Introduction to Bayesian Inference

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Based on notes by Mohan Delampady

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Outline

1. Statistical Inference
2. Frequentist Statistics
3. Conditioning on Data
4. The Bayesian Recipe
5. Inference for Binomial proportion
6. Inference With Normals/Gaussians
7. Bayesian Computations
8. Empirical Bayes Methods for High Dimensional Problems
10. Bayesian Model Selection
11. Model Selection or Model Averaging?
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What is Statistical Inference?

It is an inverse problem as in ‘Toy Example’:

**Example 1 (Toy).** Suppose a million candidate stars are examined for the presence of planetary systems associated with them. If 272 ‘successes’ are noticed, how likely that the success rate is 1%, 0.1%, 0.01%, · · · for the entire universe?

Probability models for observed data involve *direct* probabilities:

**Example 2.** An astronomical study involved 100 galaxies of which 20 are Seyfert galaxies and the rest are starburst galaxies. To illustrate generalization of certain conclusions, say 10 of these 100 galaxies are randomly drawn. How many galaxies drawn will be Seyfert galaxies?

This is exactly like an artificial problem involving an urn having 100 marbles of which 20 are red and the rest blue. 10 marbles are drawn at random with replacement (repeatedly, one by one, after replacing the one previously drawn and mixing the marbles well). How many marbles drawn will be red?
Data and Models

\[ X = \text{number of Seyfert galaxies (red marbles) in the sample (out of sample size } n = 10) \]

\[ P(X = k \mid \theta) = \binom{n}{k} \theta^k (1 - \theta)^{n-k}, \quad k = 0, 1, \ldots, n \] (1)

In (1) \( \theta \) is the proportion of Seyfert galaxies (red marbles) in the urn, which is also the probability of drawing a Seyfert galaxy at each draw. In Example 2, \( \theta = \frac{20}{100} = 0.2 \) and \( n = 10 \). So,

\[ P(X = 0 \mid \theta = 0.2) = 0.8^{10}, \]
\[ P(X = 1 \mid \theta = 0.2) = 10 \times 0.2 \times 0.8^9, \text{ and so on.} \]
In practice, as in ‘Toy Example’, $\theta$ is unknown and inference about it is the question to solve.

In the Seyfert/starburst galaxy example, if $\theta$ is not known and 3 galaxies out of 10 turned out to be Seyfert, one could ask:

how likely is $\theta = 0.1$, or 0.2 or 0.3 or . . . ?

Thus inference about $\theta$ is an inverse problem:

Causes (parameters) ←— Effects (observations)
How does this *inversion* work?

The direct probability model \( P(X = k \mid \theta) \) provides a *likelihood function* for the unknown parameter \( \theta \) when data \( X = x \) is observed:

\[
l(\theta \mid x) = f(x \mid \theta) = P(X = x \mid \theta) \quad \text{when } X \text{ is a discrete random variable} \]

**Interpretation:** \( f(x \mid \theta) \) says how likely \( x \) is under different \( \theta \) or the model \( P(\cdot \mid \theta) \), so if \( x \) is observed, then

\[
P(X = x \mid \theta) = f(x \mid \theta) = l(\theta \mid x)\]

should be able to indicate what the likelihood of different \( \theta \) values or \( P(\cdot \mid \theta) \) are for that \( x \).

As a function of \( x \) for fixed \( \theta \) \( P(X = x \mid \theta) \) is a probability mass function or density, but as a function of \( \theta \) for fixed \( x \), it has no such meaning, but just a measure of likelihood.
After an experiment is conducted and seeing data $x$, the only entity available to convey the information about $\theta$ obtained from the experiment is $l(\theta \mid x)$.

For the Urn Example we have $l(\theta \mid X = 3) \propto \theta^3(1 - \theta)^7$:

```r
> curve(dbinom(3, prob = x, size = 10), from = 0, to = 1,
+       xlab = expression(theta), ylab = "", las = 1,
+       main = expression(L(theta) \propto theta^3 * (1-theta)^7))
```

$L(\theta) \propto \theta^3(1 - \theta)^7$
Maximum Likelihood Estimation (MLE): If $l(\theta \mid x)$ measures the likelihood of different $\theta$ (or the corresponding models $P(\cdot \mid \theta)$), just find that $\theta = \hat{\theta}$ which maximizes the likelihood.

For model (1)

$$\hat{\theta} = \hat{\theta}(x) = x/n = \text{sample proportion of successes}.$$ 

This is only an estimate. How good is it? What is the possible error in estimation?
Frequentist Approach

- Consider repeating this experiment again and again.
- One can look at all possible sample data
  \[ X \sim Bin(n, \theta) \rightarrow \hat{\theta} = X / n. \]
- Utilize *long-run average behaviour* of the MLE. i.e. treat \(\hat{\theta}\) as a random quantity (function of \(X\).

\[
E(\hat{\theta}) = E(X/n) = \theta \\
Var(\hat{\theta}) = Var(X/n) = \theta(1 - \theta)/n
\]

- Gives “standard error” \(\sqrt{\hat{\theta}(1 - \hat{\theta})/n}\).
- For large \(n\), can use *Law of Large Numbers* and the *Central Limit Theorem*
Confidence Statements

Specifically, for large $n$, approximately

$$\frac{\hat{\theta} - \theta}{\sqrt{\theta(1 - \theta)/n}} \sim N(0, 1),$$

or

$$\frac{\hat{\theta} - \theta}{\sqrt{\hat{\theta}(1 - \hat{\theta})/n}} \sim N(0, 1). \quad (2)$$

From (2), an approximate 95\% confidence interval for $\theta$ (when $n$ is large) is

$$\hat{\theta} \pm 2\sqrt{\hat{\theta}(1 - \hat{\theta})/n}.$$
What Does This Mean?

Simply, if we sample again and again, in about 19 cases out of 20 this random interval

$$
\left( \hat{\theta}(X) - 2\sqrt{\hat{\theta}(X)(1 - \hat{\theta}(X))/n}, \hat{\theta}(X) + 2\sqrt{\hat{\theta}(X)(1 - \hat{\theta}(X))/n} \right)
$$

will contain the true unknown value of $\theta$.

Fine, but what can we say about the one interval that we can construct for the given sample or data $x$?
What Does This Mean?

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\[
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\]

will contain the true unknown value of \(\theta\).

Fine, but what can we say about the one interval that we can construct for the given sample or data \(x\)?

Nothing; either \(\theta\) is inside

\[
(0.3 - 2\sqrt{0.3 \times 0.7/10}, 0.3 + 2\sqrt{0.3 \times 0.7/10})
\]

or it is outside.

If \(\theta\) is treated as fixed unknown constant, conditioning on the given data \(X = x\) is meaningless.
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Conditioning on Data

- What other approach is possible, then?
- How does one condition on data?
- How does one talk about probability of a model or a hypothesis?

Example 3. (not from physics but medicine) Consider a blood test for a certain disease; result is positive \((x = 1)\) or negative \((x = 0)\). Suppose \(\theta_1\) denotes disease is present, \(\theta_2\) disease not present.

Test is not confirmatory. Instead the probability distribution of \(X\) for different \(\theta\) is:

<table>
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<th>(x = 0)</th>
<th>(x = 1)</th>
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<tr>
<td>(\theta_1)</td>
<td>0.2</td>
<td>0.8</td>
<td>Test is +ve 80% of time if ‘disease present’</td>
</tr>
<tr>
<td>(\theta_2)</td>
<td>0.7</td>
<td>0.3</td>
<td>Test is –ve 70% of time if ‘disease not present’</td>
</tr>
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</table>

If for a particular patient the test result comes out to be ‘positive’, what should the doctor conclude?
What is the Question?

What is to be answered is ‘what are the chances that the disease is present given that the test is positive?’ i.e., $P(\theta = \theta_1 | X = 1)$. What we have is $P(X = 1 | \theta = \theta_1)$ and $P(X = 1 | \theta = \theta_2)$. We have the ‘wrong’ conditional probabilities. They need to be ‘reversed’. But how?
The Bayesian Recipe

Recall Bayes Theorem: If $A$ and $B$ are two events,

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

assuming $P(B) > 0$. Therefore, $P(A \text{ and } B) = P(A|B)P(B)$, and by symmetry $P(A \text{ and } B) = P(B|A)P(A)$. Consequently, if $P(B|A)$ is given and $P(A|B)$ is desired, note

$$P(A|B) = \frac{P(A \text{ and } B)}{P(B)} = \frac{P(B|A)P(A)}{P(B)}.$$

But how can we get $P(B)$?
The Bayesian Recipe

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$$P(A|B) = \frac{P(A \text{ and } B)}{P(B)} = \frac{P(B|A)P(A)}{P(B)}.$$

But how can we get $P(B)$? Rule of total probability says,

$$P(B) = P(B \text{ and } \Omega) = P(B \text{ and } A) + P(B \text{ and } A^c)$$

$$= P(B|A)P(A) + P(B|A^c)(1 - P(A)),$$

so

$$P(A|B) = \frac{P(B|A)P(A)}{P(B|A)P(A) + P(B|A^c)(1 - P(A))} \quad (3)$$
Bayes Theorem allows one to invert a certain conditional probability to get a certain other conditional probability. How does this help us?

In our example we want \( P(\theta = \theta_1 | X = 1) \). From (3),

\[
P(\theta = \theta_1 | X = 1) = \frac{P(X = 1 | \theta = \theta_1)P(\theta = \theta_1)}{P(X = 1 | \theta_1)P(\theta = \theta_1) + P(X = 1 | \theta_2)P(\theta = \theta_2)}.
\]

(4)

So, all we need is \( P(\theta = \theta_1) \), which is simply the probability that a randomly chosen person has this disease, or just the ‘prevalence’ of this disease in the concerned population.
The doctor most likely has this information. But this is not part of the experimental data.

This is pre-experimental information or \textit{prior} information. If we have this, and are willing to incorporate it in the analysis, we get the post-experimental information or \textit{posterior} information in the form of $P(\theta|X = x)$. 
In our example, if we take $P(\theta = \theta_1) = 0.05$ or 5%, we get

\[
P(\theta = \theta_1 \mid X = 1) = \frac{0.8 \times 0.05}{0.8 \times 0.05 + 0.3 \times 0.95} = \frac{0.04}{0.325} = 0.123
\]

which is only 12.3% and $P(\theta = \theta_2 \mid X = 1) = 0.877$ or 87.7%.
In our example, if we take $P(\theta = \theta_1) = 0.05$ or 5%, we get

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which is only 12.3% and $P(\theta = \theta_2 \mid X = 1) = 0.877$ or 87.7%.

Formula (4) which shows how to ‘invert’ the given conditional probabilities, $P(X = x \mid \theta)$ into the conditional probabilities of interest, $P(\theta \mid X = x)$ is an instance of the Bayes Theorem, and hence the Theory of Inverse Probability (usage at the time of Bayes and Laplace, late eighteenth century and even by Jeffreys), is known these days as Bayesian inference.
Ingredients of Bayesian inference:

- **Likelihood function**, \( l(\theta \mid x) \); \( \theta \) can be a parameter vector
- **Prior probability**, \( \pi(\theta) \)

Combining the two, one gets the **posterior probability density** or mass function

\[
\pi(\theta \mid x) = \begin{cases} 
\frac{\pi(\theta)l(\theta \mid x)}{\sum_j \pi(\theta_j)l(\theta_j \mid x)} & \text{if } \theta \text{ is discrete}; \\
\frac{\pi(\theta)l(\theta \mid x)}{\int \pi(u)l(u \mid x) \, du} & \text{if } \theta \text{ is continuous}.
\end{cases}
\]
A more relevant example
A more relevant example

http://xkcd.com/1132/
A more relevant example

Frequentist answer?

- Null hypothesis: sun has not exploded.
- \( p \)-value = ?

Bayesian answer?
A more relevant example

Frequentist Statistician:

The probability of this result happening by chance is $\frac{1}{36} = 0.027$. Since $p < 0.05$, I conclude that the Sun has exploded.

Bayesian Statistician:

BET YOU $50 IT HASN'T.
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Example 2 contd. Suppose we have no special information available on $\theta$. Then assume $\theta$ is uniformly distributed on the interval $(0, 1)$. i.e., the prior density is $\pi(\theta) = 1, \quad 0 < \theta < 1$.

This is a choice of non-informative or vague or reference prior. Often, Bayesian inference from such a prior coincides with classical inference.
The posterior density of \( \theta \) given \( x \) is then

\[
\pi(\theta|x) = \frac{\pi(\theta) l(\theta|x)}{\int \pi(u) l(u|x) \, du} = \frac{(n+1)!}{x!(n-x)!} \theta^x (1-\theta)^{n-x}, \quad 0 < \theta < 1.
\]

As a function of \( \theta \), this is the same as the likelihood function

\[ l(\theta|x) \propto \theta^x (1-\theta)^{n-x}, \]

and so maximizing the posterior probability density will give the same estimate as the maximum likelihood estimate!
Influence of the Prior

If we had some knowledge about $\theta$ which can be summarized in the form of a Beta prior distribution with parameters $\alpha$ and $\gamma$, the posterior will also be Beta with parameters $x + \alpha$ and $n - x + \gamma$. Such priors which result in posteriors from the same ‘family’ are called ‘natural conjugate priors’.

