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Bayesian Statistics and Data Analysis
Lecture 3

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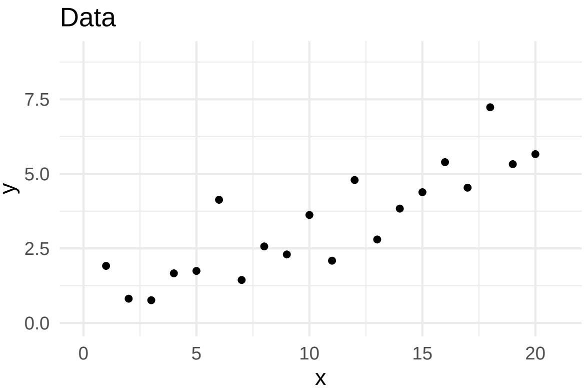
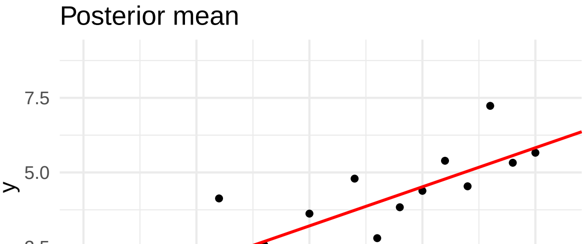
Thanks to Aki Vehtari, Aalto University

Example of uncertainty in modeling





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Monte Carlo and Posterior Draws

- Assume we can get draws from $p(\theta \mid y)$
- $\theta^{(s)}$ draws from $p(\theta \mid y)$ can be used
  - for visualization
  - to approximate expectations (integrals)

$$E_{p(\theta|y)}[\theta] = \int \theta p(\theta \mid y) \approx \frac{1}{S} \sum_{s=1}^{S} \theta^{(s)}$$

- to approximate uncertainty intervals for θ

Marginalization

- Joint posterior distribution of multiple parameters

$$p(\theta_1, \theta_2 \mid y) \propto p(y \mid \theta_1, \theta_2) p(\theta_1, \theta_2)$$

- Marginalization

$$p(\theta_1 \mid y) = \int p(\theta_1, \theta_2 \mid y) d\theta_2$$

$p(\theta_1 \mid y)$ is a marginal distribution

- Goal is often to find marginal posterior of an interesting quantity
  - a parameter $p(\theta|y)$
  - a potential observation $p(\tilde{y}|y)$

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Marginalization - predictive distribution

- Joint distribution of unknown future observation and parameters

$$
\begin{aligned}
p(\tilde{y}, \theta \mid y) &= p(\tilde{y} \mid \theta, y) p(\theta \mid y) \\
&= p(\tilde{y} \mid \theta) p(\theta \mid y) \qquad \text{(often)}
\end{aligned}
$$

- Marginalization over posterior distribution

$$
\begin{aligned}
p(\tilde{y} \mid y) &= \int p(\tilde{y} \mid \theta) p(\theta \mid y) d\theta \\
&= \int p(\tilde{y}, \theta \mid y) d\theta
\end{aligned}
$$

$p(\tilde{y} \mid y)$ is a predictive distribution

Gaussian with unknown μ and σ^2

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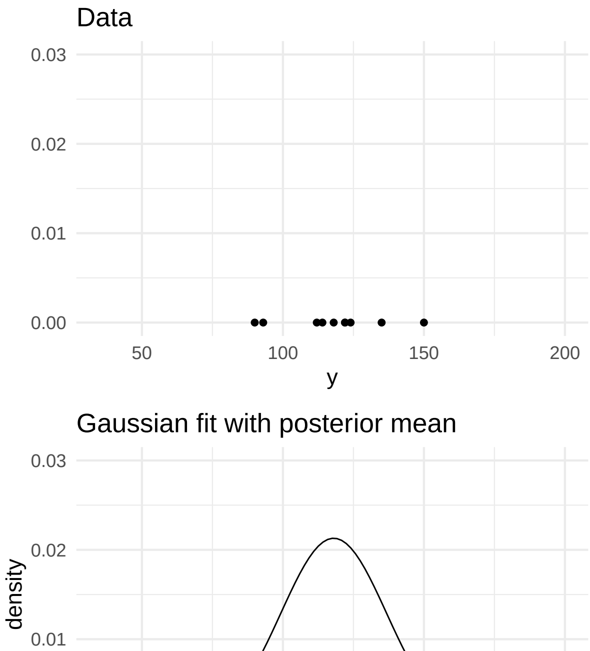
- Observation model

