

# An introduction to Bayesian statistical inference

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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)

## Reminder: 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

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

('Bayes formula')

## Reminder: Joint, marginal, conditional (2/2)

**Continuous case:** 2 continuous random variables  $U$  and  $V$

- Joint distribution:

	$v$	marginal
$u$	$p_{UV}(u, v)$	$p_U(u) = \int p_{UV}(u, v) dv$
marginal	$p_V(v) = \int p_{UV}(u, v) du$	$\int p_{UV}(u, v) du dv = 1$

- Marginal distribution: 'integrate out' the other variable

$$p_U(u) = \int p_{UV}(u, v) dv$$

- Conditional distribution: fix the value of the other variable

$$p_{V|U=u}(v) = \frac{p_{UV}(u, v)}{p_U(u)} = \frac{p_{UV}(u, v)}{\int p_{UV}(u, v) dv}$$

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## An example

### Example:

- ▶  $n$  tissue samples:  $i = 1 \dots n$
- ▶  $Y_i = \text{status}$  (0 = n, normal = tumor) of sample  $i$
- ▶  $\mathbf{x}_i = (x_{i1}, \dots, x_{ip}) = \text{vector of gene expression for sample } i \text{ (gene } j = 1 \dots p)$

**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
	 X				 Y

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Similar question for genotyping data:  $x_{ij} \in \{0, 1, 2\}$ .



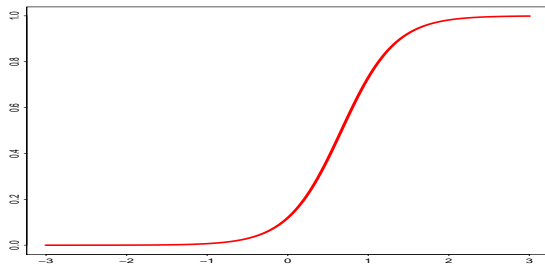
## A statistical model

**Model:** Logistic regression

- ▶ The samples are independent.
- ▶ The probability for sample  $i$  to be tumor 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

$\theta$  = 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)  $\rightarrow$  conf. 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

$\theta$  = random parameter:

- ▶ Statistical model:

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

- ▶ Inference: provide the conditional distribution of  $\theta$  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  $B$
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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 acts as the normalizing constant of the posterior  $p(\boldsymbol{\theta} | \mathbf{Y})$ .



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

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

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

# The posterior depends on the prior

## Data & Model:

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

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

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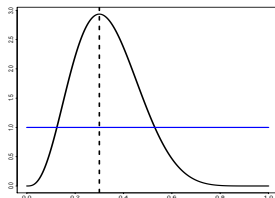
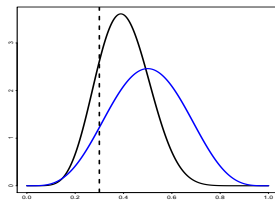
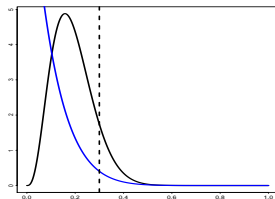
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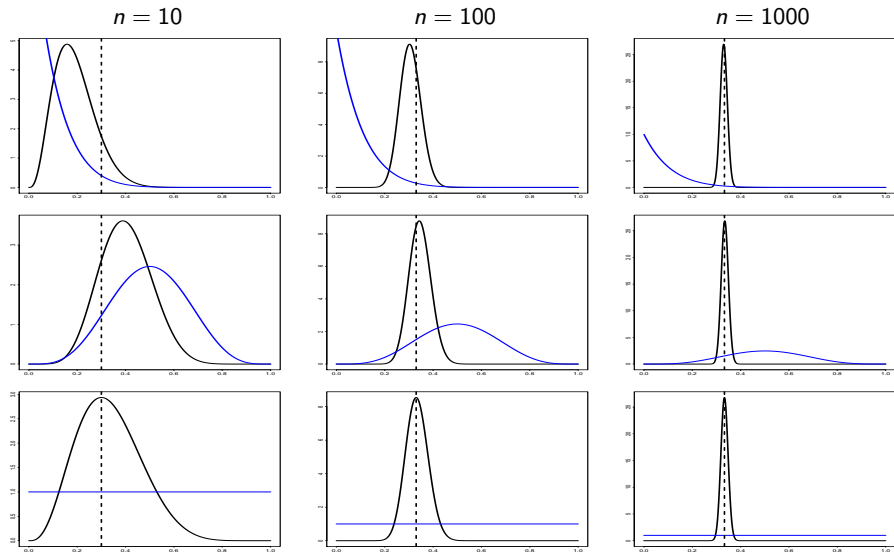
## Output:

