theta}$ = random parameter:

- Statistical model:

$$\ell(\mathbf{Y} \mid \boldsymbol{\theta}) := p(\mathbf{Y} \mid \boldsymbol{\theta}) \qquad (= \textit{likelihood})$$

- Inference: provide the conditional distribution of $\boldsymbol{\theta}$ given the observed data $\mathbf{Y}$:

$$p(\boldsymbol{\theta} \mid \mathbf{Y}) \qquad (= \textit{posterior} \text{ distribution})$$

  $\rightarrow$ credibility intervals

- Requires to define a marginal distribution:

$$\pi(\boldsymbol{\theta}) := p(\boldsymbol{\theta}) \qquad (= \textit{prior} \text{ distribution})$$

Outline

Why 'Bayes'

Bayes formula:

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

- $P(B)$ = marginal probability of B
- $P(A, B)$ = joint probability of A and B
- $P(A \mid B)$ = conditional probability of A given B [# 55]

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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.

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

$\rightarrow$ Requires to evaluate the *integrated likelihood* (i.e. marginal)

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

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

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$$p(\boldsymbol{\theta} \,|\, \mathbf{Y}) = \frac{\pi(\boldsymbol{\theta})\; \ell(\mathbf{Y} \,|\, \boldsymbol{\theta})}{p(\mathbf{Y})} \qquad \Leftrightarrow \qquad [\boldsymbol{\theta} \,|\, \mathbf{Y}] = \frac{[\boldsymbol{\theta}]\; [\mathbf{Y} \,|\, \boldsymbol{\theta}]}{[\mathbf{Y}]}$$

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3. Obviously

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

$\rightarrow$ $p(\boldsymbol{\theta} \mid \mathbf{Y})$ and $p(\boldsymbol{\theta}' \mid \mathbf{Y})$ can be compared, without computing $p(\mathbf{Y})$

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

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

The posterior depends on the prior

Data & Model:

- $Y_i = 1$ if sick, 0 otherwise
- $n = 10$ patients
- $\vdots$: number sicks $/n$

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Param:

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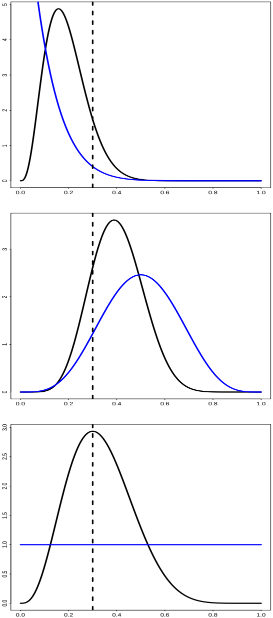

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- ⋮ : number sicks $/n$

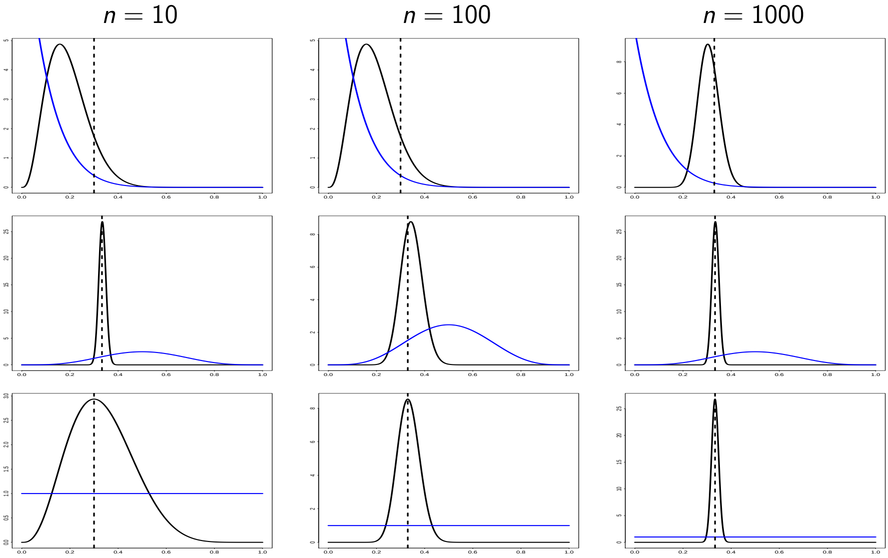
Param:

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

Output:

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

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 $\boldsymbol{\theta}$:

$$\Pr\{Y_i = 1 \,|\, \boldsymbol{\theta}\} = e^{\mathbf{x}_i^\intercal \boldsymbol{\theta}} \Big/ \left(1 + e^{\mathbf{x}_i^\intercal \boldsymbol{\theta}}\right)$$

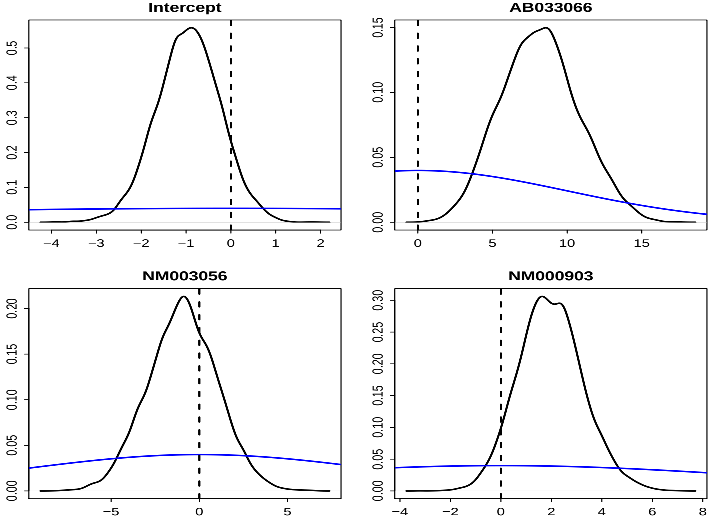
Inference:

$$\boldsymbol{\theta} \,|\, \mathbf{Y} \sim ?$$

(see later, but $p(\boldsymbol{\theta} \,|\, \mathbf{Y}) \neq \mathcal{N}(\cdot, \cdot)$, for sure.)

Bayesian inference

Output:



Outline

Posterior distribution and confidence intervals

Parameter 'estimate'.

$$\text{posterior mean:} \qquad \widehat{\theta}_j = \mathbb{E}(\theta_j \mid \mathbf{Y})$$
$$\text{posterior mode:} \qquad \widehat{\theta}_j = \arg\max_{\theta_j} \; p(\theta_j \mid \mathbf{Y})$$

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

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

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Example. [# 4]

	post.mean	post.mode	lower.CI	upper.CI
Intercept	-0.9816181	-0.8652166	-2.41342	0.3704264
AB033066	8.395169	8.587083	3.271464	13.98373
NM003056	-1.042483	-0.9854149	-5.046639	2.819764
NM000903	1.911312	1.677234	-0.4240319	4.452512

Accounting for uncertainty

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

Model answer:

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

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

Bayesian answer: *posterior predictive* probability

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

Model comparison (1/2)

Problem. Which model fits the data better:

$$M_0 : \text{none of the genes has an effect, i.e. } \boldsymbol{\theta} = (\theta_0, 0, \dots, 0)$$
$$M_1 : \text{only the fist gene has an effect, i.e. } \boldsymbol{\theta} = (\theta_0, \theta_1, 0, \dots, 0)$$
$$\dots$$
$$M_p : \text{all genes have an effect, i.e. } \boldsymbol{\theta} = (\theta_0, \theta_1, \dots, \theta_p)$$

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

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

Model comparison (2/2)

Ingredients:

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

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

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

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

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Recipe:

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

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

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

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

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

Model averaging (uncertainty on models)

Question: Probability for patient 0 to be sick?

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Model selection.

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

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

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Model averaging.