![Graph showing Beta distributions](image-url)
Robustness?

If the answer depends on choice of prior, which prior should we choose?
Robustness?

If the answer depends on choice of prior, which prior should we choose?

**Objective Bayesian Approach:**

- Invariant priors (Jeffreys)
- Reference priors (Bernardo, Jeffreys)
- Maximum entropy priors (Jaynes)

**Subjective Bayesian Approach:**

- Expert opinion, previous studies, etc.
In Example 2, what $\pi(\theta|x)$ says is that

- The uncertainty in $\theta$ can now be described in terms of an actual probability distribution (posterior distribution).
- The MLE $\hat{\theta} = x/n$ happens to be the value where the posterior is maximum (traditionally called the mode of the distribution).
- $\hat{\theta}$ can thus be interpreted as the most probable value of the unknown parameter $\theta$ conditional on the sample data $x$.
- Also called the ‘maximum a posteriori estimate (MAP)’, or the ‘highest posterior density estimate (HPD)’, or simply ‘posterior mode’.
Of course we do not need to mimic the MLE.

In fact the more common Bayes estimate is the posterior mean (which minimizes the posterior dispersion):

\[
E[(\theta - \hat{\theta}_B)^2 | x] = \min_a E[(\theta - a)^2 | x],
\]

when \( \hat{\theta}_B = E(\theta | x) \).
If we choose $\hat{\theta}_B$ as the estimate of $\theta$, we get a natural measure of variability of this estimate in the form of the posterior variance:

$$E[(\theta - E(\theta|x))^2|x].$$

Therefore the posterior standard deviation is a natural measure of estimation error. i.e., our estimate is $\hat{\theta}_B \pm \sqrt{E[(\theta - E(\theta|x))^2|x]}$.

In fact, we can say much more. For any interval around $\hat{\theta}$ we can compute the (posterior) probability of it containing the true parameter $\theta$. In other words, a statement such as

$$P(\hat{\theta}_B - k_1 \leq \theta \leq \hat{\theta}_B + k_2|x) = 0.95$$

is perfectly meaningful.

All these inferences are conditional on the given data.
In Example 2, if the prior is a Beta distribution with parameters $\alpha$ and $\gamma$, then $\theta|x$ will have a $\text{Beta}(x + \alpha, n - x + \gamma)$ distribution, so the Bayes estimate of $\theta$ will be

$$\hat{\theta}_B = \frac{(x + \alpha)}{(n + \alpha + \gamma)} = \frac{n}{n + \alpha + \gamma} \frac{x}{n} + \frac{\alpha + \gamma}{n + \alpha + \gamma} \frac{\alpha}{\alpha + \gamma}.$$ 

This is a convex combination of sample mean and prior mean, with the weights depending upon the sample size and the strength of the prior information as measured by the values of $\alpha$ and $\gamma$. 
Bayesian inference relies on the conditional probability language to revise one’s knowledge.

In the above example, prior to the collection of sample data one had some (vague, perhaps) information on $\theta$.

Then came the sample data.

Combining the model density of this data with the prior density one gets the posterior density, the conditional density of $\theta$ given the data.

From now on until further data is available, this posterior distribution of $\theta$ is the only relevant information as far as $\theta$ is concerned.
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Inference With Normals/Gaussians

**Gaussian PDF**

\[
 f(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \quad \text{over } [-\infty, \infty] \tag{6}
\]

Common abbreviated notation: \( X \sim N(\mu, \sigma^2) \)

**Parameters**

\[
 \mu = E(X) \equiv \int x f(x|\mu, \sigma^2) \, dx
\]

\[
 \sigma^2 = E((X - \mu)^2) \equiv \int (x - \mu)^2 f(x|\mu, \sigma^2) \, dx
\]
Example 4. Fit a normal/Gaussian model to the ‘globular cluster luminosity functions’ data. The set-up is as follows.

Our data consist of \( n \) measurements, \( X_i = \mu + \epsilon_i \). Suppose the noise contributions are independent, and \( \epsilon_i \sim N(0, \sigma^2) \). Denoting the random sample \((x_1, \ldots, x_n)\) by \( \mathbf{x} \),

\[
\begin{align*}
f(\mathbf{x} | \mu, \sigma^2) &= \prod_i f(x_i | \mu, \sigma^2) \\
&= \prod_i \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2} (x_i - \mu)^2} \\
&= (2\pi\sigma^2)^{-n/2} e^{-\frac{1}{2\sigma^2} \sum_{i=1}^{n} (x_i - \mu)^2} \\
&= (2\pi\sigma^2)^{-n/2} e^{-\frac{1}{2\sigma^2} \left[ \sum_{i=1}^{n} (x_i - \bar{x})^2 + n(\bar{x} - \mu)^2 \right]}.
\end{align*}
\]

Note \((\bar{X}, s^2 = \sum_{i=1}^{n} (X_i - \bar{X})^2/(n - 1))\) is sufficient for the parameters \((\mu, \sigma^2)\). This is a very substantial data compression.
Inference About a Normal Mean, $\sigma^2$ known

Not useful, but easy to understand.

$$l(\mu|\mathbf{x}) \propto f(\mathbf{x}|\mu, \sigma^2) \propto e^{-\frac{n}{2\sigma^2}(\mu-\bar{x})^2},$$

so that $\bar{X}$ is sufficient.

Also,

$$\bar{X}|\mu \sim N(\mu, \sigma^2/n).$$
If an informative prior, \( \mu \sim N(\mu_0, \tau^2) \) is chosen for \( \mu \),

\[
\pi(\mu|x) \propto l(\mu|x)\pi(\mu) \\
\propto e^{-\frac{1}{2} \left[ \frac{n(\mu - \bar{x})^2}{\sigma^2} + \frac{(\mu - \mu_0)^2}{\tau^2} \right]} \\
\propto e^{-\frac{\tau^2 + \sigma^2/n}{2\tau^2\sigma^2/n} \left( \mu - \frac{\tau^2\sigma^2/n}{\tau^2 + \sigma^2/n} \left( \frac{\mu_0}{\tau^2} + \frac{n\bar{x}}{\sigma^2} \right) \right)^2}.
\]

i.e., \( \mu|x \sim N(\hat{\mu}, \delta^2) \):

\[
\hat{\mu} = \frac{\tau^2\sigma^2/n}{\tau^2 + \sigma^2/n} \left( \frac{\mu_0}{\tau^2} + \frac{n\bar{x}}{\sigma^2} \right) \\
= \frac{\tau^2}{\tau^2 + \sigma^2/n} \bar{x} + \frac{\sigma^2/n}{\tau^2 + \sigma^2/n} \mu_0.
\]
\( \hat{\mu} \) is the Bayes estimate of \( \mu \), which is just a weighted average of sample mean \( \bar{x} \) and prior mean \( \mu_0 \).

\( \delta^2 \) is the posterior variance of \( \mu \) and

\[
\delta^2 = \frac{\tau^2 \sigma^2 / n}{\tau^2 + \sigma^2 / n} = \frac{\sigma^2}{n} \frac{\tau^2}{\tau^2 + \sigma^2 / n}.
\]

Therefore

- \( \hat{\mu} \pm \delta \) is our estimate for \( \mu \), and
- \( \hat{\mu} \pm 2\delta \) is a 95\% HPD (Bayesian) credible interval for \( \mu \).
\( \hat{\mu} \) is the Bayes estimate of \( \mu \), which is just a weighted average of sample mean \( \bar{x} \) and prior mean \( \mu_0 \).

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Therefore

- \( \hat{\mu} \pm \delta \) is our estimate for \( \mu \), and
- \( \hat{\mu} \pm 2\delta \) is a 95% HPD (Bayesian) credible interval for \( \mu \).

What happens as \( \tau^2 \to \infty \), or as the prior becomes more and more flat?

\[
\hat{\mu} \to \bar{x}, \quad \delta \to \frac{\sigma}{\sqrt{n}}.
\]

So Jeffreys’ prior \( \pi(\mu) = C \) reproduces frequentist inference.
Inference About a Normal Mean, $\sigma^2$ unknown

Our observations $X_1, \ldots X_n$ is a random sample from a Gaussian population with both mean $\mu$ and variance $\sigma^2$ unknown.

We are only interested in $\mu$.

How do we get rid of the nuisance parameter $\sigma^2$?

Bayesian inference uses posterior distribution which is a probability distribution, so $\sigma^2$ should be integrated out from the joint posterior distribution of $\mu$ and $\sigma^2$ to get the marginal posterior distribution of $\mu$. 
\[
 l(\mu, \sigma^2 | x) = (2\pi \sigma^2)^{-n/2} e^{-\frac{1}{2\sigma^2} \left[ \sum_{i=1}^{n} (x_i - \bar{x})^2 + n(\mu - \bar{x})^2 \right]}.
\]

Start with \( \pi(\mu, \sigma^2) \) and get

\[
 \pi(\mu, \sigma^2 | x) \propto \pi(\mu, \sigma^2) l(\mu, \sigma^2 | x)
\]

and then get

\[
 \pi(\mu | x) = \int_{0}^{\infty} \pi(\mu, \sigma^2 | x) \, d\sigma^2.
\]
Use Jeffreys’ prior $\pi(\mu, \sigma^2) \propto 1/\sigma^2$: Flat prior for $\mu$ which is a location or translation parameter, and an independent flat prior for $\log(\sigma)$ which is again a location parameter, being the log of a scale parameter.

$$
\pi(\mu, \sigma^2 | x) \propto \frac{1}{\sigma^2} l(\mu, \sigma^2 | x)
$$
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$$\pi(\mu, \sigma^2|x) \propto \frac{1}{\sigma^2} l(\mu, \sigma^2|x)$$

$$\pi(\mu|x) \propto \int_0^\infty (\sigma^2)^{-(n+1)/2} e^{-\frac{1}{2\sigma^2}[\sum_{i=1}^n (x_i - \bar{x})^2 + n(\mu - \bar{x})^2]} d\sigma^2$$

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

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

$$\propto \text{density of Students } t_{n-1}.$$
\[
\frac{\sqrt{n}(\mu - \bar{x})}{s} \mid \text{data} \sim t_{n-1}
\]

\[
P(\bar{x} - t_{n-1}(0.975) \frac{s}{\sqrt{n}} \leq \mu \leq \bar{x} + t_{n-1}(0.975) \frac{s}{\sqrt{n}} \mid \text{data}) = 95\%
\]

i.e., the Jeffreys’ translation-scale invariant prior reproduces frequentist inference.

What if there are some constraints on \(\mu\) such as \(-A \leq \mu \leq B\), for example, \(\mu > 0\)? We will get a truncated \(t_{n-1}\) instead, but the procedure will go through with minimal change.
Example 4 contd. (GCL Data) $n = 360$, $\bar{x} = 14.46$, $s = 1.19$. 

$$\frac{\sqrt{360}(\mu - 14.46)}{1.19} \mid \text{data} \sim t_{359}$$

$$\mu \mid \text{data} \sim N(14.46, 0.063^2)$$ approximately.