$$\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y-\theta)^2\right)$$

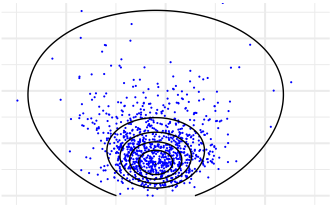
- Uninformative prior

$$p(\mu, \sigma^2) \propto \sigma^{-2}$$

Gaussian example



Joint posterior



$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma \mid y)$$

with $p(\mu, \sigma^2) \propto \sigma^{-2}$

$$p(\mu, \sigma^2 \mid y) \propto \sigma^{-2} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mu)^2\right)$$

$$p(\mu, \sigma^2 \mid y) \propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mu)^2\right)$$

$$= \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\left[\sum_{i=1}^{n}(y_i - \bar{y})^2 + n(\bar{y} - \mu)^2\right]\right)$$

where $\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

$$= \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right)$$

where $s^2 = \frac{1}{n-1}\sum^{n}(y_i - \bar{y})^2$

Gaussian: Completing the square

$$\sum_{i=1}^{n}(y_i-\mu)^2$$

$$\sum_{i=1}^{n}(y_i^2-2y_i\mu+\mu^2)$$

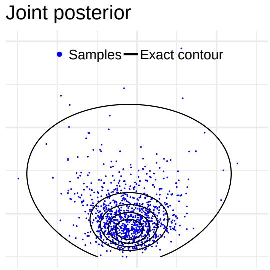
$$\sum_{i=1}^{n}(y_i^2-2y_i\mu+\mu^2-\bar{y}^2+\bar{y}^2-2y_i\bar{y}+2y_i\bar{y})$$

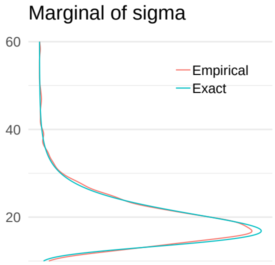
$$\sum_{i=1}^{n}(y_i^2-2y_i\bar{y}+\bar{y}^2)+\sum_{i=1}^{n}(\mu^2-2y_i\mu-\bar{y}^2+2y_i\bar{y})$$

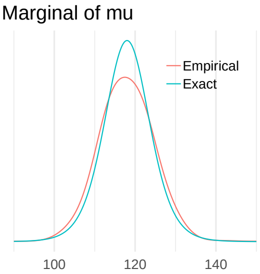
$$\sum_{i=1}^{n}(y_i-\bar{y})^2+n(\mu^2-2\bar{y}\mu-\bar{y}^2+2\bar{y}\bar{y})$$

$$\sum_{i=1}^{n}(y_i-\bar{y})^2+n(\bar{y}-\mu)^2$$

Marginal $p(\mu)$ and $p(\sigma^2)$







$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma \mid y)$$

marginals

$$p(\mu \mid y) = \int p(\mu, \sigma \mid y) d\sigma$$

$$p(\sigma \mid y) = \int p(\mu, \sigma \mid y) d\mu$$

Marginal $p(\mu|y)$ and $p(\sigma^2|y)$

Marginal posterior $p(\sigma^2 \mid y)$ (easier for σ^2 than σ)

$$
\begin{aligned}
p(\sigma^2 \mid y) &\propto \int p(\mu, \sigma^2 \mid y) d\mu \\
&\propto \int \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\left[(n-1)s^2 + n(\bar{y}-\mu)^2\right]\right) d\mu \\
&\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \cdot \\
&\quad \int \exp\left(-\frac{n}{2\sigma^2}(\bar{y}-\mu)^2\right) d\mu \\
\textit{Note!} &\quad \int \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y-\theta)^2\right) d\theta = 1 \\
&\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \sqrt{2\pi\sigma^2/n} \\
&\propto (\sigma^2)^{-(n+1)/2} \exp\left(-\frac{(n-1)s^2}{2\sigma^2}\right) \\
p(\sigma^2 \mid y) &= \text{Inv-}\chi^2(\sigma^2 \mid n-1, s^2)
\end{aligned}
$$

Gaussian - non-informative prior

Known mean

$$\sigma^2 \mid y \sim \text{Inv-}\chi^2(n, v)$$

$$\text{where} \quad v = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta)^2$$

