Chapter 4

- 4.1 Normal approximation (Laplace's method)
- 4.2 Large-sample theory
- 4.3 Counter examples
  - includes examples of difficult posteriors for MCMC, too
- 4.4 Frequency evaluation*
- 4.5 Other statistical methods*

Normal approximation (Laplace approximation)

- Often posterior converges to normal distribution when $n \to \infty$
  - bounded, non-singular, the number of parameters don't grow with n
  - we can then approximate $p(\theta|y)$ with normal distribution

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  - Laplace used this (before Gauss) to approximate the posterior of binomial model to infer ratio of girls and boys born

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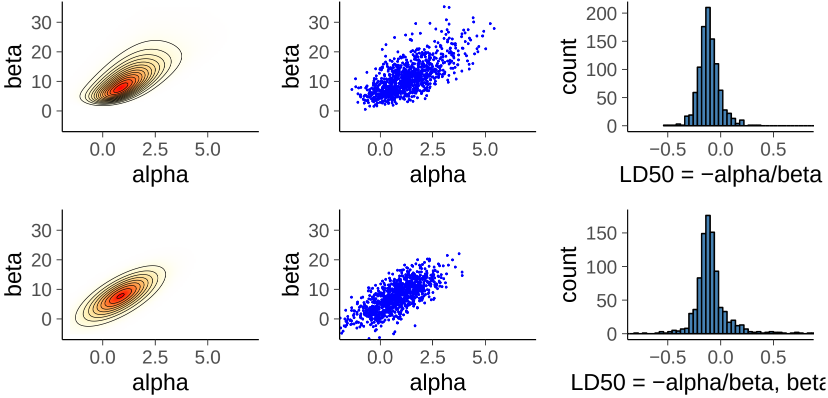

Taylor series

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$$p(\theta|y) \approx \frac{1}{\sqrt{2\pi}\sigma_\theta} \exp\left(-\frac{1}{2\sigma_\theta^2}(\theta - \hat{\theta})^2\right)$$

  - i.e. log posterior $\log p(\theta|y)$ can be approximated with a quadratic function

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  - often when $n \to \infty$, $\frac{f^{(3)}(\hat{\theta})}{3!}(\theta - \hat{\theta})^3 + \ldots$ is small

Multivariate Taylor series

- Multivariate series expansion

$$f(\theta) = f(\hat{\theta}) + \frac{df(\theta')}{d\theta'}_{\theta'=\hat{\theta}}(\theta - \hat{\theta}) + \frac{1}{2!}(\theta - \hat{\theta})^T \frac{d^2 f(\theta')}{d\theta'^2}_{\theta'=\hat{\theta}}(\theta - \hat{\theta}) + \dots$$

Normal approximation

- Taylor series expansion of the log posterior around the posterior mode $\hat{\theta}$

$$\log p(\theta|y) = \log p(\hat{\theta}|y) + \frac{1}{2}(\theta - \hat{\theta})^T \left[\frac{d^2}{d\theta^2} \log p(\theta'|y)\right]_{\theta'=\hat{\theta}} (\theta - \hat{\theta}) + \ldots$$

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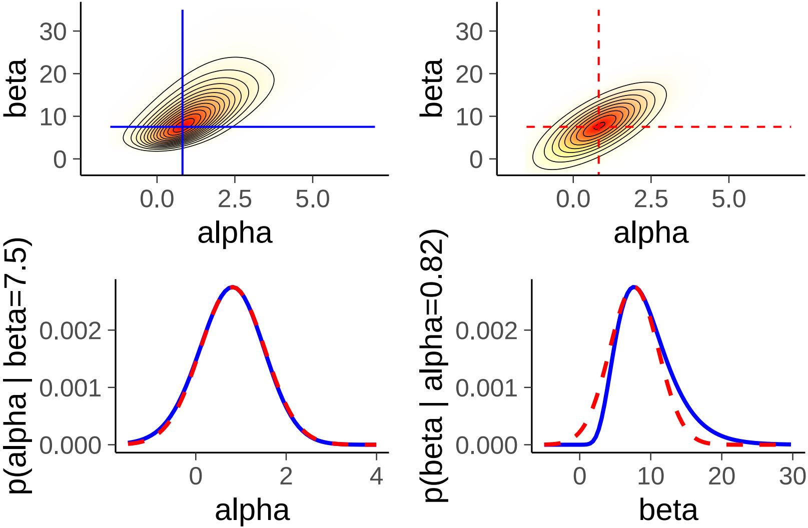