Estimate for mean GCL is $14.46 \pm 0.063$ and 95% HPD credible interval is $(14.33, 14.59)$. 
Comparing two Normal Means

**Example 5.** Check whether the mean distance indicators in the two populations of LMC datasets are different.


```r
> x <- c(18.70, 18.55, 18.55, 18.575, 18.4, 18.42, 18.45, + 18.59, 18.471, 18.54, 18.54, 18.64, 18.58)
> y <- c(18.45, 18.45, 18.44, 18.30, 18.38, 18.50, 18.55, + 18.52, 18.40, 18.45, 18.55, 18.69)
```

Model as follows:

\[ X_1, \ldots, X_{n_1} \text{ is a random sample from } N(\mu_1, \sigma_1^2). \]
\[ Y_1, \ldots, Y_{n_2} \text{ is a random sample from } N(\mu_2, \sigma_2^2) \text{ (independent).} \]

Unknown parameters: \((\mu_1, \mu_2, \sigma_1^2, \sigma_2^2)\)

Quantity of interest: \(\eta = \mu_1 - \mu_2\)

Nuisance parameters: \(\sigma_1^2\) and \(\sigma_2^2\)
Case 1. $\sigma_1^2 = \sigma_2^2$. Then sufficient statistic for $(\mu_1, \mu_2, \sigma^2)$ is

$$
\left( \bar{X}, \bar{Y}, s^2 = \frac{1}{n_1+n_2-2} \left( \sum_{i=1}^{n_1} (X_i - \bar{X})^2 + \sum_{j=1}^{n_2} (Y_j - \bar{Y})^2 \right) \right)
$$

It can be shown that

- $\bar{X} | \mu_1, \mu_2, \sigma^2 \sim N(\mu_1, \sigma^2/n_1)$,
- $\bar{Y} | \mu_1, \mu_2, \sigma^2 \sim N(\mu_2, \sigma^2/n_2)$,
- $(n_1 + n_2 - 2) s^2 | \mu_1, \mu_2, \sigma^2 \sim \sigma^2 \chi^2_{n_1+n_2-2}$,

and these three are independently distributed.
\[ \bar{X} - \bar{Y} | \mu_1, \mu_2, \sigma^2 \sim N(\eta, \sigma^2(\frac{1}{n_1} + \frac{1}{n_2})) \], \quad \eta = \mu_1 - \mu_2 \\

Use Jeffreys' location-scale invariant prior \( \pi(\mu_1, \mu_2, \sigma^2) \propto 1/\sigma^2 \)

\[ \eta | \sigma^2, x, y \sim N(\bar{x} - \bar{y}, \sigma^2(\frac{1}{n_1} + \frac{1}{n_2})) \], \quad \text{and} \\
\[ \pi(\eta, \sigma^2 | x, y) \propto \pi(\eta | \sigma^2, x, y)\pi(\sigma^2 | s^2), \tag{7} \]

Integrate out \( \sigma^2 \) from (7) as in the previous example to get

\[ \frac{\eta - (\bar{x} - \bar{y})}{s \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}} \mid x, y \sim t_{n_1+n_2-2}. \]

95% HPD credible interval for \( \eta = \mu_1 - \mu_2 \) is

\[ \bar{x} - \bar{y} \pm t_{n_1+n_2-2}(0.975)s \sqrt{\frac{1}{n_1} + \frac{1}{n_2}}, \]

same as frequentist \( t \)-interval.
Example 5 contd. We have $\bar{x} = 18.539$, $\bar{y} = 18.473$, $n_1 = 13$, $n_2 = 12$ and $s^2 = 0.0085$. $\hat{\eta} = \bar{x} - \bar{y} = 0.066$, $s\sqrt{\frac{1}{n_1} + \frac{1}{n_2}} = 0.037$, $t_{23}(0.975) = 2.069$.

95% HPD credible interval for $\eta = \mu_1 - \mu_2$: $(0.066 - 2.069 \times 0.037, 0.066 + 2.069 \times 0.037) = (-0.011, 0.142)$. 
Case 2. $\sigma_1^2$ and $\sigma_2^2$ are not known to be equal.

From the one-sample normal example, note that

$$(\bar{X}, s^2_X = \frac{1}{n_1-1} \sum_{i=1}^{n_1} (X_i - \bar{X})^2)$$

sufficient for $(\mu_1, \sigma_1^2)$, and

$$(\bar{Y}, s^2_Y = \frac{1}{n_2-1} \sum_{j=1}^{n_2} (Y_j - \bar{Y})^2)$$

sufficient for $(\mu_2, \sigma_2^2)$.

Making inference on $\eta = \mu_1 - \mu_2$ when $\sigma_1^2$ and $\sigma_2^2$ are not assumed to be equal is called the Behrens-Fisher problem for which the frequentist solution is not very straightforward, but the Bayes solution is.
It is a well-known result that

\[
\bar{X} \mid \mu_1, \sigma_1^2 \sim N(\mu_1, \sigma_1^2/n_1) \\
(n_1 - 1) s_X^2 \mid \mu_1, \sigma_1^2 \sim \sigma^2 \chi_{n_1-1}^2
\]

and are independently distributed. Similarly,

\[
\bar{Y} \mid \mu_2, \sigma_2^2 \sim N(\mu_2, \sigma_2^2/n_2) \\
(n_2 - 1) s_Y^2 \mid \mu_2, \sigma_2^2 \sim \sigma^2 \chi_{n_2-1}^2
\]

and are independently distributed.

\(X\) and \(Y\) samples are independent.

Use Jeffreys’ prior

\[
\pi(\mu_1, \mu_2, \sigma_1^2, \sigma_2^2) \propto 1/\sigma_1^2 \times 1/\sigma_2^2
\]
Calculations similar to those in one-sample case give:

\[
\frac{\sqrt{n_1}(\mu_1 - \bar{x})}{s_X} \mid \text{data} \sim t_{n_1-1},
\]

\[
\frac{\sqrt{n_2}(\mu_2 - \bar{y})}{s_Y} \mid \text{data} \sim t_{n_2-1},
\]

(8)

and these two are independent.
Posterior distribution of $\eta = \mu_1 - \mu_2$ given the data is non-standard (difference of two independent $t$ variables) but not difficult to get.

Use Monte-Carlo Sampling: Simply generate $(\mu_1, \mu_2)$ repeatedly from (8) and construct a histogram for $\eta = \mu_1 - \mu_2$.

Example 5 (LMC) contd.

```r
> xbar <- mean(x)
> ybar <- mean(y)
> n1 <- length(x)
> n2 <- length(y)
> sx <- sqrt(var(x))
> sy <- sqrt(var(y))
> mu1.sim <- xbar + sx * rt(100000, df = n1 - 1) / sqrt(n1)
> mu2.sim <- ybar + sy * rt(100000, df = n2 - 1) / sqrt(n2)
```
```r
> plot(density(mu1.sim - mu2.sim))
> s <- sqrt((1/n1 + 1/n2) * ((n1-1)*sx^2 + (n2-1)*sy^2) / (n1+n2-2))
> curve(dt((x - (xbar-ybar)) / s, df = n1 + n2 - 2) / s,
+       add = TRUE, col = "red")

```

![Density plot](image-url)
Posterior mean of $\eta = \mu_1 - \mu_2$ is

$$\hat{\eta} = E(\mu_1 - \mu_2 \mid \text{data}) = 0.0654.$$  \hspace{1cm} (9)

95% HPD credible interval for $\eta = \mu_1 - \mu_2$ is

$$= \begin{cases} 
(-0.011, 0.142) & \text{equal variance;} \\
(-0.014, 0.147) & \text{unequal variance.}
\end{cases}$$ \hspace{1cm} (10)
Outline

1. Statistical Inference
2. Frequentist Statistics
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6. Inference With Normals/Gaussians
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Bayesian Computations

Bayesian analysis requires computation of expectations and quantiles of probability distributions (posterior distributions).

Most often posterior distributions will not be standard distributions.

Then posterior quantities of inferential interest cannot be computed in closed form. Special techniques are needed.
Example M1. Suppose $X_1, X_2, \ldots, X_k$ are observed number of certain type of stars in $k$ similar regions. Model them as independent Poisson counts: $X_i \sim \text{Poisson}(\theta_i)$. $\theta_i$ are a priori considered related. $\nu_i = \log(\theta_i)$ is the $i$th element of $\nu$ and suppose 

$$\nu \sim N_k \left( \mu \mathbf{1}, \tau^2 \left\{(1 - \rho)I_k + \rho \mathbf{1} \mathbf{1}' \right\} \right),$$

where $\mathbf{1}$ is the $k$-vector with all elements being 1, and $\mu$, $\tau^2$ and $\rho$ are known constants. Then 

$$f(\mathbf{x} \mid \nu) = \exp \left( - \sum_{i=1}^{k} \{e^{\nu_i} - \nu_i x_i\} \right) / \prod_{i=1}^{k} x_i!.$$
\[ \pi(\boldsymbol{\nu}) \propto \exp \left( -\frac{1}{2\tau^2} (\boldsymbol{\nu} - \mu \mathbf{1})' \left( (1 - \rho) I_k + \rho \mathbf{1} \mathbf{1}' \right)^{-1} (\boldsymbol{\nu} - \mu \mathbf{1}) \right) \]

\[ \pi(\boldsymbol{\nu} \mid x) \propto \exp \left\{ -\sum_{i=1}^{k} \left\{ e^{\nu_i} - \nu_i x_i \right\} - \frac{(\nu - \mu \mathbf{1})'((1 - \rho) I_k + \rho \mathbf{1} \mathbf{1}')^{-1}(\nu - \mu \mathbf{1})}{2\tau^2} \right\}. \]

To obtain the posterior mean of \( \theta_j \), compute

\[ E^\pi(\theta_j \mid x) = E^\pi(\exp(\nu_j) \mid x) = \frac{\int_{\mathcal{R}^k} \exp(\nu_j) g(\nu \mid x) \, d\nu}{\int_{\mathcal{R}^k} g(\nu \mid x) \, d\nu}, \]

where \( g(\nu \mid x) = \exp \left\{ -\sum_{i=1}^{k} \left\{ e^{\nu_i} - \nu_i x_i \right\} - \frac{(\nu - \mu \mathbf{1})'((1 - \rho) I_k + \rho \mathbf{1} \mathbf{1}')^{-1}(\nu - \mu \mathbf{1})}{2\tau^2} \right\}. \)
This is a ratio of two \( k \)-dimensional integrals, and as \( k \) grows, the integrals become less and less easy to work with. Numerical integration techniques fail to be an efficient technique in this case. This problem, known as the \textit{curse of dimensionality}, is due to the fact that the size of the part of the space that is not relevant for the computation of the integral grows very fast with the dimension. Consequently, the error in approximation associated with this numerical method increases as the power of the dimension \( k \), making the technique inefficient.

The recent popularity of Bayesian approach to statistical applications is mainly due to advances in statistical computing. These include the E-M algorithm and the Markov chain Monte Carlo (MCMC) sampling techniques.
Monte Carlo Sampling

Consider an expectation that is not available in closed form. To estimate a population mean, gather a large sample from this population and consider the corresponding sample mean. The Law of Large Numbers guarantees that the estimate will be good provided the sample is large enough. Specifically, let $f$ be a probability density function (or a mass function) and suppose the quantity of interest is a finite expectation of the form

$$E_f h(X) = \int_{\chi} h(x)f(x) \, dx \quad (11)$$

(or the corresponding sum in the discrete case). If i.i.d. observations $X_1, X_2, \ldots$ can be generated from the density $f$, then

$$\bar{h}_m = \frac{1}{m} \sum_{i=1}^{m} h(X_i) \quad (12)$$

converges in probability to $E_f h(X)$. This justifies using $\bar{h}_m$ as an approximation for $E_f h(X)$ for large $m$. 
To provide a measure of accuracy or the extent of error in the approximation, compute the standard error. If $\text{Var}_f h(\mathbf{X})$ is finite, then $\text{Var}_f(\bar{h}_m) = \frac{\text{Var}_f h(\mathbf{X})}{m}$. Further, $\text{Var}_f h(\mathbf{X}) = E_f h^2(\mathbf{X}) - (E_f h(\mathbf{X}))^2$ can be estimated by

$$s_m^2 = \frac{1}{m} \sum_{i=1}^{m} (h(\mathbf{X}_i) - \bar{h}_m)^2,$$

and hence the standard error of $\bar{h}_m$ can be estimated by

$$\frac{1}{\sqrt{m}} s_m = \frac{1}{m} \left( \sum_{i=1}^{m} (h(\mathbf{X}_i) - \bar{h}_m)^2 \right)^{1/2}.$$
Confidence intervals for $E_fh(X)$: Using CLT

$$\frac{\sqrt{m} \left( \bar{h}_m - E_f h(X) \right)}{s_m} \xrightarrow{m \to \infty} N(0, 1), \text{ so}$$

$$\left( \bar{h}_m - z_{\alpha/2} s_m / \sqrt{m}, \bar{h}_m + z_{\alpha/2} s_m / \sqrt{m} \right)$$

can be used as an approximate $100(1 - \alpha)%$ confidence interval for $E_f h(X)$, with $z_{\alpha/2}$ denoting the $100(1 - \alpha/2)%$ quantile of standard normal.
If we want to approximate the posterior mean, try to generate i.i.d. observations from the posterior distribution and consider the mean of this sample. This is rarely useful because most often the posterior distribution will be a non-standard distribution which may not easily allow sampling from it. What are some other possibilities?
Example M2. Suppose $X$ is $N(\theta, \sigma^2)$ with known $\sigma^2$ and a Cauchy($\mu, \tau$) prior on $\theta$ is considered appropriate. Then

$$
\pi(\theta \mid x) \propto \exp\left( -\frac{(\theta - x)^2}{2\sigma^2} \right) \left( \tau^2 + (\theta - \mu)^2 \right)^{-1},
$$

and hence the posterior mean is

$$
E^\pi(\theta \mid x) = \frac{\int_{-\infty}^{\infty} \theta \exp\left( -\frac{(\theta - x)^2}{2\sigma^2} \right) \left( \tau^2 + (\theta - \mu)^2 \right)^{-1} \, d\theta}{\int_{-\infty}^{\infty} \exp\left( -\frac{(\theta - x)^2}{2\sigma^2} \right) \left( \tau^2 + (\theta - \mu)^2 \right)^{-1} \, d\theta}
$$

$$
= \frac{\int_{-\infty}^{\infty} \theta \left\{ \frac{1}{\sigma} \phi \left( \frac{\theta - x}{\sigma} \right) \right\} \left( \tau^2 + (\theta - \mu)^2 \right)^{-1} \, d\theta}{\int_{-\infty}^{\infty} \left\{ \frac{1}{\sigma} \phi \left( \frac{\theta - x}{\sigma} \right) \right\} \left( \tau^2 + (\theta - \mu)^2 \right)^{-1} \, d\theta},
$$