Unknown mean

$$\sigma^2 \mid y \sim \text{Inv-}\chi^2(n-1, s^2)$$

$$\text{where} \quad s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2$$

Gaussian - non-informative prior

- Marginal posterior $p(\mu \mid y)$

$$p(\mu \mid y) = \int_0^\infty p(\mu \mid \sigma^2, y) p(\sigma^2 \mid y) d\sigma^2$$

- Marginal posterior of μ, a mixture of normal distributions where mixing density is the marginal posterior of σ^2

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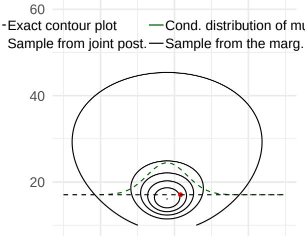
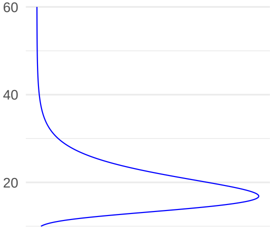
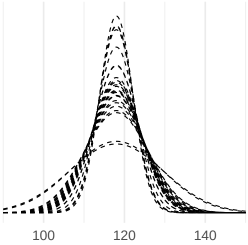
Joint posterior



Marginal of sigma



Cond distr of mu for 25 draws



Factorization

$$p(\mu, \sigma^2 \mid y) = p(\mu \mid \sigma^2, y) p(\sigma^2 \mid y)$$

$$(\sigma^2)^{(s)} \sim p(\sigma^2 \mid y)$$

$$p(\mu \mid (\sigma^2)^{(s)}, y) = \mathcal{N}(\mu \mid \bar{y}, (\sigma^2)^{(s)}/n)$$

$$p(\mu \mid y) \approx \frac{1}{S} \sum_{s=1}^{S} \mathcal{N}(\mu \mid \bar{y}, (\sigma^2)^{(s)}/$$

Cond distr of mu for 25 draws

Marginal posterior $p(\mu \mid y)$

$$p(\mu \mid y) = \int_0^\infty p(\mu, \sigma^2 \mid y) d\sigma^2$$

$$\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\left[(n-1)s^2 + n(\bar{y}-\mu)^2\right]\right) d\sigma^2$$

Transformation (integration by substitution)

$$A = (n-1)s^2 + n(\mu - \bar{y})^2 \quad \text{and} \quad z = \frac{A}{2\sigma^2}$$

$$dz = \left(-\frac{A}{2(\sigma^2)^2}\right) d\sigma^2$$

$$p(\mu \mid y) \propto A^{-n/2} \int_0^\infty z^{(n-2)/2} \exp(-z) dz$$

Recognize gamma integral $\Gamma(u) = \int_0^\infty x^{u-1} \exp(-x) dx$

$$\propto \left[(n-1)s^2 + n(\mu - \bar{y})^2\right]^{-n/2}$$

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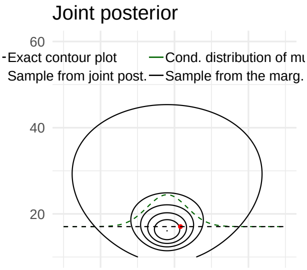
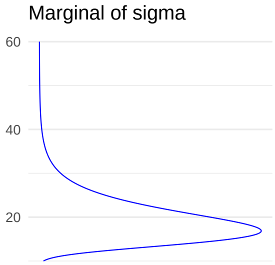
Marginal posterior $p(\mu \mid y)$

$$p(\mu|y) \propto [(n-1)s^2 + n(\mu - \bar{y})^2]^{-n/2}$$

$$\propto \left[1 + \frac{n(\mu - \bar{y})^2}{(n-1)s^2}\right]^{-n/2}$$

$$p(\mu \mid y) = t_{n-1}(\mu \mid \bar{y}, s^2/n) \quad \text{Student's } t$$



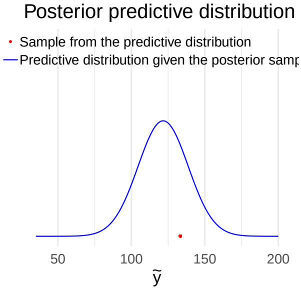


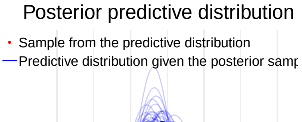
Predictive distribution for new $\tilde{y}$

$$p(\tilde{y}|y) = \int p(\tilde{y}|\mu,\sigma) p(\mu,\sigma|y) d\mu\sigma$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu,\sigma|y)$$