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





# Dependency vanishes when $n$ increases



## Back to logistic regression

### Model

- Prior: coefficients  $\theta_j$  all independent:

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

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

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

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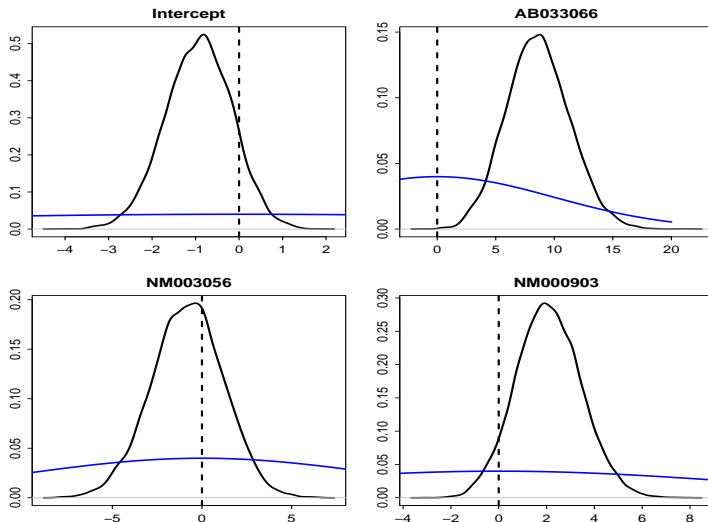
### Inference:

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

(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  $\theta$  is random:  $P(H_0 | \mathbf{Y}) = 0$

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Parameter estimate. For the same reason:

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

(because  $\theta$  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%):

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

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**Example.** [# ??]

	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 sample 0 (with profile  $\mathbf{x}_0$ ) to be tumor?

**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  $M$ :

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

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

- 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)

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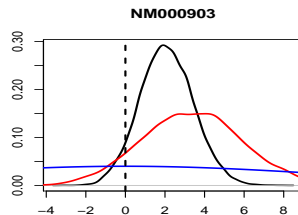
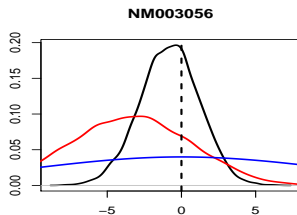
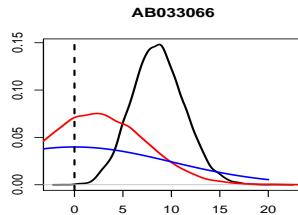
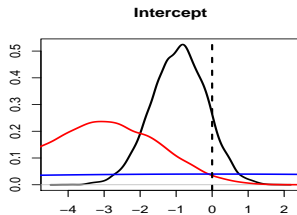
$$p(\theta | \mathbf{Y}_1, \mathbf{Y}_2) = \frac{p(\theta | \mathbf{Y}_1)p(\mathbf{Y}_2 | \theta, \mathbf{Y}_1)}{p(\mathbf{Y}_2 | \mathbf{Y}_1)}$$

**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)



## Posterior distribution

**Aim:** Evaluate

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

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

**Main problem:** evaluate

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

which requires to evaluate

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

# 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)

## Nice case: Conjugate priors

Example: Bernoulli<sup>1</sup>

**Prior:**  $\theta$  = probability to carry a disease.

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

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

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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