- Keep all models
- Compute

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

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:

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

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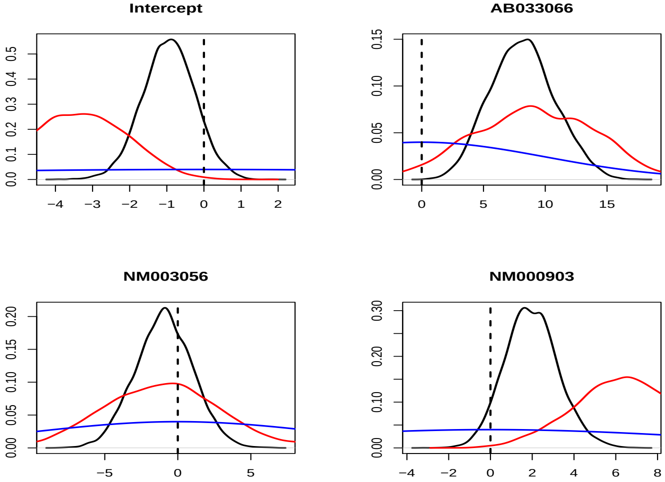
In practice:

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

Combining experiments

Output: $n_1 = n_2 = 39$



Outline

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: $f(\boldsymbol{\theta}) = \theta_j^2$ $\qquad$ ($+$ posterior mean)

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Main problem: evaluate

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

which requires to evaluate

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

Outline

Nice case: Conjugate priors

Example: Bernoulli[1]

Prior: $\theta =$ probability to be sick.

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

[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

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

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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	$\alpha,\, \beta$	$\alpha + \sum_{i=1}^n x_i,\, \beta + n - \sum_{i=1}^n x_i$	$\alpha - 1$ successes, $\beta - 1$ failures[note 1]	$p(\tilde{x} = 1) = \frac{\alpha'}{\alpha' + \beta'}$
Binomial	p (probability)	Beta	$\alpha,\, \beta$	$\alpha + \sum_{i=1}^n x_i,\, \beta + \sum_{i=1}^n N_i - \sum_{i=1}^n x_i$	$\alpha - 1$ successes, $\beta - 1$ failures[note 1]	$\operatorname{BetaBin}(\tilde{x}\mid\alpha', \beta')$ (beta-binomial)
Negative Binomial with known failure number r	p (probability)	Beta	$\alpha,\, \beta$	$\alpha + \sum_{i=1}^n x_i,\, \beta + rn$	$\alpha - 1$ total successes, $\beta - 1$ failures[note 1] (i.e. $\frac{\beta - 1}{r}$ experiments, assuming r stays fixed)	
Poisson	λ (rate)	Gamma	$k,\, \theta$	$k + \sum_{i=1}^n x_i,\; \frac{\theta}{n\theta + 1}$	k total occurrences in $1/\theta$ intervals	$\operatorname{NB}(\tilde{x}\mid k', \frac{\theta'}{1+\theta'})$ (negative binomial)
Poisson	λ (rate)	Gamma	$\alpha,\, \beta$ [note 3]	$\alpha + \sum_{i=1}^n x_i,\; \beta + n$	α total occurrences in β intervals	$\operatorname{NB}(\tilde{x}\mid \alpha', \frac{1}{1+\beta'})$ (negative binomial)
Categorical	$\boldsymbol{p}$ (probability vector), k (number of categories, i.e. size of $\boldsymbol{p}$)	Dirichlet	$\boldsymbol{\alpha}$	$\boldsymbol{\alpha} + (c_1, \ldots, c_k)$, 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	$\boldsymbol{p}$ (probability vector), k (number of categories, i.e. size of $\boldsymbol{p}$)	Dirichlet	$\boldsymbol{\alpha}$	$\boldsymbol{\alpha} + \sum_{i=1}^n \mathbf{x}_i$	$\alpha_i - 1$ occurrences of category i[note 1]	$\operatorname{DirMult}(\tilde{\mathbf{x}}\mid\boldsymbol{\alpha}')$ (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	$\alpha,\, \beta$	$\alpha + n,\, \beta + \sum_{i=1}^n x_i$	$\alpha - 1$ 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	$\mu_0,\ \sigma_0^2$	$\left(\frac{\mu_0}{\sigma_0^2}+\frac{\sum_{i=1}^n x_i}{\sigma^2}\right)\Big/\left(\frac{1}{\sigma_0^2}+\frac{n}{\sigma^2}\right),$ $\left(\frac{1}{\sigma_0^2}+\frac{n}{\sigma^2}\right)^{-1}$	mean was estimated from observations with total precision (sum of all individual precisions) $1/\sigma_0^2$ and with sample mean μ_0	$\mathcal{N}(\tilde{x}\mid\mu_0',\sigma_0^{2\prime}+\sigma^2)$[5]
Normal with known precision τ	μ (mean)	Normal	$\mu_0,\ \tau_0$	$\left(\tau_0\mu_0+\tau\sum_{i=1}^n x_i\right)\Big/(\tau_0+n\tau),\ \tau_0+n\tau$	mean was estimated from observations with total precision (sum of all individual precisions) τ_0 and with sample mean μ_0	$\mathcal{N}\left(\tilde{x}\mid\mu_0',\frac{1}{\tau_0'}+\frac{1}{\tau}\right)$[5]
Normal with known mean μ	σ^2 (variance)	Inverse gamma	$\alpha,\ \beta$ [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)	$t_{2\alpha'}(\tilde{x}\mid\mu,\sigma^2=\beta'/\alpha')$[5]
Normal with known mean μ	σ^2 (variance)	Scaled inverse chi-squared	$\nu,\ \sigma_0^2$	$\nu+n,\ \frac{\nu\sigma_0^2+\sum_{i=1}^n(x_i-\mu)^2}{\nu+n}$	variance was estimated from ν observations with sample variance σ_0^2	$t_{\nu'}(\tilde{x}\mid\mu,\sigma_0^{2\prime})$[5]
Normal with known mean μ	τ (precision)	Gamma	$\alpha,\ \beta$[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)	$t_{2\alpha'}(\tilde{x}\mid\mu,\sigma^2=\beta'/\alpha')$[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	$t_{2\alpha'}\left(\tilde{x}\mid\mu',\frac{\beta'(\nu'+1)}{\alpha'\nu'}\right)$[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	$t_{2\alpha'}\left(\tilde{x}\mid\mu',\frac{\beta'(\nu'+1)}{\alpha'\nu'}\right)$[5]
Multivariate normal with known covariance matrix $\boldsymbol{\Sigma}$	$\boldsymbol{\mu}$ (mean vector)	Multivariate normal	$\boldsymbol{\mu}_0,\ \boldsymbol{\Sigma}_0$	$\left(\boldsymbol{\Sigma}_0^{-1}+n\boldsymbol{\Sigma}^{-1}\right)^{-1}\left(\boldsymbol{\Sigma}_0^{-1}\boldsymbol{\mu}_0+n\boldsymbol{\Sigma}^{-1}\bar{\mathbf{x}}\right),$ $\left(\boldsymbol{\Sigma}_0^{-1}+n\boldsymbol{\Sigma}^{-1}\right)^{-1}$ ▪ $\bar{\mathbf{x}}$ is the sample mean	mean was estimated from observations with total precision (sum of all individual precisions) $\boldsymbol{\Sigma}_0^{-1}$ and with sample mean $\boldsymbol{\mu}_0$	$\mathcal{N}(\tilde{\mathbf{x}}\mid\boldsymbol{\mu}_0',\boldsymbol{\Sigma}_0'+\boldsymbol{\Sigma})$[5]