where $\phi$ denotes the density of standard normal.
$E^π(θ | x)$ is the ratio of expectation of $h(θ) = θ/(τ^2 + (θ - μ)^2)$ to that of $h(θ) = 1/(τ^2 + (θ - μ)^2)$, both expectations being with respect to the $N(x, σ^2)$ distribution. Therefore, we simply sample $θ_1, θ_2, \ldots$ from $N(x, σ^2)$ and use

$$E^π(θ | x) = \frac{\sum_{i=1}^{m} θ_i (τ^2 + (θ_i - μ)^2)^{-1}}{\sum_{i=1}^{m} (τ^2 + (θ_i - μ)^2)^{-1}}$$

as our Monte Carlo estimate of $E^π(θ | x)$. Note that (11) and (12) are applied separately to both the numerator and denominator, but using the same sample of $θ$’s. It is unwise to assume that the problem has been completely solved. The sample of $θ$’s generated from $N(x, σ^2)$ will tend to concentrate around $x$, whereas to satisfactorily account for the contribution of the Cauchy prior to the posterior mean, a significant portion of the $θ$’s should come from the tails of the posterior distribution.
Why not express the posterior mean in the form

\[ E^\pi(\theta \mid x) = \frac{\int_{-\infty}^{\infty} \theta \exp\left(-\frac{(\theta-x)^2}{2\sigma^2}\right) \pi(\theta) \, d\theta}{\int_{-\infty}^{\infty} \exp\left(-\frac{(\theta-x)^2}{2\sigma^2}\right) \pi(\theta) \, d\theta}, \]

and then sample \( \theta \)'s from \( \text{Cauchy}(\mu, \tau) \) and use the approximation

\[ \hat{E}^\pi(\theta \mid x) = \frac{\sum_{i=1}^{m} \theta_i \exp\left(-\frac{(\theta_i-x)^2}{2\sigma^2}\right)}{\sum_{i=1}^{m} \exp\left(-\frac{(\theta_i-x)^2}{2\sigma^2}\right)}? \]

However, this is also not satisfactory because the tails of the posterior distribution are not as heavy as those of the Cauchy prior, and there will be excess sampling from the tails relative to the center. So the convergence of the approximation will be slower resulting in a larger error in approximation (for a fixed \( m \)).
Ideally, therefore, sampling should be from the posterior distribution itself. With this view in mind, a variation of the above theme, called Monte Carlo importance sampling has been developed.
Consider (11) again. Suppose that it is difficult or expensive to sample directly from $f$, but there exists a probability density $u$ that is very close to $f$ from which it is easy to sample. Then we can rewrite (11) as

$$E_f h(X) = \int_X h(x)f(x) \, dx = \int_X h(x)\frac{f(x)}{u(x)} u(x) \, dx$$

$$= \int_X \{h(x)w(x)\} u(x) \, dx = E_u \{h(X)w(X)\},$$

where $w(x) = f(x)/u(x)$. Now apply (12) with $f$ replaced by $u$ and $h$ replaced by $hw$. In other words, generate i.i.d. observations $X_1, X_2, \ldots$ from the density $u$ and compute

$$\bar{hw}_m = \frac{1}{m} \sum_{i=1}^{m} h(X_i)w(X_i).$$

The sampling density $u$ is called the importance function.
A severe drawback of the standard Monte Carlo sampling/importance sampling: complete determination of the functional form of the posterior density is needed for implementation.

Situations where posterior distributions are incompletely specified or are specified indirectly cannot be handled: joint posterior distribution of the vector of parameters is specified in terms of several conditional and marginal distributions, but not directly.

This covers a large range of Bayesian analysis because a lot of Bayesian modeling is hierarchical so that the joint posterior is difficult to calculate but the conditional posteriors given parameters at different levels of hierarchy are easier to write down (and hence sample from).
Markov Chains in MCMC

A sequence of random variables \( \{X_n\}_{n \geq 0} \) is a Markov chain if for any \( n \), given the current value, \( X_n \), the past \( \{X_j, j \leq n - 1\} \) and the future \( \{X_j : j \geq n + 1\} \) are independent. In other words,

\[
P(A \cap B \mid X_n) = P(A \mid X_n)P(B \mid X_n),
\]

where \( A \) and \( B \) are events defined respectively in terms of the past and the future.

Important subclass: Markov chains with time homogeneous or stationary transition probabilities: the probability distribution of \( X_{n+1} \) given \( X_n = x \), and the past, \( X_j : j \leq n - 1 \) depends only on \( x \) and does not depend on the values of \( X_j : j \leq n - 1 \) or \( n \).

If the set \( S \) of values \( \{X_n\} \) can take, known as the state space, is countable, this reduces to specifying the transition probability matrix \( P \equiv ((p_{ij})) \) where for any two values \( i, j \) in \( S \), \( p_{ij} \) is the probability that \( X_{n+1} = j \) given \( X_n = i \), i.e., of moving from state \( i \) to state \( j \) in one time unit.
For state space $S$ that is not countable, specify a transition kernel or transition function $P(x, \cdot)$ where $P(x, A)$ is the probability of moving from $x$ into $A$ in one step, i.e., $P(X_{n+1} \in A \mid X_n = x)$.

Given the transition probability and the probability distribution of the initial value $X_0$, one can construct the joint probability distribution of $\{X_j : 0 \leq j \leq n\}$ for any finite $n$. i.e.,

$$P(X_0 = i_0, X_1 = i_1, \ldots, X_{n-1} = i_{n-1}, X_n = i_n)$$

$$= P(X_n = i_n \mid X_0 = i_0, \ldots, X_{n-1} = i_{n-1})$$

$$\times P(X_0 = i_0, X_1 = i_1, \ldots X_{n-1} = i_{n-1})$$

$$= p_{i_{n-1}i_n} P(X_0 = i_0, \ldots, X_{n-1} = i_{n-1})$$

$$= P(X_0 = i_0) p_{i_0i_1} p_{i_1i_2} \cdots p_{i_{n-1}i_n}.$$
A probability distribution $\pi$ is called \textit{stationary} or \textit{invariant} for a transition probability $P$ or the associated Markov chain $\{X_n\}$ if it is the case that when the probability distribution of $X_0$ is $\pi$ then the same is true for $X_n$ for all $n \geq 1$. Thus in the countable state space case a probability distribution $\pi = \{\pi_i : i \in S\}$ is stationary for a transition probability matrix $P$ if for each $j$ in $S$,

$$P(X_1 = j) = \sum_{i} P(X_1 = j \mid X_0 = i)P(X_0 = i)$$

$$= \sum_{i} \pi_i p_{ij} = P(X_0 = j) = \pi_j. \quad (14)$$

In vector notation it says $\pi = (\pi_1, \pi_2, \ldots)$ is a left eigenvector of the matrix $P$ with eigenvalue 1 and

$$\pi = \pi P. \quad (15)$$
Similarly, if $S$ is a continuum, a probability distribution $\pi$ with density $p(x)$ is *stationary* for the transition kernel $P(\cdot, \cdot)$ if

$$
\pi(A) = \int_A p(x) \, dx = \int_S P(x, A) p(x) \, dx
$$

for all $A \subset S$.

A Markov chain $\{X_n\}$ with a countable state space $S$ and transition probability matrix $P \equiv ((p_{ij}))$ is said to be *irreducible* if for any two states $i$ and $j$ the probability of the Markov chain visiting $j$ starting from $i$ is positive, i.e., for some $n \geq 1, p_{ij}^{(n)} \equiv P(X_n = j \mid X_0 = i) > 0$.

A similar notion of *irreducibility*, known as Harris or Doeblin irreducibility exists for the general state space case also.
Theorem (Law of Large Lumbers for Markov Chains).

\( \{X_n\}_{n \geq 0} \) is a Markov chain with a countable state space \( S \) and a transition probability matrix \( P \). Suppose it is *irreducible* and has a stationary probability distribution \( \pi \equiv (\pi_i : i \in S) \) as defined in (14). Then, for any bounded function \( h : S \to \mathbb{R} \) and for any initial distribution of \( X_0 \)

\[
\frac{1}{n} \sum_{i=0}^{n-1} h(X_i) \to \sum_{j} h(j)\pi_j \tag{16}
\]

in probability as \( n \to \infty \).

A similar law of large numbers (LLN) holds when the state space \( S \) is not countable. The limit value in (16) will be the integral of \( h \) with respect to the stationary distribution \( \pi \). A sufficient condition for the validity of this LLN is that the Markov chain \( \{X_n\} \) be Harris irreducible and have a stationary distribution \( \pi \).
A probability distribution $\pi$ on a set $S$ is given. Want to compute the “integral of $h$ with respect to $\pi$”, which reduces to $\sum_j h(j)\pi_j$ in the countable case.

**Look for an irreducible Markov chain $\{X_n\}$ with state space $S$ and stationary distribution $\pi$.** Starting from some initial value $X_0$, run the Markov chain $\{X_j\}$ for a period of time, say $0, 1, 2, \ldots n - 1$ and consider as an estimate

$$\mu_n = \frac{1}{n} \sum_{0}^{n-1} h(X_j).$$

By the LLN (16), $\mu_n$ will be close to $\sum_j h(j)\pi_j$ for large $n$. 
This technique is called *Markov chain Monte Carlo* (MCMC).

To approximate $\pi(A) \equiv \sum_{j \in A} \pi_j$ for some $A \subset S$ simply consider

$$
\pi_n(A) \equiv \frac{1}{n} \sum_{0}^{n-1} I_A(X_j) \to \pi(A),
$$

where $I_A(X_j) = 1$ if $X_j \in A$ and 0 otherwise.
An irreducible Markov chain \( \{X_n\} \) with a countable state space \( S \) is called *aperiodic* if for some \( i \in S \) the greatest common divisor, g.c.d. \( \{n : p_{ii}^{(n)} > 0\} = 1 \). Then, in addition to the LLN (16), the following result on the convergence of \( P(X_n = j) \) holds.

\[
\sum_j \left| P(X_n = j) - \pi_j \right| \to 0
\]  

(18)

as \( n \to \infty \), for any initial distribution of \( X_0 \). In other words, for large \( n \) the probability distribution of \( X_n \) will be close to \( \pi \). There exists a result similar to (18) for the general state space case also.
This suggests that instead of doing one run of length $n$, one could do $N$ independent runs each of length $m$ so that $n = Nm$ and then from the $i^{th}$ run use only the $m^{th}$ observation, say, $X_{m,i}$ and consider the estimate

$$
\hat{\mu}_{N,m} \equiv \frac{1}{N} \sum_{i=1}^{N} h(X_{m,i}).
$$

(19)
Metropolis-Hastings Algorithm

Very general MCMC method with wide applications. Idea is not to directly simulate from the given target density (which may be computationally difficult), but to simulate an easy Markov chain that has this target density as the stationary distribution.

Let $\pi$ be the target probability distribution on $S$, a finite or countable set. Let $Q \equiv (\{q_{ij}\})$ be a transition probability matrix such that for each $i$, it is computationally easy to generate a sample from the distribution $\{q_{ij} : j \in S\}$. Generate a Markov chain $\{X_n\}$ as follows. If $X_n = i$, first sample from the distribution $\{q_{ij} : j \in S\}$ and denote that observation $Y_n$. Then, choose $X_{n+1}$ from the two values $X_n$ and $Y_n$ according to

$$P(X_{n+1} = Y_n | X_n, Y_n) = \rho(X_n, Y_n) = 1 - P(X_{n+1} = X_n | X_n, Y_n),$$

where the “acceptance probability” $\rho(\cdot, \cdot)$ is given by

$$\rho(i, j) = \min \left\{ \frac{\pi_j q_{ji}}{\pi_i q_{ij}}, 1 \right\} \text{ for all } (i, j) \text{ such that } \pi_i q_{ij} > 0.$$
\( \{X_n\} \) is a Markov chain with transition probability matrix 
\( P = ((p_{ij})) \) given by

\[
p_{ij} = \begin{cases} 
q_{ij} \rho_{ij} & j \neq i, \\
1 - \sum_{k \neq i} p_{ik}, & j = i.
\end{cases}
\]  

(20)

\( Q \) is called the “proposal transition probability” and \( \rho \) the “acceptance probability”. A significant feature of this transition mechanism \( P \) is that \( P \) and \( \pi \) satisfy

\[
\pi_i p_{ij} = \pi_j p_{ji} \quad \text{for all } i, j.
\]  

(21)

This implies that for any \( j \)

\[
\sum_i \pi_i p_{ij} = \pi_j \sum_i p_{ji} = \pi_j,
\]  

(22)

or, \( \pi \) is a stationary probability distribution for \( P \).
Suppose $S$ is irreducible with respect to $Q$ and $\pi_i > 0$ for all $i$ in $S$. It can then be shown that $P$ is irreducible, and because it has a stationary distribution $\pi$, LLN (16) is available. This algorithm is thus a very flexible and useful one. The choice of $Q$ is subject only to the condition that $S$ is irreducible with respect to $Q$. A sufficient condition for the aperiodicity of $P$ is that $p_{ii} > 0$ for some $i$ or equivalently

$$\sum_{j \neq 1} q_{ij} \rho_{ij} < 1.$$ 

A sufficient condition for this is that there exists a pair $(i, j)$ such that $\pi_i q_{ij} > 0$ and $\pi_j q_{ji} < \pi_i q_{ij}$.