$$\tilde{y}^{(s)} \sim p(\tilde{y}|\mu^{(s)},\sigma^{(s)})$$





Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

$$
\begin{aligned}
p(\tilde{y} \mid \sigma^2, y) &= \int p(\tilde{y} \mid \mu, \sigma^2) p(\mu \mid \sigma^2, y) d\mu \\
&= \int \mathcal{N}(\tilde{y} \mid \mu, \sigma^2) \mathcal{N}(\mu \mid \bar{y}, \sigma^2/n) d\mu \\
&= \mathcal{N}(\tilde{y} \mid \bar{y}, (1 + \tfrac{1}{n})\sigma^2)
\end{aligned}
$$

this is up to scaling factor same as $p(\mu \mid \sigma^2, y)$

$$
p(\tilde{y} \mid y) = t_{n-1}(\tilde{y} \mid \bar{y}, (1 + \tfrac{1}{n})s^2)
$$

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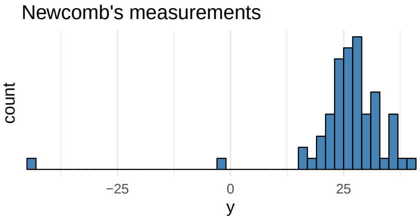
Simon Newcomb's light of speed experiment in 1882

Newcomb measured ($n = 66$) the time required for light to travel from his laboratory on the Potomac River to a mirror at the base of the Washington Monument and back, a total distance of 7422 meters.



Normal model

Gaussian - conjugate prior

- Conjugate prior has to have a form $p(\sigma^2)p(\mu \mid \sigma^2)$
- Handy parameterization

$$\mu \mid \sigma^2 \sim \mathrm{N}(\mu_0, \sigma^2/\kappa_0)$$
$$\sigma^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$$

which can be written as

$$p(\mu, \sigma^2) = \text{N-Inv-}\chi^2(\mu_0, \sigma_0^2/\kappa_0; \nu_0, \sigma_0^2)$$

- μ and σ^2 are a priori dependent
  - if σ^2 is large, then μ has wide prior

Gaussian - conjugate prior

Joint posterior (exercise 3.9)

$$p(\mu, \sigma^2 \mid y) = \text{N-Inv-}\chi^2(\mu_n, \sigma_n^2/\kappa_n; \nu_n, \sigma_n^2)$$

where

$$\begin{aligned}
\mu_n &= \frac{\kappa_0}{\kappa_0 + n}\mu_0 + \frac{n}{\kappa_0 + n}\bar{y} \\
\kappa_n &= \kappa_0 + n \\
\nu_n &= \nu_0 + n \\
\nu_n\sigma_n^2 &= \nu_0\sigma_0^2 + (n-1)s^2 + \frac{\kappa_0 n}{\kappa_0 + n}(\bar{y} - \mu_0)^2
\end{aligned}$$

Gaussian - conjugate prior

- Conditional $p(\mu \mid \sigma^2, y)$

$$\begin{aligned}\mu \mid \sigma^2, y &\sim \mathrm{N}(\mu_n, \sigma^2/\kappa_n)\\ &= \mathrm{N}\left(\frac{\frac{\kappa_0}{\sigma^2}\mu_0 + \frac{n}{\sigma^2}\bar{y}}{\frac{\kappa_0}{\sigma^2} + \frac{n}{\sigma^2}}, \frac{1}{\frac{\kappa_0}{\sigma^2} + \frac{n}{\sigma^2}}\right)\end{aligned}$$

- Marginal $p(\sigma^2 \mid y)$

$$\sigma^2 \mid y \sim \text{Inv-}\chi^2(\nu_n, \sigma_n^2)$$

- Marginal $p(\mu \mid y)$

$$\mu \mid y \sim t_{\nu_n}(\mu \mid \mu_n, \sigma_n^2/\kappa_n)$$

Multinomial model for categorical data

- Extension of binomial to K categories
- Observation model (Categorical distribution, $n = 1$)
  $y_i = (0, 1, 0, 0, 0)$ - what is K here?