en.wikipedia.org/wiki/Conjugate_prior

Outline

Computing integrals

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

Goal: compute

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

where

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

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We need to evaluate integrals of the form

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

Monte Carlo

Principle. To evaluate

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In practice:

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

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

- 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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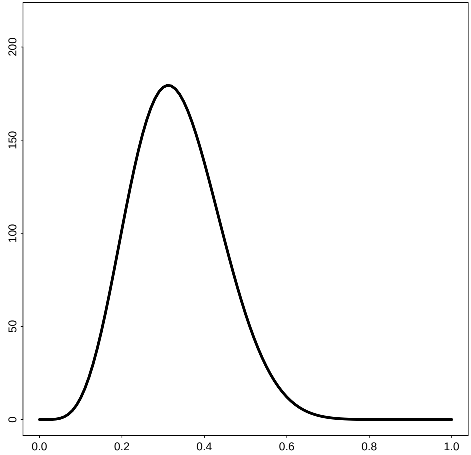
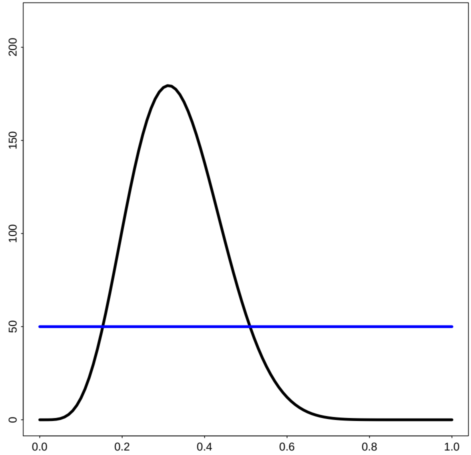
$\rightarrow$ unbiased estimate of $\mathbb{E}[f(\boldsymbol{\theta})]$ with variance $\propto \sum_m W(\theta^m)^2/M$.