Recall that if $P$ is aperiodic, then both the LLN (16) and (18) hold.
If $S$ is not finite or countable but is a continuum and the target distribution $\pi(\cdot)$ has a density $p(\cdot)$, then one proceeds as follows: Let $Q$ be a transition function such that for each $x$, $Q(x, \cdot)$ has a density $q(x, y)$. Then proceed as in the discrete case but set the “acceptance probability” $\rho(x, y)$ to be

$$\rho(x, y) = \min \left\{ \frac{p(y)q(y, x)}{p(x)q(x, y)}, 1 \right\}$$

for all $(x, y)$ such that $p(x)q(x, y) > 0$.

A particularly useful feature of the above algorithm is that it is enough to know $p(\cdot)$ up to a multiplicative constant as the “acceptance probability” $\rho(\cdot, \cdot)$ needs only the ratios $p(y)/p(x)$ or $\pi_i/\pi_j$.

This assures us that in Bayesian applications it is not necessary to have the normalizing constant of the posterior density available for computation of the posterior quantities of interest.
Gibbs Sampling

Most of the new problems that Bayesians are asked to solve are high-dimensional: e.g. micro-arrays, image processing. Bayesian analysis of such problems involve target (posterior) distributions that are high-dimensional multivariate distributions.

In image processing, typically one has \( N \times N \) square grid of pixels with \( N = 256 \) and each pixel has \( k \geq 2 \) possible values. Each configuration has \( (256)^2 \) components and the state space \( S \) has \( k(256)^2 \) configurations. How does one simulate a random configuration from a target distribution over such a large \( S \)?

*Gibbs sampler* is a technique especially suitable for generating an irreducible aperiodic Markov chain that has as its stationary distribution a target distribution in a high-dimensional space having some special structure.

The most interesting aspect of this technique: to run this Markov chain, it suffices to generate observations from *univariate distributions*. 
The *Gibbs sampler* in the context of a bivariate probability distribution can be described as follows. Let $\pi$ be a target probability distribution of a bivariate random vector $(X, Y)$. For each $x$, let $P(x, \cdot)$ be the conditional probability distribution of $Y$ given $X = x$. Similarly, let $Q(y, \cdot)$ be the conditional probability distribution of $X$ given $Y = y$. Note that for each $x$, $P(x, \cdot)$ is a univariate distribution, and for each $y$, $Q(y, \cdot)$ is also a univariate distribution. Now generate a bivariate Markov chain $Z_n = (X_n, Y_n)$ as follows:

Start with some $X_0 = x_0$. Generate an observation $Y_0$ from the distribution $P(x_0, \cdot)$. Then generate an observation $X_1$ from $Q(Y_0, \cdot)$. Next generate an observation $Y_1$ from $P(X_1, \cdot)$ and so on. At stage $n$ if $Z_n = (X_n, Y_n)$ is known, then generate $X_{n+1}$ from $Q(Y_n, \cdot)$ and $Y_{n+1}$ from $P(X_{n+1}, \cdot)$.
If \( \pi \) is a discrete distribution concentrated on 
\( \{(x_i, y_j) : 1 \leq i \leq K, 1 \leq j \leq L\} \) and if \( \pi_{ij} = \pi(x_i, y_j) \) then
\[
P(x_i, y_j) = \pi_{ij}/\pi_i.
\]
and
\[
Q(y_j, x_i) = \pi_{ij}/\pi_j,
\]
where
\[
\pi_i = \sum_j \pi_{ij}, \quad \pi_j = \sum_i \pi_{ij}.
\]
Thus the transition probability matrix
\[
R = ((r_{ij}(k\ell)))
\]
for the \( \{Z_n\} \) chain is given by
\[
r_{ij}(k\ell) = Q(y_j, x_k)P(x_k, y_\ell)
\]
\[
= \frac{\pi_{kj}}{\pi_i} \frac{\pi_{k\ell}}{\pi_j}.
\]
Verify that this chain is irreducible, aperiodic, and has \( \pi \) as its stationary distribution. Thus LLN (16) and (18) hold in this case.
Thus for large \( n \), \( Z_n \) can be viewed as a sample from a distribution that is close to \( \pi \) and one can approximate
\[
\sum_{i,j} h(i, j) \pi_{ij}
\]
by
\[
\sum_{1=1}^{n} h(X_i, Y_i)/n.
\]
Illustration: Consider sampling from 
\[
\begin{pmatrix} X \\ Y \end{pmatrix} \sim N_2\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \right).
\]
The conditional distribution of \( X \) given \( Y = y \) and that of \( Y \) given \( X = x \) are

\[
X \mid Y = y \sim N(\rho y, 1 - \rho^2) \quad \text{and} \quad Y \mid X = x \sim N(\rho x, 1 - \rho^2). \tag{23}
\]

Using this property, Gibbs sampling proceeds as follows: Generate \((X_n, Y_n)\), \(n = 0, 1, 2, \ldots\), by starting from an arbitrary value \(x_0\) for \(X_0\), and repeat the following steps for \(i = 0, 1, \ldots, n\).

1. Given \(x_i\) for \(X\), draw a random deviate from \(N(\rho x_i, 1 - \rho^2)\) and denote it by \(Y_i\).
2. Given \(y_i\) for \(Y\), draw a random deviate from \(N(\rho y_i, 1 - \rho^2)\) and denote it by \(X_{i+1}\).
The theory of Gibbs sampling tells us that if $n$ is large, then $(x_n, y_n)$ is a random draw from a distribution that is close to $N_2\left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \right)$. 
Multivariate extension: \( \pi \) is a probability distribution of a \( k \)-dimensional random vector \((X_1, X_2, \ldots, X_k)\). If \( u = (u_1, u_2, \ldots, u_k) \) is any \( k \)-vector, let 
\( u_{-i} = (u_1, u_2, \ldots, u_{i-1}, u_{i+1}, \ldots, u_k) \) be the \( k-1 \) dimensional vector resulting by dropping the \( i \)th component \( u_i \). Let \( \pi_i(\cdot \mid x_{-i}) \) denote the univariate conditional distribution of \( X_i \) given that 
\( X_{-i} \equiv (X_1, X_2, X_{i-1}, X_{i+1}, \ldots, X_k) = x_{-i} \). Starting with some initial value for \( X_0 = (x_{01}, x_{02}, \ldots, x_{0k}) \) generate 
\( X_1 = (X_{11}, X_{12}, \ldots, X_{1k}) \) sequentially by generating \( X_{11} \) according to the univariate distribution \( \pi_1(\cdot \mid x_{0-1}) \) and then generating \( X_{12} \) according to \( \pi_2(\cdot \mid (X_{11}, x_{03}, x_{04}, \ldots, x_{0k})) \) and so on.
The most important feature to recognize here is that all the univariate conditional distributions, $X_i \mid X_{-i} = x_{-i}$, known as full conditionals should easily allow sampling from them. This is the case in most hierarchical Bayes problems. Thus, the Gibbs sampler is particularly well adapted for Bayesian computations with hierarchical priors.
Rao-Blackwellization

The variance reduction idea of the famous *Rao-Blackwell theorem* in the presence of auxiliary information can be used to provide improved estimators when MCMC procedures are adopted.

**Theorem (Rao-Blackwell)** Let $\delta(X_1, X_2, \ldots, X_n)$ be an estimator of $\theta$ with finite variance. Suppose that $T$ is sufficient for $\theta$, and let $\delta^*(T)$, defined by $\delta^*(t) = E(\delta(X_1, X_2, \ldots, X_n) \mid T = t)$, be the conditional expectation of $\delta(X_1, X_2, \ldots, X_n)$ given $T = t$. Then

$$E(\delta^*(T) - \theta)^2 \leq E(\delta(X_1, X_2, \ldots, X_n) - \theta)^2.$$  

The inequality is strict unless $\delta = \delta^*$, or equivalently, $\delta$ is already a function of $T$. 
By the property of iterated conditional expectation,

\[ E(\delta^*(T)) = E\left[ E(\delta(X_1, X_2, \ldots, X_n) \mid T) \right] = E(\delta(X_1, X_2, \ldots, X_n)). \]

Therefore, to compare the mean squared errors (MSE) of the two estimators, compare their variances only. Now,

\[
\begin{align*}
\text{Var}(\delta(X_1, X_2, \ldots, X_n)) &= \text{Var}[E(\delta \mid T)] + E[\text{Var}(\delta \mid T)] \\
&= \text{Var}(\delta^*) + E[\text{Var}(\delta \mid T)] > \text{Var}(\delta^*),
\end{align*}
\]

unless \( \text{Var}(\delta \mid T) = 0 \), which is the case only if \( \delta \) is a function of \( T \).
The Rao–Blackwell theorem involves two key steps: variance reduction by conditioning and conditioning by a sufficient statistic. The first step is based on the analysis of variance formula: For any two random variables $S$ and $T$, because

$$\text{Var}(S) = \text{Var}(E(S \mid T)) + E(\text{Var}(S \mid T)),$$

one can reduce the variance of a random variable $S$ by taking conditional expectation given some auxiliary information $T$. This can be exploited in MCMC.
\((X_j, Y_j), j = 1, 2, \ldots, N\): a single run of the Gibbs sampler algorithm with a target distribution of a bivariate random vector \((X, Y)\). Let \(h(X)\) be a function of the \(X\) component of \((X, Y)\) and let its mean value be \(\mu\). Goal is to estimate \(\mu\). A first estimate is the sample mean of the \(h(X_j), j = 1, 2, \ldots, N\). From the MCMC theory, as \(N \to \infty\), this estimate will converge to \(\mu\) in probability. The computation of variance of this estimator is not easy due to the (Markovian) dependence of the sequence \(\{X_j, j = 1, 2, \ldots, N\}\). Suppose we make \(n\) independent runs of Gibbs sampler and generate \((X_{ij}, Y_{ij}), j = 1, 2, \ldots, N; i = 1, 2, \ldots, n\). Suppose that \(N\) is sufficiently large so that \((X_{iN}, Y_{iN})\) can be regarded as a sample from the limiting target distribution of the Gibbs sampling scheme. Thus \((X_{iN}, Y_{iN}), i = 1, 2, \ldots, n\) form a random sample from the target distribution. Consider a second estimate of \(\mu\)—the sample mean of \(h(X_{iN}), i = 1, 2, \ldots, n\).
This estimator ignores part of the MCMC data but has the advantage that the variables $h(X_{iN}), i = 1, 2, \ldots, n$ are independent and hence the variance of their mean is of order $n^{-1}$. Now applying the variance reduction idea of the Rao-Blackwell theorem by using the auxiliary information $Y_{iN}, i = 1, 2, \ldots, n$, one can improve this estimator as follows:

Let $k(y) = E(h(X) \mid Y = y)$. Then for each $i$, $k(Y_{iN})$ has a smaller variance than $h(X_{iN})$ and hence the following third estimator,

$$\frac{1}{n} \sum_{i=1}^{n} k(Y_{iN}),$$

has a smaller variance than the second one. A crucial fact to keep in mind here is that the exact functional form of $k(y)$ be available for implementing this improvement.
(Example M2 continued.) \( X \mid \theta \sim N(\theta, \sigma^2) \) with known \( \sigma^2 \) and \( \theta \sim \text{Cauchy}(\mu, \tau) \). Simulate \( \theta \) from the posterior distribution, but sampling directly is difficult.