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

---

<sup>1</sup>#15: 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 <sup>[note 1]</sup>	Posterior predictive <sup>[note 2]</sup>
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 <sup>[note 1]</sup>	$p(\tilde{x} = 1) = \frac{\alpha'}{\alpha' + \beta'}$
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 <sup>[note 1]</sup>	BetaBin( $\tilde{x} \alpha', \beta'$ ) (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 <sup>[note 1]</sup> (i.e. $\frac{\beta-1}{r}$ experiments, assuming $r$ stays fixed)	
Poisson	$\lambda$ (rate)	Gamma	$k, \theta$	$k + \sum_{i=1}^n x_i, \frac{\theta}{n\theta + 1}$	$k$ total occurrences in $1/\theta$ intervals	NB( $\tilde{x} k', \frac{\theta'}{1+\theta'}$ ) (negative binomial)
Poisson	$\lambda$ (rate)	Gamma	$\alpha, \beta$ <sup>[note 3]</sup>	$\alpha + \sum_{i=1}^n x_i, \beta + n$	$\alpha$ total occurrences in $\beta$ intervals	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 $i$ <sup>[note 1]</sup>	$p(\tilde{x} = i) = \frac{\alpha_i'}{\sum_i \alpha_i'}$ $= \frac{\alpha_i + c_i}{\sum_i \alpha_i + n}$
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 $i$ <sup>[note 1]</sup>	DirMult( $\tilde{\mathbf{x}} \boldsymbol{\alpha}'$ ) (Dirichlet-multinomial)
Hypergeometric with known total population size $N$	$M$ (number of target members)	Beta-binomial <sup>[4]</sup>	$n = N, \alpha, \beta$	$\alpha + \sum_{i=1}^n x_i, \beta + \sum_{i=1}^n N_i - \sum_{i=1}^n x_i$	$\alpha - 1$ successes, $\beta - 1$ failures <sup>[note 1]</sup>	
Geometric	$p_0$ (probability)	Beta	$\alpha, \beta$	$\alpha + n, \beta + \sum_{i=1}^n x_i$	$\alpha - 1$ experiments, $\beta - 1$ total failures <sup>[note 1]</sup>	