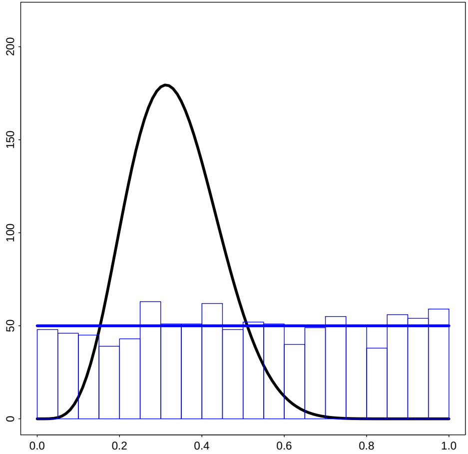
Importance Sampling (a picture)



Importance Sampling (a picture)



Importance Sampling (a picture)



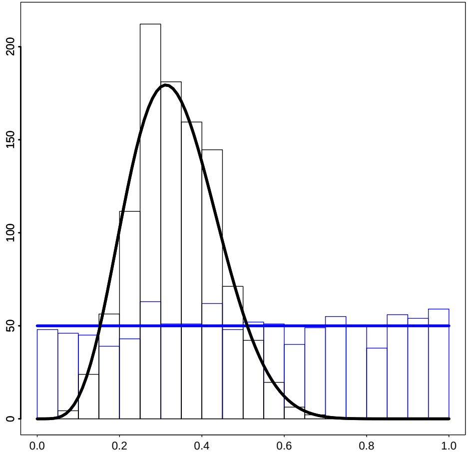
Importance Sampling (a picture)

Efficiency of sampling:

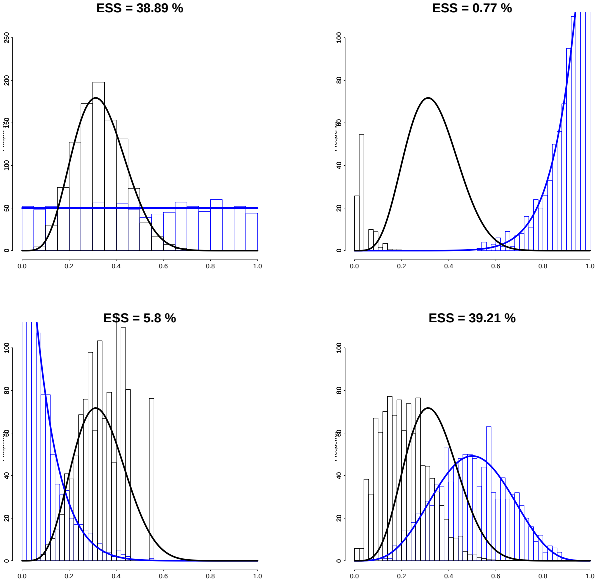
$$ESS = \overline{W}^2 / \overline{W^2}$$