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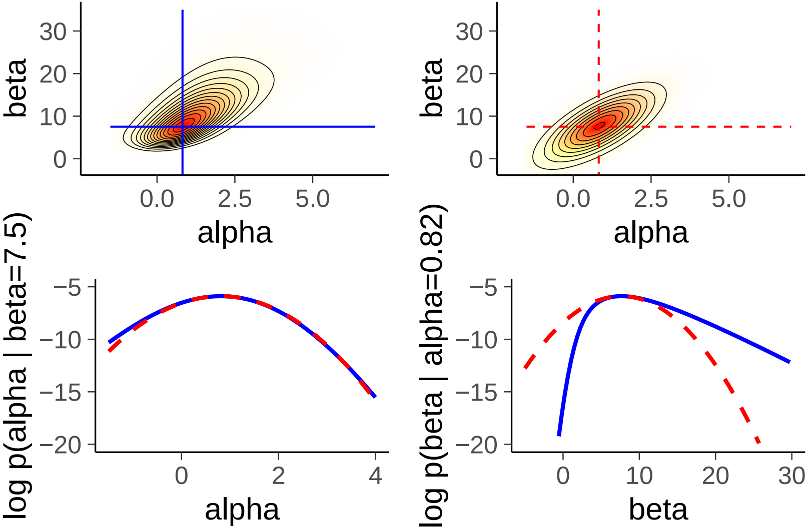

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Hessian $H(\theta) = -I(\theta)$

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  - $I(\hat{\theta})$ is the second derivatives at the mode and thus describes the curvature at the mode
  - if the mode is inside the parameter space, $I(\hat{\theta})$ is positive
  - if θ is a vector, then $I(\theta)$ is a matrix

Normal approximation

- BDA3 Ch 4 has an example where it is easy to compute first and second derivatives and there is easy analytic solution to find where the first derivatives are zero

Normal approximation – example

- Normal distribution, unknown mean and variance
  - uniform prior $(\mu, \log\sigma)$
  - normal approximation for the posterior of $(\mu, \log\sigma)$

$$\log p(\mu, \log\sigma | y) = \text{constant} - n\log\sigma - \frac{1}{2\sigma^2}[(n-1)s^2 + n(\bar{y}-\mu)^2]$$

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from which it is easy to compute the mode

$$(\hat{\mu}, \log\hat{\sigma}) = \left(\bar{y}, \frac{1}{2}\log\left(\frac{n-1}{n}s^2\right)\right)$$

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  matrix of the second derivatives at $(\hat{\mu}, \log\hat{\sigma})$

$$
\begin{pmatrix} -n/\hat{\sigma}^2 & 0 \\ 0 & -2n \end{pmatrix}
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Normal approximation – example

- Normal distribution, unknown mean and variance
  posterior mode

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  normal approximation

$$p(\mu, \log \sigma | y) \approx \mathrm{N}\left(\begin{pmatrix} \mu \\ \log \sigma \end{pmatrix} \middle| \begin{pmatrix} \bar{y} \\ \log \hat{\sigma} \end{pmatrix}, \begin{pmatrix} \hat{\sigma}^2/n & 0 \\ 0 & 1/(2n) \end{pmatrix}\right)$$

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  - e.g. in R, demo4_1.R:

```
bioassayfun <- function(w, df) {
  z <- w[1] + w[2]*df$x
  -sum(df$y*(z) - df$n*log1p(exp(z)))
}

theta0 <- c(0,0)
optimres <- optim(w0, bioassayfun, gr=NULL, df1, hessian=T)
thetahat <- optimres$par
Sigma <- solve(optimres$hessian)
```

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  - e.g. Gaussian latent variable models, such as Gaussian processes (Ch 21) and Gaussian Markov random fields
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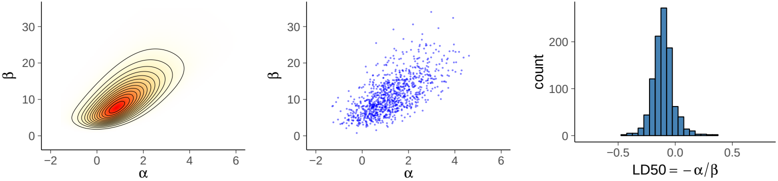
- Accuracy can be improved by importance sampling (Ch 10)