[en.wikipedia.org/wiki/Conjugate\\_prior](https://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 <sup>[note 4]</sup>
Normal with known variance $\sigma^2$	$\mu$ (mean)	Normal	$\mu_0, \sigma_0^2$	$\left( \frac{\mu_0}{\sigma_0^2} + \frac{\sum_{i=1}^n x_i}{\sigma^2} \right) / \left( \frac{1}{\sigma_0^2} + \frac{n}{\sigma^2} \right),$ $\left( \frac{1}{\sigma_0^2} + \frac{n}{\sigma^2} \right)^{-1}$	mean was estimated from observations with total precision (sum of all individual precisions) $1/\sigma_0^2$ and with sample mean $\mu_0$	$\mathcal{N}(\tilde{x}   \mu'_0, \sigma_0'^2 + \sigma^2)^{[5]}$
Normal with known precision $\tau$	$\mu$ (mean)	Normal	$\mu_0, \tau_0$	$\left( \tau_0 \mu_0 + \tau \sum_{i=1}^n x_i \right) / (\tau_0 + n\tau), \tau_0 + n\tau$	mean was estimated from observations with total precision (sum of all individual precisions) $\tau_0$ and with sample mean $\mu_0$	$\mathcal{N}\left(\tilde{x}   \mu'_0, \frac{1}{\tau_0} + \frac{1}{\tau}\right)^{[5]}$
Normal with known mean $\mu$	$\sigma^2$ (variance)	Inverse gamma	$\alpha, \beta$ <sup>[note 5]</sup>	$\alpha + \frac{n}{2}, \beta + \frac{\sum_{i=1}^n (x_i - \mu)^2}{2}$	variance was estimated from $2\alpha$ observations with sample variance $\beta/\alpha$ (i.e. with sum of squared deviations $2\beta$ , where deviations are from known mean $\mu$ )	$t_{2\alpha'}(\tilde{x}   \mu, \sigma^2 = \beta'/\alpha')^{[5]}$
Normal with known mean $\mu$	$\sigma^2$ (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 $\nu$ observations with sample variance $\sigma_0^2$	$t_{\nu'}(\tilde{x}   \mu, \sigma_0'^2)^{[5]}$
Normal with known mean $\mu$	$\tau$ (precision)	Gamma	$\alpha, \beta$ <sup>[note 3]</sup>	$\alpha + \frac{n}{2}, \beta + \frac{\sum_{i=1}^n (x_i - \mu)^2}{2}$	precision was estimated from $2\alpha$ observations with sample variance $\beta/\alpha$ (i.e. with sum of squared deviations $2\beta$ , where deviations are from known mean $\mu$ )	$t_{2\alpha'}(\tilde{x}   \mu, \sigma^2 = \beta'/\alpha')^{[5]}$
Normal <sup>[note 6]</sup>	$\mu$ and $\sigma^2$ 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 $\nu$ observations with sample mean $\mu_0$ ; variance was estimated from $2\alpha$ observations with sample mean $\mu_0$ and sum of squared deviations $2\beta$	$t_{2\alpha'}\left(\tilde{x}   \mu', \frac{\beta'(\nu' + 1)}{\alpha'\nu'}\right)^{[5]}$
Normal	$\mu$ and $\tau$ 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 $\nu$ observations with sample mean $\mu_0$ , and precision was estimated from $2\alpha$ observations with sample mean $\mu_0$ and sum of squared deviations $2\beta$	$t_{2\alpha'}\left(\tilde{x}   \mu', \frac{\beta'(\nu' + 1)}{\alpha'\nu'}\right)^{[5]}$
Multivariate normal with known covariance matrix $\Sigma$	$\boldsymbol{\mu}$ (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) $\Sigma_0^{-1}$ and with sample mean $\boldsymbol{\mu}_0$	$\mathcal{N}(\bar{\mathbf{x}}   \boldsymbol{\mu}', \Sigma_0' + \Sigma)^{[5]}$

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## 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

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where

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

We need to evaluate integrals of the form

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

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Principle. To evaluate

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

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



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Main trick = weighting particles.

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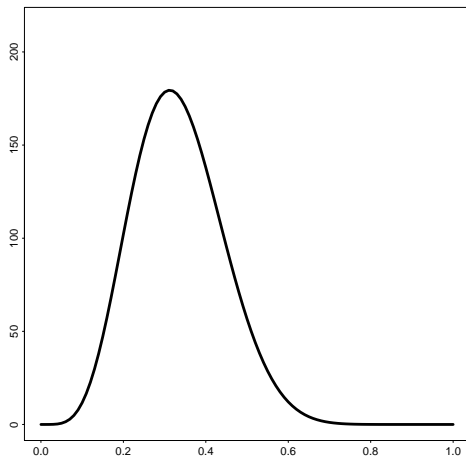
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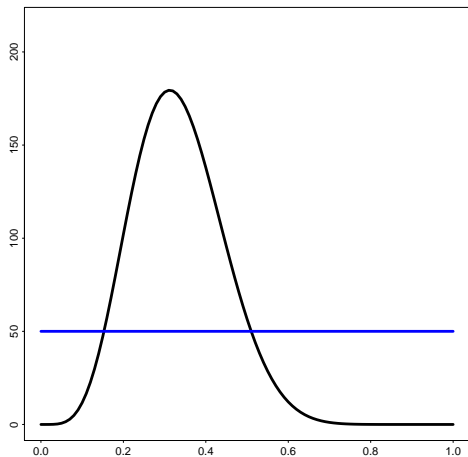
$$\widehat{\mathbb{E}}[f(\boldsymbol{\theta})] = \frac{1}{B} \sum_b W(\boldsymbol{\theta}^b)f(\boldsymbol{\theta}^b)$$