$q' = q$

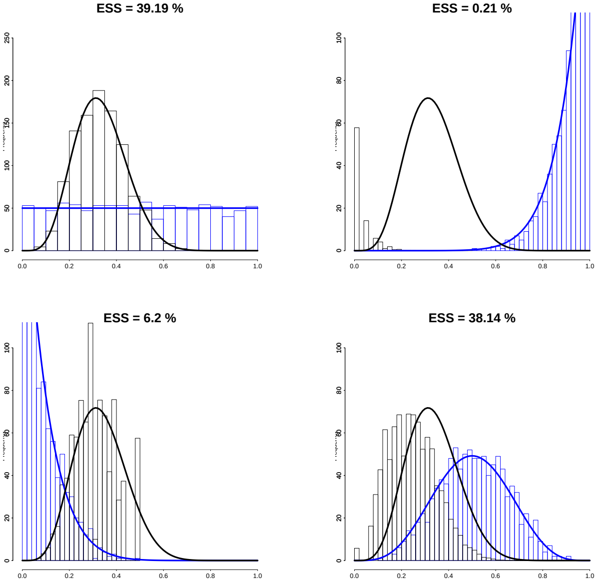
$$\Rightarrow \quad ESS = 1$$



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

$$\mathbb{E}[f(\boldsymbol{\theta}) \mid \mathbf{Y}] = \int f(\boldsymbol{\theta}) p(\boldsymbol{\theta}, \mathbf{Y}) \, \mathrm{d}\boldsymbol{\theta} \Big/ p(\mathbf{Y}) \; = \; \dots$$
$$= \int f(\boldsymbol{\theta}) \frac{\pi(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathbf{Y})}{q(\boldsymbol{\theta})} q(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta} \Big/ \int \frac{\pi(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathbf{Y})}{q(\boldsymbol{\theta})} q(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta}$$

1. sample
$$(\boldsymbol{\theta}^1, \dots, \boldsymbol{\theta}^M) \text{ iid } \sim q$$
2. compute the weights
$$W(\boldsymbol{\theta}^m) = \pi(\boldsymbol{\theta}^m) p(\boldsymbol{\theta}^m \mid \mathbf{Y}) \, / q(\boldsymbol{\theta}^m)$$
3. get
$$\widehat{\mathbb{E}}[f(\boldsymbol{\theta}) \mid \mathbf{Y}] = \sum_m W(\boldsymbol{\theta}^m) f(\boldsymbol{\theta}^m) \Big/ \sum_m W(\boldsymbol{\theta}^m)$$

$\rightarrow$ slightly biased.

Good proposals

Choosing q is critical

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Typical choices

- Prior

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

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

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- MLE:

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

$\rightarrow$ fine, as long as MLE is available

Good proposals

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Typical choices

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$$q(\boldsymbol{\theta}) = \mathcal{N}(\widehat{\boldsymbol{\theta}}_{MLE}, \mathbb{V}_\infty(\widehat{\boldsymbol{\theta}}_{MLE}))$$
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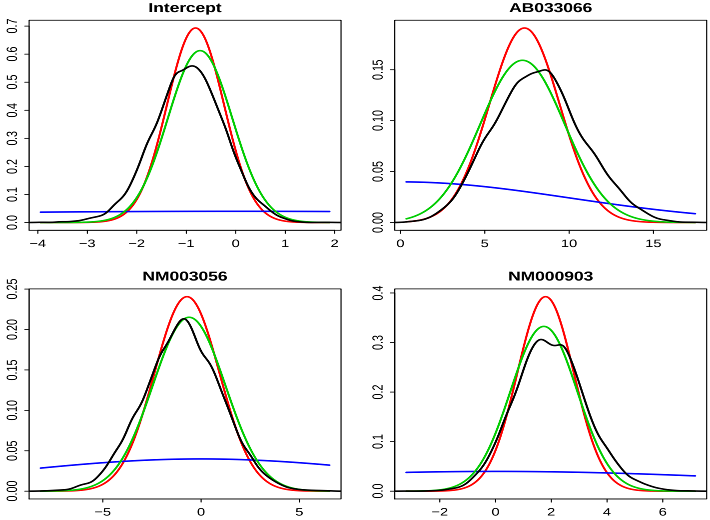
- Variational Bayes, expectation propagation, ...:
$$q(\boldsymbol{\theta}) = \arg\min_{q \in \mathcal{Q}} KL\left[q(\boldsymbol{\theta}) \,||\, p(\boldsymbol{\theta} \mid \mathbf{Y}\right]$$
$\rightarrow$ fast and reasonably accurate

Variational Bayes as prior

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



Outline

Limit distribution of Markov chain

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

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

$$p\left(\{\phi^t\}\right) = \nu(\phi^0) \times \kappa(\phi^1 \mid \phi^0) \times \kappa(\phi^2 \mid \phi^1) \times \kappa(\phi^3 \mid \phi^2) \times \dots$$

then

- it admits a unique stationary distribution μ:

$$\phi^{t-1} \sim \mu \qquad \Rightarrow \qquad \phi^t \sim \mu$$

- ϕ^t converges towards μ in distribution

$$\phi^t \xrightarrow[t\to\infty]{\Delta} \mu$$

for any initial distribution ν

Use for Bayesian inference

Aim. Sample from

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

Idea.