Example: Importance sampling in Bioassay

Grid



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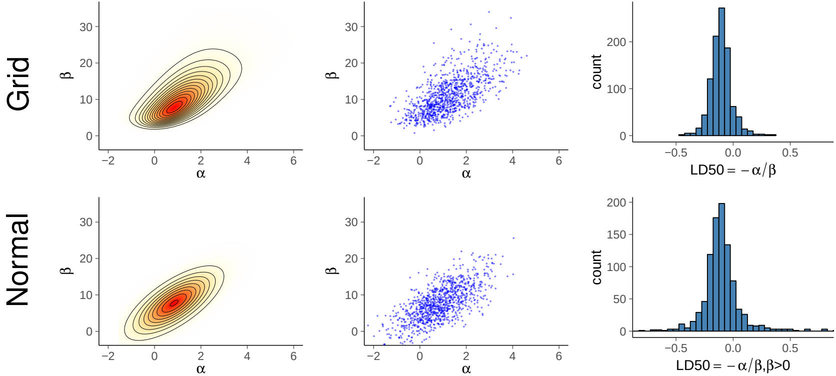

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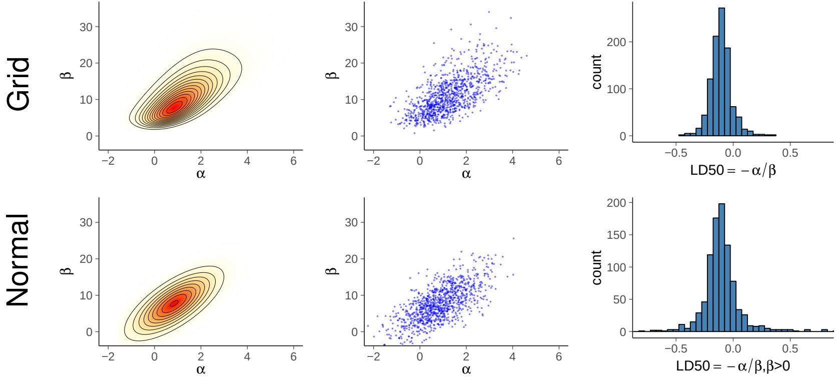

But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

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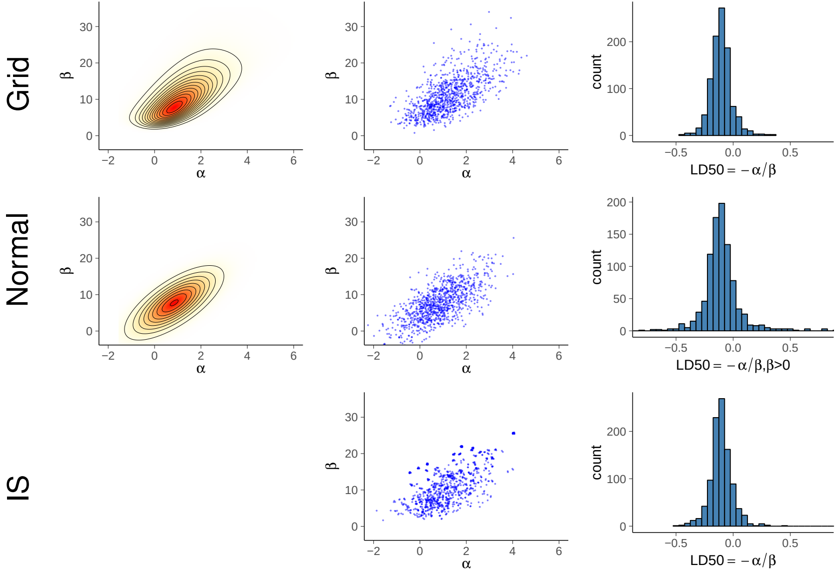

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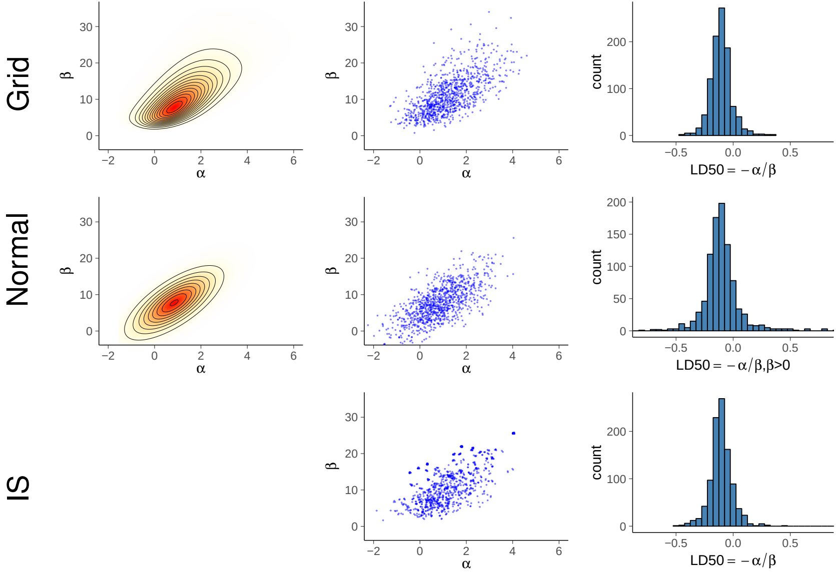