Gibbs sampling: Cauchy is a scale mixture of normal densities, with the scale parameter having a Gamma distribution.

\[
\pi(\theta) \propto (\tau^2 + (\theta - \mu)^2)^{-1} \propto \int_0^\infty \left( \frac{\lambda}{2\pi \tau^2} \right)^{1/2} \exp \left( -\frac{\lambda}{2\tau^2} (\theta - \mu)^2 \right) \lambda^{1/2-1} \exp(-\frac{\lambda}{2}) \ d\lambda,
\]

so that \( \pi(\theta) \) may be considered the marginal prior density from the joint prior density of \((\theta, \lambda)\) where

\[
\theta \mid \lambda \sim N(\mu, \tau^2/\lambda) \quad \text{and} \quad \lambda \sim \text{Gamma}(1/2, 1/2).
\]

This implicit hierarchical prior structure implies: \( \pi(\theta \mid x) \) is the marginal density from \( \pi(\theta, \lambda \mid x) \).
Full conditionals of $\pi(\theta, \lambda \mid x)$ are standard distributions:

$$\theta \mid \lambda, x \sim N \left( \frac{\tau^2}{\tau^2 + \lambda \sigma^2} x + \frac{\lambda \sigma^2}{\tau^2 + \lambda \sigma^2} \mu, \frac{\tau^2 \sigma^2}{\tau^2 + \lambda \sigma^2} \right), \quad (24)$$

$$\lambda \mid \theta, x \sim \lambda \mid \theta \sim \text{Exponential} \left( \frac{\tau^2 + (\theta - \mu)^2}{2\tau^2} \right). \quad (25)$$

Thus, the Gibbs sampler will use (24) and (25) to generate $(\theta, \lambda)$ from $\pi(\theta, \lambda \mid x)$. 
Example M5. $X$ = number of defectives in the daily production of a product. $(X \mid Y, \theta) \sim \text{binomial}(Y, \theta)$, where $Y$, a day’s production, is Poisson with known mean $\lambda$, and $\theta$ is the probability that any product is defective. The difficulty is that $Y$ is not observable, and inference has to be made on the basis of $X$ only. Prior: $(\theta \mid Y = y) \sim \text{Beta}(\alpha, \gamma)$, with known $\alpha$ and $\gamma$ independent of $Y$. Bayesian analysis here is not difficult because the posterior distribution of $\theta \mid X = x$ can be obtained as follows. First, $X \mid \theta \sim \text{Poisson}(\lambda \theta)$. Next, $\theta \sim \text{Beta}(\alpha, \gamma)$. Therefore,

$$
\pi(\theta \mid X = x) \propto \exp(-\lambda \theta)\theta^{x+\alpha-1}(1 - \theta)^{\gamma-1}, 0 < \theta < 1. (26)
$$
This is not a standard distribution, and hence posterior quantities cannot be obtained in closed form. Instead of focusing on $\theta \mid X$ directly, view it as a marginal component of $(Y, \theta \mid X)$. Check that the full conditionals of this are given by $Y \mid X = x, \theta \sim x + \text{Poisson}(\lambda(1 - \theta))$, and $\theta \mid X = x, Y = y \sim \text{Beta}(\alpha + x, \gamma + y - x)$ both of which are standard distributions.
Example M5 continued. It is actually possible here to sample from the posterior distribution using the accept-reject Monte Carlo method:

Let \( g(x)/K \) be the target density, where \( K \) is the possibly unknown normalizing constant of the unnormalized density \( g \). Suppose \( h(x) \) is a density that can be simulated by a known method and is close to \( g \), and suppose there exists a known constant \( c > 0 \) such that \( g(x) < ch(x) \) for all \( x \). Then, to simulate from the target density, the following two steps suffice.

Step 1. Generate \( Y \sim h \) and \( U \sim U(0, 1) \);
Step 2. Accept \( X = Y \) if \( U \leq g(Y)/(ch(Y)) \); return to Step 1 otherwise.

The optimal choice for \( c \) is \( \sup \{g(x)/h(x)\} \).
In Example M5, from (26),
\[ g(\theta) = \exp(-\lambda \theta) \theta^{x+\alpha-1} (1 - \theta)^{\gamma-1} I\{0 \leq \theta \leq 1\}, \]
so that \( h(\theta) \) may be chosen to be the density of Beta\((x + \alpha, \gamma)\).
Then, with the above-mentioned choice for \( c \), if 
\( \theta \sim \text{Beta}(x + \alpha, \gamma) \) is generated in Step 1, its ‘acceptance probability’ in Step 2 is simply \( \exp(-\lambda \theta) \).

Even though this method works here, let us see how the Metropolis-Hastings algorithm can be applied.

The required Markov chain is generated by taking the transition density \( q(z, y) = q(y \mid z) = h(y) \), independently of \( z \). Then the acceptance probability is
\[
\rho(z, y) = \min \left\{ \frac{g(y)h(z)}{g(z)h(y)}, 1 \right\} \\
= \min \left\{ \exp \left( -\lambda(y - z) \right), 1 \right\}.
\]
The steps involved in this “independent” M-H algorithm are:

Start at $t = 0$ with a value $x_0$ in the support of the target distribution; in this case, $0 < x_0 < 1$. Given $x_t$, generate the next value in the chain as given below.

(a) Draw $Y_t$ from $\text{Beta}(x + \alpha, \gamma)$.
(b) Let

$$x(t+1) = \begin{cases} 
Y_t & \text{with probability } \rho_t \\
x_t & \text{otherwise},
\end{cases}$$

where $\rho_t = \min\{\exp(-\lambda(Y_t - x_t)), 1\}$.
(c) Set $t = t + 1$ and go to step (a).

Run this chain until $t = n$, a suitably chosen large integer. In our example, for $x = 1$, $\alpha = 1$, $\gamma = 49$ and $\lambda = 100$, we simulated such a Markov chain. The resulting frequency histogram is shown in Figure below, with the true posterior density super-imposed on it.
Figure: M-H frequency histogram and true posterior density.
Outline

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Empirical Bayes Methods for High Dimensional Problems

This is becoming popular again, this time for ‘high dimensional’ problems. Astronomers routinely estimate characteristics of millions of similar astronomical objects – distance, radial velocity whatever. Consider the data:

\[
(X_1 = \begin{pmatrix} X_{11} \\ X_{12} \\ \vdots \\ X_{1n} \end{pmatrix}, X_2 = \begin{pmatrix} X_{21} \\ X_{22} \\ \vdots \\ X_{2n} \end{pmatrix}, \ldots, X_p = \begin{pmatrix} X_{p1} \\ X_{p2} \\ \vdots \\ X_{pn} \end{pmatrix}).
\]

\(X_j\) represents \(n\) repeated independent observations on the \(j\)th object, \(j = 1, 2, \ldots, p\). The important point is \(n\) is small, 2, 5, or 10, whereas \(p\) is large, such as a million.

Suppose \(X_{j1}, \ldots, X_{jn}\) measure \(\mu_j\) with variability \(\sigma^2\).

Problem: Maximum likelihood can give wrong estimates
Take $n = 2$ and suppose
\[
\begin{pmatrix} X_{j1} \\ X_{j2} \end{pmatrix} \sim N \left( \begin{pmatrix} \mu_j \\ \mu_j \end{pmatrix}, \begin{pmatrix} \sigma^2 & 0 \\ 0 & \sigma^2 \end{pmatrix} \right), \quad j = 1, 2, \ldots, p.
\]
i.e., we measure $\mu_j$ with 2 independent measurements, each coming with a $N(0, \sigma^2)$ error added to it; we do this for a very large number $p$ of objects. What is the MLE of $\sigma^2$?

\[
l(\mu_1, \ldots, \mu_p; \sigma^2 \mid x_1, \ldots, x_p) = f(x_1, \ldots, x_p \mid \mu_1, \ldots, \mu_p; \sigma^2)
\]

\[
= \prod_{j=1}^p \prod_{i=1}^2 f(x_{ji} \mid \mu_j, \sigma^2)
\]

\[
= (2\pi\sigma^2)^{-p} \exp\left(-\frac{1}{2\sigma^2} \sum_{j=1}^p \sum_{i=1}^2 (x_{ji} - \mu_j)^2\right)
\]

\[
= (2\pi\sigma^2)^{-p} \exp\left(-\frac{1}{2\sigma^2} \sum_{j=1}^p \left[ \sum_{i=1}^2 (x_{ji} - \bar{x}_j)^2 + 2(\bar{x}_j - \mu_j)^2 \right]\right).
\]
\[ \hat{\mu}_j = \bar{x}_j = (x_{j1} + x_{j2})/2 \text{ and} \]
\[
\hat{\sigma}^2 = \frac{1}{2p} \sum_{j=1}^{p} \sum_{i=1}^{2} (x_{ji} - \bar{x}_j)^2
\]
\[
= \frac{1}{2p} \sum_{j=1}^{p} \left[ \left( x_{j1} - \frac{x_{j1} + x_{j2}}{2} \right)^2 + \left( x_{j2} - \frac{x_{j1} + x_{j2}}{2} \right)^2 \right]
\]
\[
= \frac{1}{2p} \sum_{j=1}^{p} 2 \left( \frac{x_{j1} - x_{j2}}{2} \right)^2 = \frac{1}{4p} \sum_{j=1}^{p} (x_{j1} - x_{j2})^2.
\]

Since \( X_{j1} - X_{j2} \sim N(0, 2\sigma^2) \), \( j = 1, 2 \ldots \),
\[
\frac{1}{p} \sum_{j=1}^{p} (X_{j1} - X_{j2})^2 \xrightarrow{p \to \infty} 2\sigma^2, \text{ so that}
\]
\[
\hat{\sigma}^2 = \frac{1}{4p} \sum_{j=1}^{p} (X_{j1} - X_{j2})^2 \xrightarrow{p \to \infty} \frac{\sigma^2}{2}, \text{ and not } \sigma^2.
\]
Good estimates for $\sigma^2$ do exist, for example,

$$\frac{1}{2p} \sum_{j=1}^{p} (X_{j1} - X_{j2})^2 \xrightarrow{p \to \infty} 2\sigma^2.$$  

What is going wrong here?

This is not a small $p$, large $n$ problem, but a small $n$, large $p$ problem. i.e. a high dimensional problem, so needs care!

As $p \to \infty$, there are too many parameters to estimate and the likelihood function is unable to see where information lies, so tries to distribute it everywhere.

What is the way out? Go Bayesian!
There is a lot of information available on $\sigma^2$ (note $\sum_{j=1}^p (X_{j1} - X_{j2})^2 \sim 2\sigma^2 \chi_p^2$) but very little on individual $\mu_j$. However, if $\mu_j$ are ‘similar’, there is a lot of information on where they come from, because we get to see $p$ samples, $p$ large.

Suppose we are interested in $\mu_j$. How can we use the above information? Model as follows:

\[
\bar{X}_j \mid \mu_j, \sigma^2 \sim N(\mu_j, \sigma^2/2), \quad j = 1, \ldots p, \text{ independent observations.}
\]

$\sigma^2$ may be assumed known, since a reliable estimate

\[
\hat{\sigma}^2 = \frac{1}{2p} \sum_{j=1}^p (X_{j1} - X_{j2})^2
\]

is available. Express the information that $\mu_j$ are ‘similar’ in the form:

$\mu_j, j = 1, \ldots p$ is a random sample (collection) from $N(\eta, \tau^2)$.

Where do we get the $\eta$ and $\tau^2$, the prior mean and prior variance?

Marginally (or in predictive sense) $\bar{X}_j, j = 1, \ldots p$ is a random sample from $N(\mu_0, \tau^2 + \sigma^2/2)$. Use this random sample.
Estimate $\eta$ by $\hat{\eta} = \bar{X} = \frac{1}{p} \sum \bar{X}_j$ and $\tau^2$ by $\hat{\tau}^2 = \left( \frac{1}{p-1} \sum_{j=1}^{p} (\bar{X}_j - \bar{X})^2 - \sigma^2/2 \right)^+.

Now one could pretend that the prior for $(\mu_1, \ldots, \mu_p)$ is $N(\hat{\eta}, \hat{\tau}^2)$ and compute the Bayes estimates for $\mu_j$:

$$E(\mu_j \mid X_1, \ldots, X_p) = (1 - \hat{B}) \bar{X}_j + \hat{B} \bar{X},$$

where $\hat{B} = \frac{\sigma^2/2}{\sigma^2/2 + \hat{\tau}^2}$. If instead of 2 observations, each sample has $n$ observations, replace 2 by $n$. This is called Empirical Bayes since the prior is estimated using data. There is also a fully Bayesian counter-part called Hierarchical Bayes.
Consider a simpler, abstract problem instead. Suppose $X$ having density $f(x \mid \theta)$ is observed, with $\theta$ being an unknown element of the parameter space $\Theta$. We are interested in comparing two models $M_0$ and $M_1$:

\begin{align*}
M_0 & : \ X \text{ has density } f(x \mid \theta) \text{ where } \theta \in \Theta_0; \\
M_1 & : \ X \text{ has density } f(x \mid \theta) \text{ where } \theta \in \Theta_1. 
\end{align*} 

(27)

Simplify even further, and assume we want to test

\begin{align*}
M_0 : \theta = \theta_0 \text{ versus } M_1 : \theta \neq \theta_0,
\end{align*} 

(28)

Frequentist: A (classical) significance test is derived. It is based on a test statistic $T(X)$, large values of which are deemed to provide evidence against the null hypothesis, $M_0$. If data $X = x$ is observed, with corresponding $t = T(x)$, the P-value is

$$
\alpha = P_{\theta_0} (T(X) \geq T(x)).
$$
Example 6. Consider a random sample $X_1, \ldots, X_n$ from $N(\theta, \sigma^2)$, where $\sigma^2$ is known. Then $\bar{X}$ is sufficient for $\theta$ and it has the $N(\theta, \sigma^2/n)$ distribution. Noting that

$$T = T(\bar{X}) = \left| \sqrt{n} \left( \bar{X} - \theta_0 \right) / \sigma \right|$$

is a natural test statistic to test (28), one obtains the usual P-value as $\alpha = 2[1 - \Phi(t)]$, where $t = \left| \sqrt{n} (\bar{x} - \theta_0) / \sigma \right|$ and $\Phi$ is the standard normal cumulative distribution function.