$$p(y \mid \theta) \propto \prod_{k=1}^{K} \theta_j^{y_j},$$

$$\text{where } \sum_{k}^{K} \theta_k = 1\,, \text{ and } \forall \theta_k > 0$$

- What is important when choosing the prior for θ?
- Conjugate prior: The Dirichlet distribution

$$p(\theta) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1},$$

$$\text{where } \forall \alpha_k > 0$$

Multinomial model for categorical data: The posterior

- The posterior $p(\theta|y)$

$$\begin{aligned} p(\theta \mid y) &\propto p(y \mid \theta)p(\theta) \\ &\propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \prod_{i}^{n} \prod_{k=1}^{K} \theta_k^{y_{k,i}} \\ &= \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \prod_{k=1}^{K} \theta_k^{\sum_i^n y_{k,i}} \\ &= \prod_{k=1}^{K} \theta_k^{\alpha_k - 1 + \sum_i^n y_{k,i}} \end{aligned}$$

- The posterior is $p(\theta|y) = \mathrm{Dir}(\alpha + \sum y)$

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Multivariate Gaussian

- Observation model

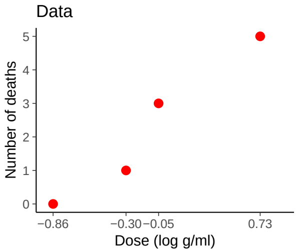
$$p(y \mid \mu, \Sigma) \propto \mid \Sigma \mid^{-1/2} \exp\left(-\frac{1}{2}(y-\mu)^T\Sigma^{-1}(y-\mu)\right),$$

where $y \in \mathcal{R}^D$

- See BDA3 p. 72–
- New recommended LKJ-prior mentioned in Appendix A, see more in Stan manual

Bioassay

Dose, x_i (log g/ml)	Number of animals, n_i	Number of deaths, y_i
-0.86	5	0
-0.30	5	1
-0.05	5	3
0.73	5	5



Find out lethal dose 50% (LD50)

- used to classify how hazardous chemical is
- 1984 EEC directive has 4 levels

Bayesian methods help to

- reduce the number of animals needed
- easy to make sequential experiment and stop as soon as desired accuracy is obtained

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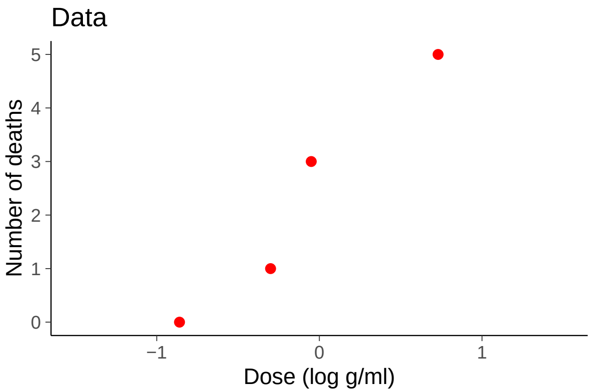
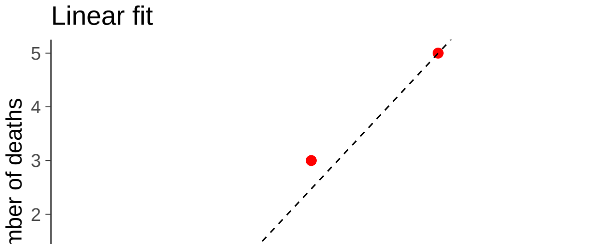
Bioassay





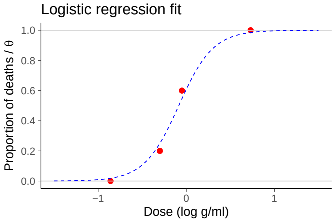
Bioassay

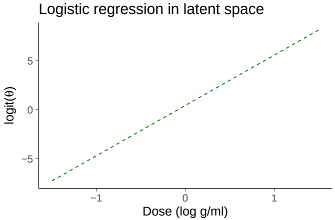
$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i)$$