Grid sd(LD50) $\approx$ 0.1, IS sd(LD50) $\approx$ 0.1

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- RStanARM has an option `algorithm='optimizing'`
  - since version 2.19.2 (2019-10-03)
    - + Pareto-k diagnostic
    - + importance resampling (IR)

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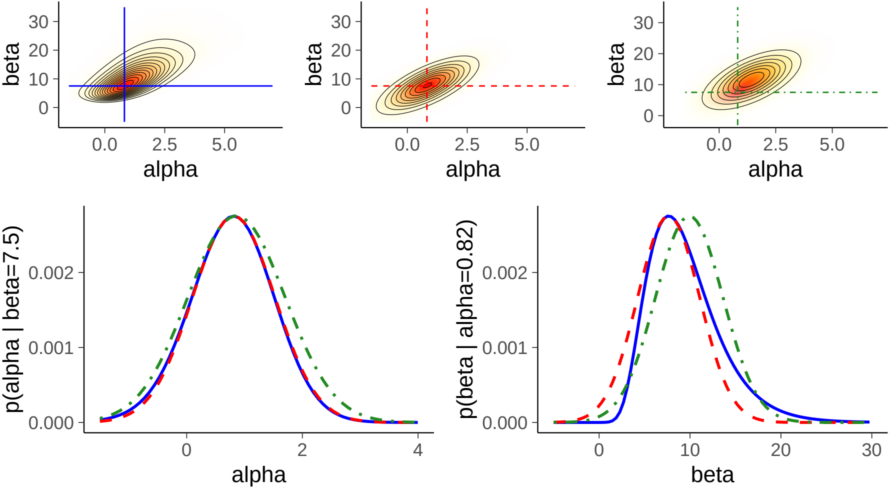
- Instead of mode and Hessian at mode, e.g.
  - variational inference (Ch 13)
    - CS-E4820 - Machine Learning: Advanced Probabilistic Methods
    - CS-E4895 - Gaussian Processes
    - Stan has the ADVI algorithm, and soon Pathfinder algorithm
    - instead of normal, methods with flexible flow transformations
  - expectation propagation (Ch 13)
  - speed of these is usually between optimization and MCMC

Distributional approximations

Exact, Normal at mode, Normal with variational inference



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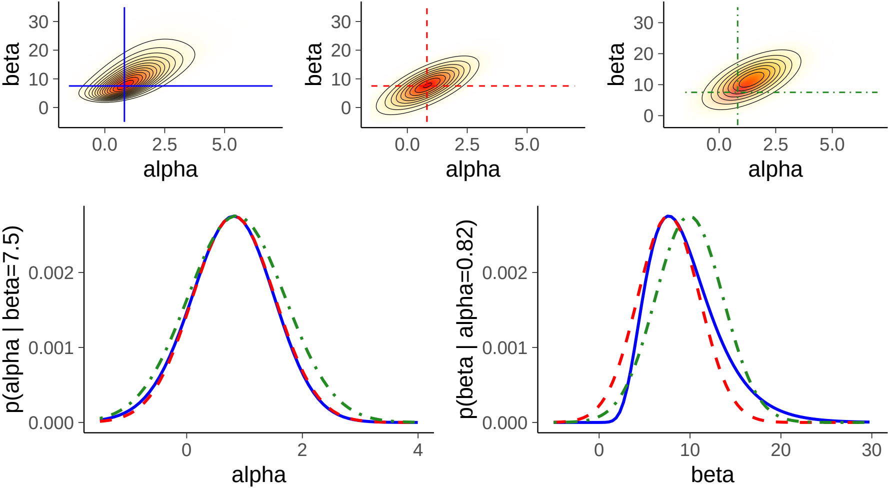