What is a P-value and what does it say? P-value is the probability under a (simple) null hypothesis of obtaining a value of a test statistic that is at least as extreme as that observed in the sample data.

To compute a P-value we take the observed value of the test statistic to the reference distribution and check if it is likely or unlikely under $M_0$. 
Example 7. Rutherford and Geiger (1910) gave the following observed numbers of intervals of 1/8 minute when 0, 1, . . . \(\alpha\)-particles are ejected by a specimen. Check if Poisson fits well.

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<thead>
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<td>203</td>
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<tr>
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<td>139</td>
<td>45</td>
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<tr>
<td>Exp.</td>
<td>254</td>
<td>140</td>
<td>68</td>
<td>29</td>
<td>11</td>
<td>4</td>
</tr>
</tbody>
</table>

Test statistic:  
\[
T = \sum_{j=1}^{k} \frac{(O_i - E_i)^2}{E_i} \sim \chi^2_{k-2} \text{ approximately for large } n,
\]

where \(k\) is the number of cells, \(O_i\) is the observed and \(E_i\) is the expected count (estimated) for the \(i\)th cell.
Estimated Poisson intensity rate = \((\text{total number of particles ejected})/\text{(total number of intervals)}\) = \(100097/2608 \approx 3.87\). 

\(k = 13\).

P-value = \(P(T \geq 14.03) \approx 0.21\) (under \(\chi^2_{11}\)).
Likelihood Ratio Criterion

Standard likelihood ratio criterion for comparing $M_0$ and $M_1$ is

$$\lambda_n = \frac{f(x | \hat{\theta}_0)}{f(x | \hat{\theta})} = \frac{\max_{\theta \in \Theta_0} f(x | \theta)}{\max_{\theta \in \Theta_0 \cup \Theta_1} f(x | \theta)}.$$  \hspace{1cm} (29)

$0 < \lambda_n \leq 1$, and large values of $\lambda_n$ provide evidence for $M_0$. Reject $M_0$ for small values.

Use $\lambda_n$ (or a function of $\lambda_n$) as a test statistic if its distribution under $M_0$ can be derived. Otherwise, use the large sample result:

$$-2 \log(\lambda_n) \xrightarrow{\mathcal{L}} \chi^2_{p_1 - p_0},$$

under $M_0$ where $p_0$ and $p_1$ are dimensions of $\Theta_0$ and $\Theta_0 \cup \Theta_1$. 
Outline

1. Statistical Inference
2. Frequentist Statistics
3. Conditioning on Data
4. The Bayesian Recipe
5. Inference for Binomial proportion
6. Inference With Normals/Gaussians
7. Bayesian Computations
8. Empirical Bayes Methods for High Dimensional Problems
10. Bayesian Model Selection
11. Model Selection or Model Averaging?
12. References
Bayesian Model Selection

How does the Bayesian approach work?

\[ X \sim f(x \mid \theta) \] and we want to test

\[ M_0 : \theta \in \Theta_0 \quad \text{versus} \quad M_1 : \theta \in \Theta_1. \quad (30) \]

If \( \Theta_0 \) and \( \Theta_1 \) are of the same dimension (e.g.: \( M_0 : \theta \leq 0 \) and \( M_1 : \theta > 0 \)), choose a prior density that assigns positive prior probability to \( \Theta_0 \) and \( \Theta_1 \). Then calculate the posterior probabilities \( P\{\Theta_0 \mid x\} \), \( P\{\Theta_1 \mid x\} \) as well as the posterior odds ratio, namely,

\[ P\{\Theta_0 \mid x\} / P\{\Theta_1 \mid x\}. \]

Find a threshold like 1/9 or 1/19, etc. to decide what constitutes evidence against \( H_0 \).

Alternatively, let \( \pi_0 \) and \( 1 - \pi_0 \) be the prior probabilities of \( \Theta_0 \) and \( \Theta_1 \). Let \( g_i(\theta) \) be the prior p.d.f. of \( \theta \) under \( \Theta_i \) (or \( M_i \)), so that

\[ \int_{\Theta_i} g_i(\theta) \, d\theta = 1. \]
The prior in the previous approach is nothing but
\[ \pi(\theta) = \pi_0 g_0(\theta) I\{\theta \in \Theta_0\} + (1 - \pi_0) g_1(\theta) I\{\theta \in \Theta_1\}. \]

Need not require any longer that \(\Theta_0\) and \(\Theta_1\) are of the same dimension. Sharp null hypotheses are also covered. Proceed as before and report posterior probabilities or posterior odds. To compute these posterior quantities, note that the marginal density of \(X\) under the prior \(\pi\) can be expressed as
\[
m_{\pi}(x) = \int_{\Theta} f(x \mid \theta) \pi(\theta) \, d\theta
\]
\[
= \pi_0 \int_{\Theta_0} f(x \mid \theta) g_0(\theta) \, d\theta + (1 - \pi_0) \int_{\Theta_1} f(x \mid \theta) g_1(\theta) \, d\theta
\]
and hence the posterior density of \(\theta\) given the data \(X = x\) as
\[
\pi(\theta \mid x) = \frac{f(x \mid \theta) \pi(\theta)}{m_{\pi}(x)} = \begin{cases} 
\pi_0 f(x \mid \theta) g_0(\theta) / m_{\pi}(x) & \text{if } \theta \in \Theta_0 \\
(1 - \pi_0) f(x \mid \theta) g_1(\theta) / m_{\pi}(x) & \text{if } \theta \in \Theta_1
\end{cases}
\]
It follows then that

\[
P^\pi(M_0 \mid x) = P^\pi(\Theta_0 \mid x) = \frac{\pi_0}{m_\pi(x)} \int_{\Theta_0} f(x \mid \theta) g_0(\theta) \, d\theta
\]

\[
= \frac{\pi_0 \int_{\Theta_0} f(x \mid \theta) g_0(\theta) \, d\theta}{\pi_0 \int_{\Theta_0} f(x \mid \theta) g_0(\theta) \, d\theta + (1 - \pi_0) \int_{\Theta_1} f(x \mid \theta) g_1(\theta) \, d\theta}
\]

\[
P^\pi(M_1 \mid x) = P^\pi(\Theta_1 \mid x) = \frac{(1 - \pi_0)}{m_\pi(x)} \int_{\Theta_1} f(x \mid \theta) g_1(\theta) \, d\theta
\]

\[
= \frac{(1 - \pi_0) \int_{\Theta_1} f(x \mid \theta) g_1(\theta) \, d\theta}{\pi_0 \int_{\Theta_0} f(x \mid \theta) g_0(\theta) \, d\theta + (1 - \pi_0) \int_{\Theta_1} f(x \mid \theta) g_1(\theta) \, d\theta}
\]

One may also report the Bayes factor, which does not depend on \( \pi_0 \). The Bayes factor of \( M_0 \) relative to \( M_1 \) is defined as

\[
BF_{01} = \frac{P(\Theta_0 \mid x)}{P(\Theta_1 \mid x)} / \frac{P(\Theta_0)}{P(\Theta_1)} = \frac{\int_{\Theta_0} f(x \mid \theta) g_0(\theta) \, d\theta}{\int_{\Theta_1} f(x \mid \theta) g_1(\theta) \, d\theta}.
\]
Note:

- $BF_{10} = 1/BF_{01}$.
- Posterior odds ratio of $M_0$ relative to $M_1$:
  \[
  \frac{P(\Theta_0 \mid x)}{P(\Theta_1 \mid x)} = \left( \frac{\pi_0}{1 - \pi_0} \right) BF_{01}.
  \]
- Posterior odds ratio of $M_0$ relative to $M_1 = BF_{01}$ if $\pi_0 = \frac{1}{2}$.
- The smaller the value of $BF_{01}$, the stronger the evidence against $M_0$.

Testing as a model selection problem using Bayes factor illustrated below: Jeffreys test.
Jeffreys Test for Normal Mean; $\sigma^2$ Unknown

$X_1, X_2, \ldots, X_n$ a random sample from $N(\mu, \sigma^2)$. We want to test

$$M_0 : \mu = \mu_0 \text{ versus } M_1 : \mu \neq \mu_0$$

where $\mu_0$ is some specified number.

Parameter $\sigma^2$ is common in the two models corresponding to $M_0$ and $M_1$ and $\mu$ occurs only in $M_1$. Take the prior $g_0(\sigma) = 1/\sigma$ for $\sigma$ under $M_0$. Under $M_1$, take the same prior for $\sigma$ and add a conditional prior for $\mu$ given $\sigma$, namely

$$g_1(\mu \mid \sigma) = \frac{1}{\sigma} g_2\left(\frac{\mu}{\sigma}\right).$$

where $g_2(\cdot)$ is a p.d.f. Jeffreys suggested we should take $g_2$ to be Cauchy, so

$$g_0(\sigma) = \frac{1}{\sigma} \quad \text{under } M_0$$

$$g_1(\mu, \sigma) = \frac{1}{\sigma} g_1(\mu \mid \sigma) = \frac{1}{\sigma} \frac{1}{\sigma \pi (1 + \mu^2/\sigma^2)} \quad \text{under } M_1.$$
**Example 8.** Einstein’s theory of gravitation predicts the amount of deflection of light deflected by gravitation. Eddington’s expedition in 1919 (and other groups in 1922 and 1929) provided 4 observations: \( x_1 = 1.98, x_2 = 1.61, x_3 = 1.18, x_4 = 2.24 \) (all in seconds as measures of angular deflection). Suppose they are normally distributed around their predicted value \( \mu \). Then \( X_1, \cdots, X_4 \) are independent and identically distributed as \( N(\mu, \sigma^2) \). Einstein’s prediction is \( \mu = 1.75 \). Test \( M_0 : \mu = 1.75 \) versus \( M_1 : \mu \neq 1.75 \), where \( \sigma^2 \) is unknown.

Use the conventional priors of Jeffreys to calculate the Bayes factor.

\[
BF_{01} = 2.98.
\]

The calculations with the given data lend some support to Einstein’s prediction. However, the evidence in the data isn’t very strong.
BIC

When we compare two models $M_0 : \theta \in \Theta_0$ and $M_1 : \theta \in \Theta_1$, what does the Bayes factor

$$BF_{01} = \frac{\int_{\Theta_0} f(x | \theta) g_0(\theta) \, d\theta}{\int_{\Theta_1} f(x | \theta) g_1(\theta) \, d\theta} = \frac{m_0(x)}{m_1(x)}$$

measure?

$m_0(x)$ measures how well $M_0$ fits the data $x$ whereas $m_1(x)$ measures how well $M_1$ fits the same data, so $BF_{01}$ is the relative strength of the two models in the predictive sense. This can be difficult to compute for complicated models, so any good approximation is welcome.

Approximate marginal density $m(x)$ of $X$ for large sample size $n$:

$$m(x) = \int \pi(\theta)f(x | \theta) \, d\theta = ?$$
Laplace’s Method

\[ m(\mathbf{x}) = \int \pi(\theta) f(\mathbf{x} | \theta) \, d\theta = \int \pi(\theta) \prod_{i=1}^{n} f(x_i | \theta) \, d\theta \]

\[ = \int \pi(\theta) \exp\left(\sum_{i=1}^{n} \log f(x_i | \theta)\right) \, d\theta = \int \pi(\theta) \exp(nh(\theta)) \, d\theta. \]

where \( h(\theta) = \frac{1}{n} \sum_{i=1}^{n} \log f(x_i | \theta) \).

Consider any integral of the form

\[ I = \int_{-\infty}^{\infty} q(\theta) e^{nh(\theta)} \, d\theta \]

where \( q \) and \( h \) are smooth functions of \( \theta \) with \( h \) having a unique maximum at \( \hat{\theta} \).