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

## Importance Sampling (a picture)

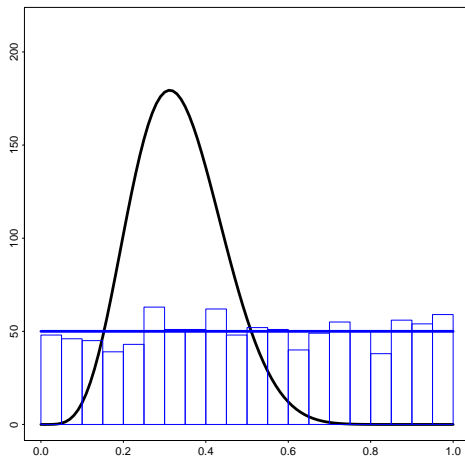


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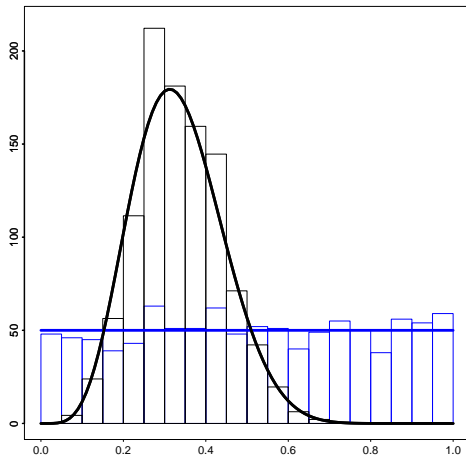
# Importance Sampling (a picture)

Efficiency of sampling:

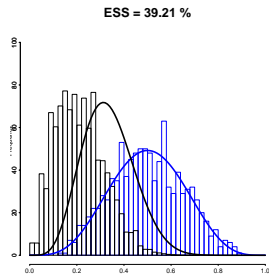
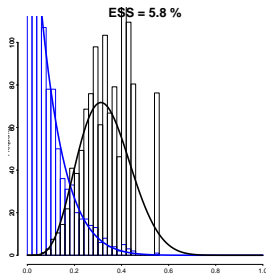
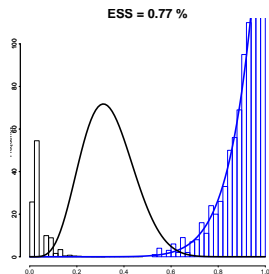
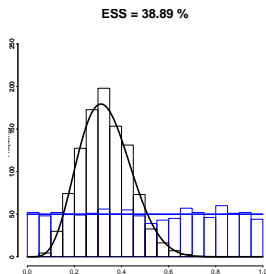
$$ESS = \overline{W}^2 / \overline{W^2}$$

$$q' = q$$

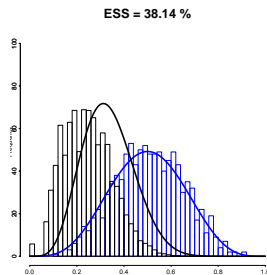
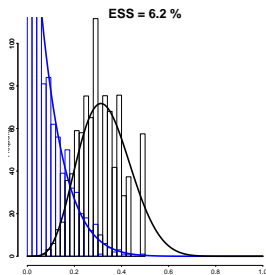
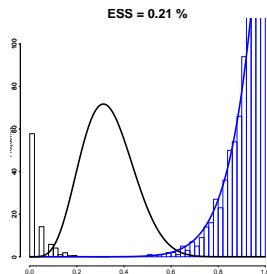
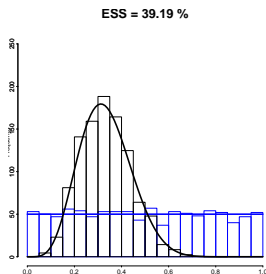
$$\Rightarrow ESS = 1$$