$$\text{logit}(\theta_i) = \log\left(\frac{\theta_i}{1-\theta_i}\right)$$

$$= \alpha + \beta x_i$$

$$\theta_i = \frac{1}{1+\exp(-(\alpha+\beta x_i))}$$





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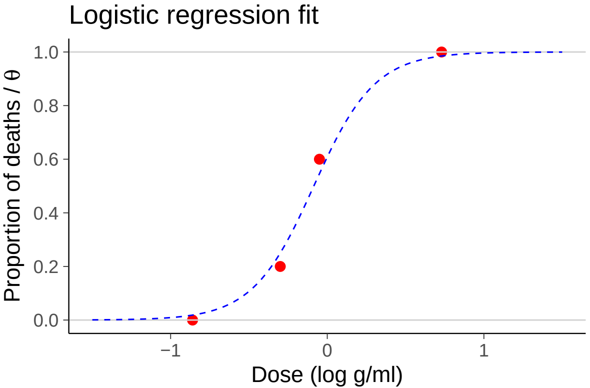
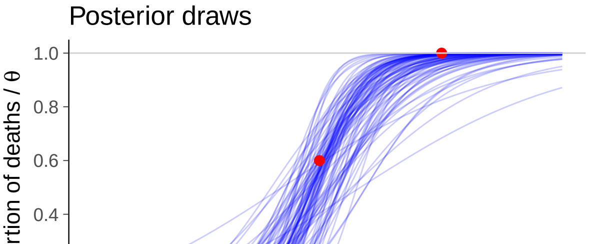
Bioassay: Lethal Dose 50%





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Bioassay posterior

Binomial model

$$y_i \mid \theta_i \sim \mathrm{Bin}(\theta_i, n_i)$$

Link function

$$\mathrm{logit}(\theta_i) = \alpha + \beta x_i$$

Likelihood

$$\begin{aligned} p(y_i \mid \alpha, \beta, n_i, x_i) &\propto \theta_i^{y_i}[1-\theta_i]^{n_i-y_i} \\ &\propto [\mathrm{logit}^{-1}(\alpha+\beta x_i)]^{y_i}[1-\mathrm{logit}^{-1}(\alpha+\beta x_i)]^{n_i-y_i} \end{aligned}$$

Posterior

$$p(\alpha, \beta \mid y, n, x) \propto p(\alpha, \beta) \prod_{i=1}^{n} p(y_i \mid \alpha, \beta, n_i, x_i)$$

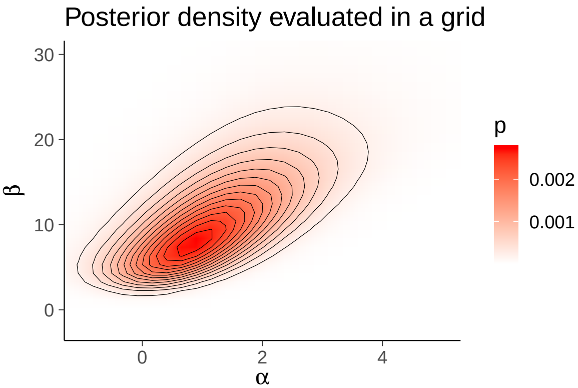
No analytic posterior distribution? What can we do?

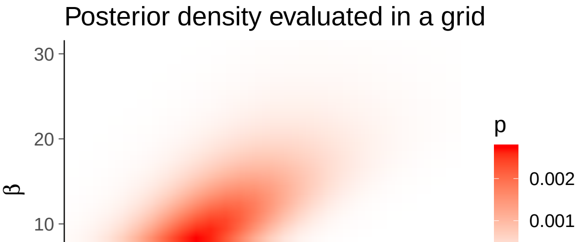
Grid evaluation

1. Setup an area (can be hard) for α and β that capture most mass (here $\alpha = [-1, 5]$ and $\beta = [0, 30]$)
2. Compute unnormalized $p(\alpha^{(g)}, \beta^{(g)} \mid y, n, x)$, here $\tilde{p}$, at the grid points g
3. Sum up $\tilde{p}$ over the whole grid (for all $g \in \{1, ..., G\}$)
4. Compute (normalize) the pmf approximation of the posterior $\hat{p}$

g	$(\alpha,\ \beta)$	$\tilde{p}$	$\hat{p}$
1	(0, -1)	0.02	0.0002
2	(0, -0.8)	0.03	0.0003
...	...	...	...
G	(30, 5)	0.001	0.00001
$\sum_g^G$	-	100	1

Bioassay (with uniform prior on α, β)





Grid sampling

- Draws can be used to estimate expectations, for example

$$E[x_{\mathrm{LD50}}] = E[-\alpha/\beta] \approx \frac{1}{S}\sum_{s=1}^{S}\frac{\alpha^{(s)}}{\beta^{(s)}}$$

- Instead of sampling, grid could be used to evaluate functions directly, for example

$$\mathrm{E}[-\alpha/\beta] \approx \sum_{t=1}^{T} w_{\mathrm{cell}}^{(t)}\frac{\alpha^{(t)}}{\beta^{(t)}},$$

  where $w_{\mathrm{cell}}^{(t)}$ is the normalized probability of a grid cell t, and $\alpha^{(t)}$ and $\beta^{(t)}$ are center locations of grid cells

- Grid sampling gets computationally too expensive in high dimensions