If \( h \) has a unique sharp maximum at \( \hat{\theta} \), then most contribution to the integral \( I \) comes from the integral over a small neighborhood \((\hat{\theta} - \delta, \hat{\theta} + \delta)\) of \( \hat{\theta} \).
Study the behavior of $I$ as $n \to \infty$. As $n \to \infty$, we have

$$I \sim I_1 = \int_{\hat{\theta} - \delta}^{\hat{\theta} + \delta} q(\theta) e^{nh(\theta)} \, d\theta.$$ 

Laplace’s method involves Taylor series expansion of $q$ and $h$ about $\hat{\theta}$:

$$I \sim \int_{\hat{\theta} - \delta}^{\hat{\theta} + \delta} \left[ q(\hat{\theta}) + (\theta - \hat{\theta}) q'(\hat{\theta}) + \frac{1}{2} (\theta - \hat{\theta})^2 q''(\hat{\theta}) + \cdots \right]$$

$$\times \exp \left[ nh(\hat{\theta}) + nh'(\hat{\theta})(\theta - \hat{\theta}) + \frac{n}{2} h''(\hat{\theta})(\theta - \hat{\theta})^2 + \cdots \right]$$

$$\sim e^{nh(\hat{\theta})} q(\hat{\theta}) \int_{\hat{\theta} - \delta}^{\hat{\theta} + \delta} \left[ 1 + (\theta - \hat{\theta}) q'(\hat{\theta})/q(\hat{\theta}) + \frac{1}{2} (\theta - \hat{\theta})^2 \frac{q''(\hat{\theta})}{q(\hat{\theta})} \right]$$

$$\times \exp \left[ \frac{n}{2} h''(\hat{\theta})(\theta - \hat{\theta})^2 \right] \, d\theta.$$ 

Assume $c = -h''(\hat{\theta}) > 0$ and use a change of variable $t = \sqrt{nc}(\theta - \hat{\theta})$: 
\[ I \sim e^{nh(\hat{\theta})} q(\hat{\theta}) \frac{1}{\sqrt{nc}} \times \int_{-\delta \sqrt{nc}}^{\delta \sqrt{nc}} \left[ 1 + \frac{t}{\sqrt{nc}} q'(\hat{\theta})/q(\hat{\theta}) + \frac{t^2}{2nc} q''(\hat{\theta})/q(\hat{\theta}) \right] e^{-t^2/2} dt \]

\[ \sim e^{nh(\hat{\theta})} \frac{\sqrt{2\pi}}{\sqrt{nc}} q(\hat{\theta}) \left[ 1 + \frac{q''(\hat{\theta})}{2ncq(\hat{\theta})} \right] \]

\[ = e^{nh(\hat{\theta})} \frac{\sqrt{2\pi}}{\sqrt{nc}} q(\hat{\theta}) \left[ 1 + O(n^{-1}) \right]. \tag{32} \]

Apply (32) to \( m(x) = \int \pi(\theta)f(x \mid \theta) \, d\theta = \int \pi(\theta) \exp(nh(\theta)) \, d\theta \), with \( q = \pi \) and ignore terms that stay bounded.

\[ \log(m(x)) \approx nh(\hat{\theta}) - \frac{1}{2} \log n = \log(f(x \mid \hat{\theta})) - \frac{1}{2} \log n. \]
What Happens When $\theta$ is $p > 1$ Dimensional?

Simply replace (32) by its $p$ dimensional counter part:

$$I = e^{nh(\hat{\theta})}(2\pi)^{p/2}n^{-p/2} \det(\Delta_h(\hat{\theta}))^{-1/2}q(\hat{\theta})(1 + O(n^{-1}))$$

where $\Delta_h(\theta)$ denotes the Hessian of $-h$, i.e.,

$$\Delta_h(\theta) = \left(-\frac{\partial^2}{\partial \theta_i \partial \theta_j} h(\theta)\right)_{p \times p}.$$

Now apply this to

$$m(x) = \int \cdots \int \pi(\theta)f(x \mid \theta) \, d\theta = \int \cdots \int \pi(\theta) \exp(nh(\hat{\theta})) \, d\theta,$$

with $q = \pi$ and ignore terms that stay bounded. Then

$$\log(m(x)) \approx nh(\hat{\theta}) - \frac{p}{2} \log n = \log(f(x \mid \hat{\theta})) - \frac{p}{2} \log n.$$
Schwarz (1978) proposed a criterion, known as the BIC, based on (32) ignoring the terms that stay bounded as the sample size $n \to \infty$ (and general dimension $p$ for $\theta$):

$$BIC = \log f(x | \hat{\theta}) - (p/2) \log n$$

This serves as an approximation to the logarithm of the integrated likelihood of the model and is free from the choice of prior.

$2 \log BF_{01}$ is a commonly used evidential measure to compare the support provided by the data $x$ for $M_0$ relative to $M_1$. Under the above approximation we have,

$$2 \log(BF_{01}) \approx 2 \log \left( \frac{f(x | \hat{\theta}_0)}{f(x | \hat{\theta}_1)} \right) - (p_0 - p_1) \log n. \quad (33)$$

This is the approximate Bayes factor based on the Bayesian information criterion (BIC) due to Schwarz (1978). The term $(p_0 - p_1) \log n$ can be considered a penalty for using a more complex model.
AIC

Recall the likelihood ratio criterion: \( \lambda_n = \frac{f(x | \hat{\theta}_0)}{f(x | \hat{\theta})} \)

\[ P(M_0 \text{ is rejected} | M_0) = P(\lambda_n < c) \approx P(\chi^2_{p_1 - p_0} > -2 \log(c)) > 0, \]

so, from a frequentist point of view, a criterion based solely on the likelihood ratio does not converge to a sure answer under \( M_0 \).

Akaike (1983) suggested a penalized likelihood criterion:

\[
2 \log \left( \frac{f(x | \hat{\theta}_0)}{f(x | \hat{\theta}_1)} \right) - 2(p_0 - p_1) \tag{34}
\]

which is based on the Akaike information criterion (AIC), namely,

\[
AIC = 2 \log f(x | \hat{\theta}) - 2p
\]

for a model \( f(x | \theta) \). The penalty for using a complex model is not as drastic as that in BIC.
Example 9. Velocities (km/second) of 82 galaxies in six well-separated conic sections of the Corona Borealis region. How many clusters?
Consider mixture of normals:

\[
f(x \mid \theta) = \prod_{i=1}^{n} f(x_i \mid \theta) = \prod_{i=1}^{n} \left( \sum_{j=1}^{k} p_j \phi(x_i \mid \mu_j, \sigma_j^2) \right),
\]

where \( k \) is the number of mixture components, \( p_j \) is the weight given to the \( j \)th component, \( N(\mu_j, \sigma_j^2) \).

Models to consider:

\( M_k : X \) has density \( \sum_{j=1}^{k} p_j \phi(x_i \mid \mu_j, \sigma_j^2), \quad k = 1, 2 \ldots \)

i.e., \( M_k \) is a \( k \) component normal mixture.
Bayesian model selection procedure computes
\[ m(x \mid M_k) = \int \pi(\theta_k) f(x \mid \theta_k) \, d\theta_k, \]
for each \( k \) of interest and picks the one which gives the largest value.

**Example 9 contd.** Chib (1995), JASA:

<table>
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<th>( k )</th>
<th>( \sigma_j^2 )</th>
<th>( \log(m(x \mid M_k)) )</th>
</tr>
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<td>( \sigma_j^2 = \sigma^2 )</td>
<td>-240.464</td>
</tr>
<tr>
<td>3</td>
<td>( \sigma_j^2 = \sigma^2 )</td>
<td>-228.620</td>
</tr>
<tr>
<td>3</td>
<td>( \sigma_j^2 ) unrestricted</td>
<td>-224.138</td>
</tr>
</tbody>
</table>

3 component normal mixture model with unequal variances seems best.
From the Bayesian point of view, a natural approach to model uncertainty is to include all models, $M_k$, under consideration for future decisions.

i.e., Bypass the model-choice step entirely.

Unsuitable for scientific inference where selection of a model is a must.

Suitable for prediction purposes, since underestimation of uncertainty resulting from choosing model $\hat{M}_k$ is eliminated.
We have $\Theta = \bigcup_k \Theta_k,$

$$f(y \mid \theta) = f_k(y \mid \theta_k) \text{ if } \theta \in \Theta_k \text{ and}$$

$$\pi(\theta) = p_k g_k(\theta_k) \text{ if } \theta \in \Theta_k,$$

where $p_k = P_{\pi}(M_k)$ is the prior probability of $M_k$ and $g_k$ integrates to 1 over $\Theta_k$. Therefore, given the sample $x = (x_1, \ldots x_n),$ 

$$\pi(\theta \mid x) = \frac{f(x \mid \theta)\pi(\theta)}{m(x)}$$

$$= \sum_k p_k \frac{m(x)}{f_k(x \mid \theta_k) g_k(\theta_k) I_{\Theta_k}(\theta_k)}$$

$$= \sum_k P(M_k \mid x) g_k(\theta_k \mid x) I_{\Theta_k}(\theta_k).$$
Predictive density $m(y \mid x)$ given the sample $x = (x_1, \ldots x_n)$ is what is needed. This is given by

\[
m(y \mid x) = \int_{\Theta} f(y \mid \theta) \pi(\theta \mid x) \, d\theta
\]

\[
= \sum_k P(M_k \mid x) \int_{\Theta_k} f_k(y \mid \theta_k) g_k(\theta_k \mid x) \, d\theta_k
\]

\[
= \sum_k P(M_k \mid x) m_k(y \mid x),
\]

which is clearly obtained by averaging over all models.
Model fitting is like describing the data in a compact form. A model is better if it can provide a more compact description, or if it can compress the data more, or if it can be transmitted with fewer bits. Given a set of models to describe a data set, the best model is the one which provides the shortest description length.

In general one needs \( \log_2(n) \) bits to transmit \( n \), but patterns can reduce the description length.

- **100 · · · 0**: 1 followed by a million 0’s
- **1010 · · · 10**: pair 10 repeated a million times
If data \( x \) is known to arise from a probability density \( p \), then the optimal code length (in an average sense) is given by \(-\log p(x)\).

The optimal code length of \(-\log p(x)\) is valid only in the discrete case. What happens in the continuous case? Discretize \( x \) and denote it by \([x] = [x]_\delta\) where \( \delta \) denotes the precision. This means we consider

\[
P([x] - \delta/2 \leq X \leq [x] + \delta/2) = \int_{[x]-\delta/2}^{[x]+\delta/2} p(u) \, du \approx \delta p(x)
\]

instead of \( p(x) \) itself as far as coding of \( x \) is considered when \( x \) is one-dimensional. In the \( r \)-dimensional case, replace the density \( p(x) \) by the probability of the \( r \)-dimensional cube of side \( \delta \) containing \( x \), namely \( p([x])\delta^r \approx p(x)\delta^r \), so that the optimal code length changes to \(-\log p(x) - r \log \delta\).
MDL for Estimation or Model Fitting

Consider data $x \equiv x^n = (x_1, x_2, \ldots, x_n)$, and suppose

$$\mathcal{F} = \{ f(x^n | \theta) : \theta \in \Theta \}$$

is the collection of models of interest. Further, let $\pi(\theta)$ be a prior density for $\theta$. Given a value of $\theta$ (or a model), the optimal code length for describing $x^n$ is $-\log f(x^n | \theta)$, but since $\theta$ is unknown, its description requires a further $-\log \pi(\theta)$ bits on average. Therefore the optimal code length is obtained upon minimizing

$$DL(\theta) = -\log \pi(\theta) - \log f(x^n | \theta),$$

(35)

so that MDL amounts to seeking that model which minimizes the sum of

(i) the length, in bits, of the description of the model, and
(ii) the length, in bits, of data when encoded with the help of the model.
The posterior density of $\theta$ given the data $x^n$ is

$$
\pi(\theta \mid x^n) = \frac{f(x^n \mid \theta)\pi(\theta)}{m(x^n)},
$$

(36)

where $m(y)$ is the marginal or predictive density. Minimizing

$$
DL(\theta) = -\log \pi(\theta) - \log f(x^n \mid \theta) = -\log \{f(x^n \mid \theta)\pi(\theta)\}
$$

over $\theta$ is equivalent to maximizing $\pi(\theta \mid x^n)$. Thus MDL for estimation or model fitting is equivalent to finding the highest posterior density (HPD) estimate of $\theta$.

Consider the case of $\mathcal{F}$ having model parameters of different dimensions. Consider the continuous case and discretization. Denote $k$-dimensional $\theta$ by $\theta^k = (\theta_1, \theta_2, \ldots, \theta_k)$. Then
\[ DL(\theta^k) \]
\[ = - \log \{ \pi([\theta^k]_{\delta_\pi}) \delta^k \} - \log \{ f([x^n]_{\delta_f} | [\theta^k]_{\delta_\pi}) \delta^n_f \} \]
\[ = - \log \pi([\theta^k]_{\delta_\pi}) - k \log \delta_\pi - \log f([x^n]_{\delta_f} | [\theta^k]_{\delta_\pi}) - n \log \delta_f \]
\[ \approx - \log \pi(\theta^k) - k \log \delta_\pi - \log f(x^n | \theta^k) - n \log \delta_f. \]

Note that the term \(- n \log \delta_f\) is common across all models, so it can be ignored. However, the term \(- k \log \delta_\pi\) indicating the dimension of \(\theta\) in the model varies and is influential. According to Rissanen, \(\delta_\pi = 1/\sqrt{n}\) is optimal, in which case

\[ DL(\theta^k) \approx - \log f(x^n | \theta^k) - \log \pi(\theta^k) + \frac{k}{2} \log n + \text{ constant}. \]

(37)
References

1. Tom Loredo’s site: http://www.astro.cornell.edu/staff/loredo/bayes/
4. Bayesian Logical Data Analysis for Physical Sciences by P.C. Gregory, Cambridge University Press, 2005