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

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

- Choose 'any' initial ν and simulate $\{\boldsymbol{\theta}^t\}_{t \geq 0}$

- Until it 'reaches' its stationary distribution

Metropolis-Hastings

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

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  1. sample $\boldsymbol{\theta}' \sim \lambda(\cdot \mid \boldsymbol{\theta}^{t-1})$;

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  2. compute the Metropolis-Hastings ratio (acceptance probability)

$$\alpha(\boldsymbol{\theta}', \boldsymbol{\theta}^{t-1}) = \frac{\lambda(\boldsymbol{\theta}^{t-1} \mid \boldsymbol{\theta}')}{\lambda(\boldsymbol{\theta}' \mid \boldsymbol{\theta}^{t-1})} \frac{p(\boldsymbol{\theta}' \mid \mathbf{Y})}{p(\boldsymbol{\theta}^{t-1} \mid \mathbf{Y})}$$

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Properties.

1. λ and α defined a Markov chain with stationary distribution $\mu(\boldsymbol{\theta}) = p(\boldsymbol{\theta} \mid \mathbf{Y})$.
2. If $\lambda(\cdot \mid \boldsymbol{\theta})$ is symmetric, α reduce to $\pi(\boldsymbol{\theta}')\ell(\mathbf{Y} \mid \boldsymbol{\theta}')/[\pi(\boldsymbol{\theta}^{t-1})\ell(\mathbf{Y} \mid \boldsymbol{\theta}^{t-1})]$

Metropolis-Hastings for logistic regression

Model.

$$\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}_p, 100\,\mathbf{I}_p)$$

$$\mathbf{Y} \,|\, \boldsymbol{\theta} \sim \ell(\mathbf{Y} \,|\, \boldsymbol{\theta}) = \prod_i \left(\frac{e^{\mathbf{x}_i^\intercal \boldsymbol{\theta}}}{1 + e^{\mathbf{x}_i^\intercal \boldsymbol{\theta}}}\right)^{y_i} \left(\frac{e^{\mathbf{x}_i^\intercal \boldsymbol{\theta}}}{1 + e^{\mathbf{x}_i^\intercal \boldsymbol{\theta}}}\right)^{1-y_i}$$

Metropolis-Hastings for logistic regression

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Property.

Gibbs

Outline

Outline

Outline

When the likelihood is intractable

References

Outline

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

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

Joint, Marginal, Conditional (2/2)

Continuous case: 2 continuous random variables X and Y

- Joint distribution:

	y	marginal
x	$p_{XY}(x,y)$	$p_X(x) = \int p_{XY}(x,y)\,\mathrm{d}y$
marginal	$p_Y(y) = \int p_{XY}(x,y)\,\mathrm{d}x$	$\int p_{XY}(x,y)\,\mathrm{d}x\,\mathrm{d}y = 1$

- Marginal distribution: 'integrate out' the other variable

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

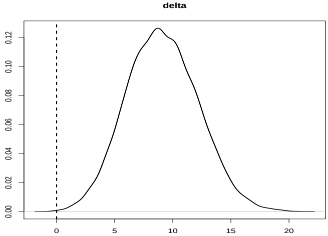
- Conditional distribution: fix the value of the other variable

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

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	9.389825	8.824822	3.539045	15.84367

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))))
```

Monte Carlo: Illustration (2/3)

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- Easy to implement

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

- Unbiased: $\mathbb{E}\left[\widehat{\mathbb{E}}(g(\boldsymbol{\theta}))\right] = \mathbb{E}(g(\boldsymbol{\theta}))$

Monte Carlo: Illustration (2/3)

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- Easy to implement

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

- Unbiased: $\mathbb{E}\left[\widehat{\mathbb{E}}(g(\boldsymbol{\theta}))\right] = \mathbb{E}(g(\boldsymbol{\theta}))$
- Precision proportional to $1/\sqrt{M}$

Monte Carlo: Illustration (2/3)

Properties.

- Easy to implement

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

- 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	–