# 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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- MLE:

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

→ fine, as long as MLE is available



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Choosing  $q$  is critical

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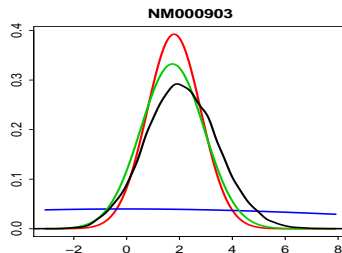
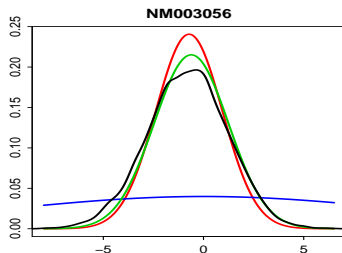
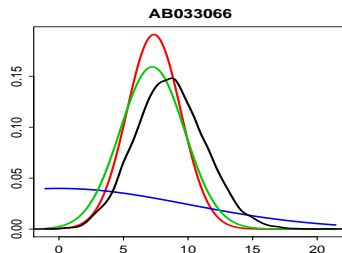
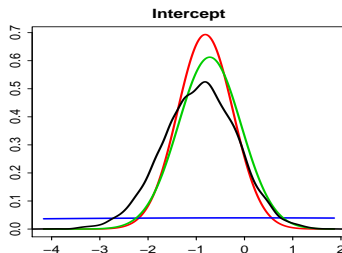
- Variational Bayes, expectation propagation, ...:

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

→ fast and reasonably accurate

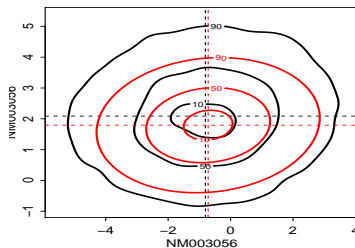
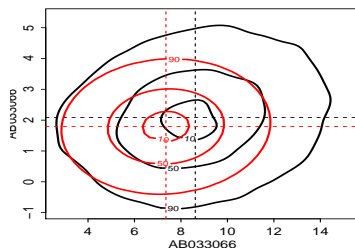
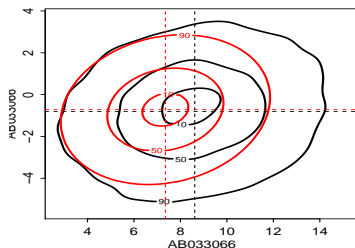
# Variational Bayes & ML as a prior

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



# Variational Bayes as a prior: joint distribution

— : VB, — : posterior



# 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)

## 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**  $\mu$ :

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

- ▶  $\phi^b$  converges towards  $\mu$  in distribution

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

for **any initial distribution**  $\nu$

## 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  $\nu$  and simulate  $\{\boldsymbol{\theta}^b\}_{b \geq 0}$
- ▶ Until it 'reaches' its stationary distribution

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

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

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

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**Properties.**

1.  $\lambda$  and  $\alpha$  define a Markov chain with stationary distribution  $\mu(\theta) = p(\theta | \mathbf{Y})$ .
2. If  $\lambda(\cdot | \theta)$  is symmetric,  $\alpha$  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.

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



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  theta.tmp = rmvnorm(1, mean=theta.sample[b-1, ], sigma=Sigma.shift)[1, ]
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## Sanity checks

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

### ► Acceptance rate

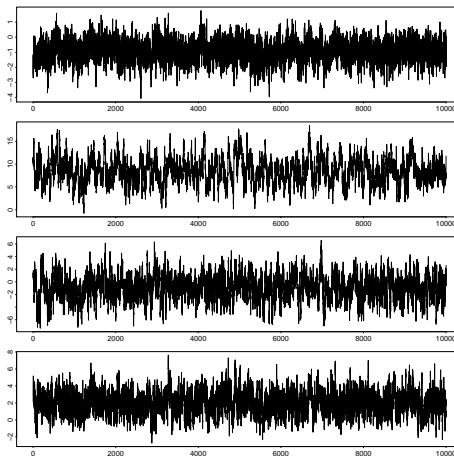
variance shift	0.1	0.5	1
acceptance rate	0.035	0.011	0.004