Grid sd(LD50) ≈ 0.090,
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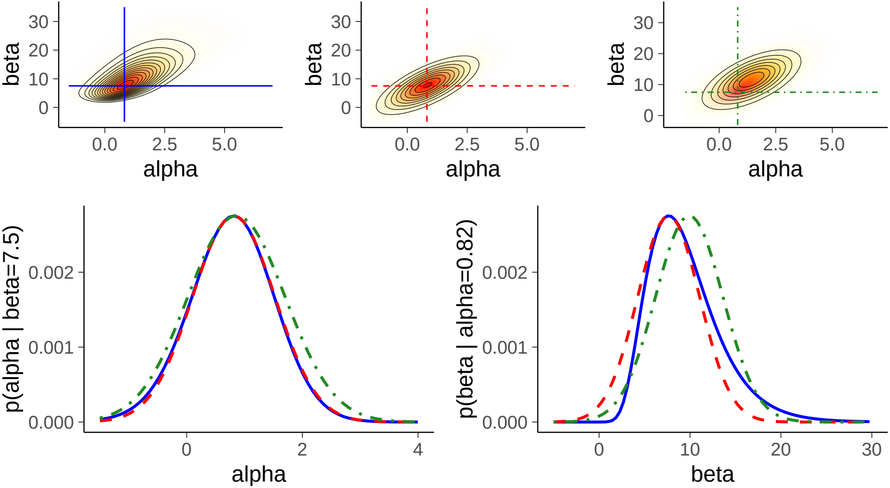

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  - with increasing number of posterior dimensions, the stochastic divergence estimate gets worse and flows have problems, too (Dhaka, Catalina, Andersen, Welandawe, Huggins, and Vehtari, 2021)

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    - eventually likelihood dominates the prior
    - the higher order terms in Taylor series increase slower than the second order term
  - see counter examples

Large sample theory

- Assume "true" underlying data distribution $f(y)$
  - observations $y_1, \ldots, y_n$ are independent samples from the joint distribution $f(y)$
  - "true" data distribution $f(y)$ is not always well defined
  - in the following we proceed as if there were true underlying data distribution
  - for the theory the exact form of $f(y)$ is not important as long at it has certain regularity conditions

Large sample theory

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  - a point doesn't have uncertainty
  - the same result as for maximum likelihood estimate

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- But a finite data from this data generating process may lack the joint height and weight observations, and thus the the finite data likelihood doesn't have information about ρ
- If the likelihood is weakly informative for some parameters, priors and integration are more important

Large sample theory – counter examples

- If the number of parameter increases as the number of observation increases
  - in some models number of parameters depends on the number of observations
  - e.g. time series models $y_t \sim \mathrm{N}(\theta_t, \sigma^2)$ and θ_t has prior in time
  - posterior of θ_t does not converge to a point, if additional observations do not bring enough information

Large sample theory – counter examples

- Aliasing (valetoisto in Finnish)
  - special case of under-identifiability where likelihood repeats in separate points
  - e.g. mixture of normals

$$p(y_i|\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \lambda) = \lambda \, \mathrm{N}(\mu_1, \sigma_1^2) + (1 - \lambda) \, \mathrm{N}(\mu_2, \sigma_2^2)$$

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- For MCMC makes the convergence diagnostics more difficult, as it is difficult to identify aliasing from other multimodality

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- Improper posterior
  - asymptotic results assume that probability sums to 1
  - e.g. Binomial model, with $\mathrm{Beta}(0, 0)$ prior and observation $y = n$
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- Should have a positive prior probability/density where needed

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  - if θ_0 is on the edge of the parameter space, Taylor series expansion has to be truncated, and normal approximation does not necessarily hold
  - e.g. $y_i \sim \mathrm{N}(\theta, 1)$ with a restriction $\theta \geq 0$ and assume that $\theta_0 = 0$
    - posterior of θ is left truncated normal distribution with $\mu = \bar{y}$
    - in the limit $n \to \infty$ posterior is half normal distribution
- Can be easy or difficult for MCMC

Frequency evaluations

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  - Calibration
    - α%-posterior interval has the true value in α% cases
    - α%-predictive interval has the true future values in α% cases
    - approximate calibration with shorter intervals for likely true values more important than exact calibration with very bad intervals for all possible values.

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  - unbiased estimate for strictly positive parameter can be negative
- Confidence interval is defined to have true value inside the interval in $\alpha\%$ cases of repeated data generation from the data generating mechanism
  - doesn’t need be useful to have perfect calibration

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- Bayesian inference
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  - a consistent way to add prior information
- A lot of machine learning is not pure frequentist or Bayesian