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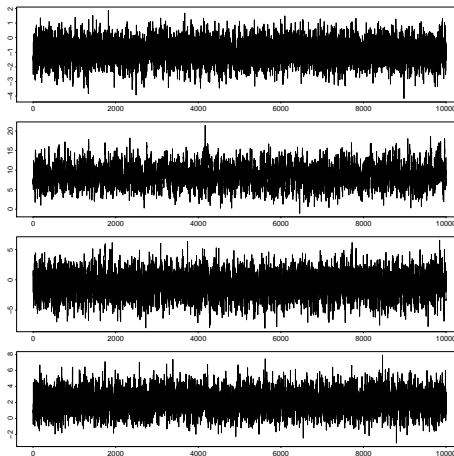
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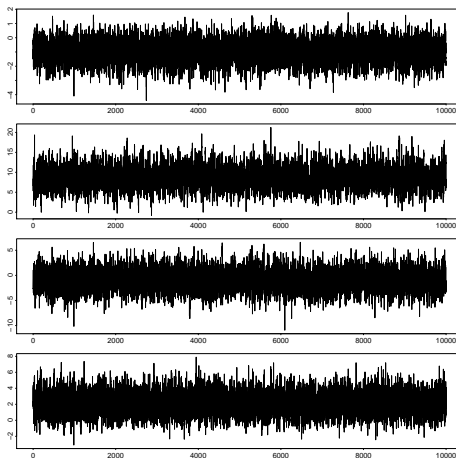
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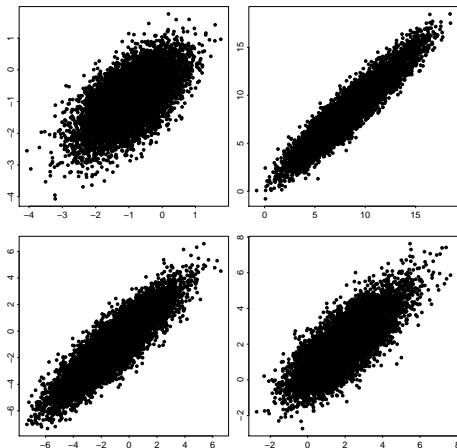
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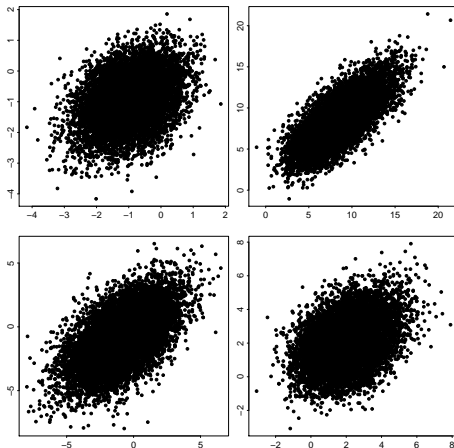
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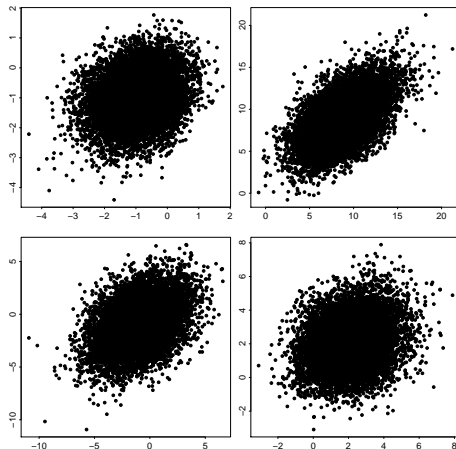
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# Gibbs

**Framework.** We do not know how to sample the whole vector  $\theta$ :

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

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

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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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**Property.**

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

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## 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
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- Monte Carlo Markov chains (MCMC)

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

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- ▶  $p(\theta | \mathbf{Y})$  (parameter inference)
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### Sequential Monte Carlo.

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

# 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)

## 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

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

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

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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  $\varepsilon$

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- ▶ 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)
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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

## 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

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- ▶ 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	—

