Laplace Approximation

Zeel B Patel, Nipun Batra

August 27, 2023

IIT Gandhinagar

Outline

Brook Taylor

Pierre-Simon Laplace

Overall idea

- Posterior distribution $p(\boldsymbol{\theta}|\mathcal{D})$ might be intractable but we can compute the MAP estimate.
- We know that posterior would be in form: $p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} p(\mathcal{D}, \boldsymbol{\theta})$, where Z is the normalizing constant.
- We can approximate this posterior using Taylor series expansion around the MAP estimate and it turns out that, after making a few assumptions, the resulting distribution is a Gaussian: $p(\boldsymbol{\theta}|\mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}_{MAP}, H^{-1})$, where H is the Hessian matrix of the log joint evaluated at $\boldsymbol{\theta}_{MAP}$.

Taylor Series Expansion

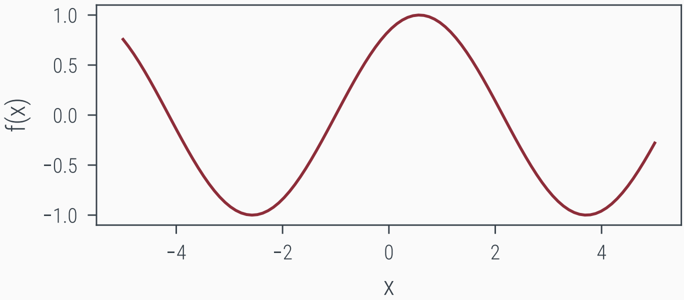
1D Taylor Series

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \frac{f'''(x_0)}{3!}(x - x_0)^3 + \ldots$$

Taylor Approximation of a 1D Function

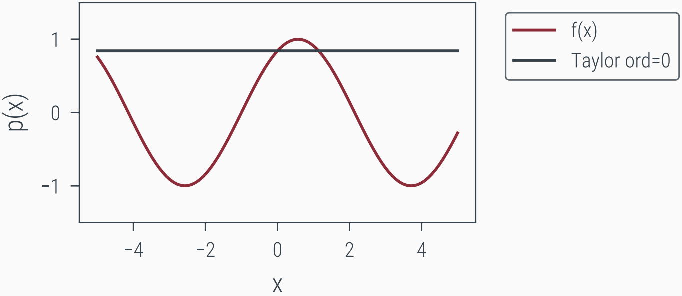
Consider the following function:

$$f(x) = \sin(1 + x)$$



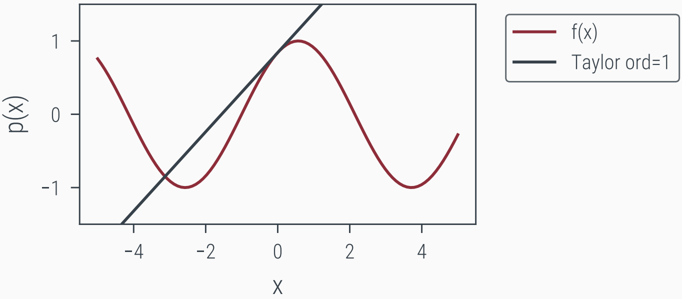
Taylor Approximation of a 1D Function

Taylor approximation at $x_0 = 0$:



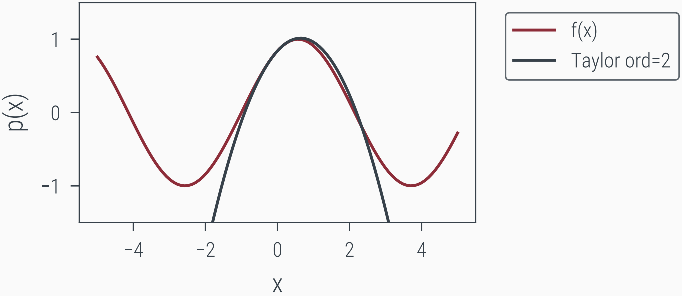
Taylor Approximation of a 1D Function

Taylor approximation at $x_0 = 0$:



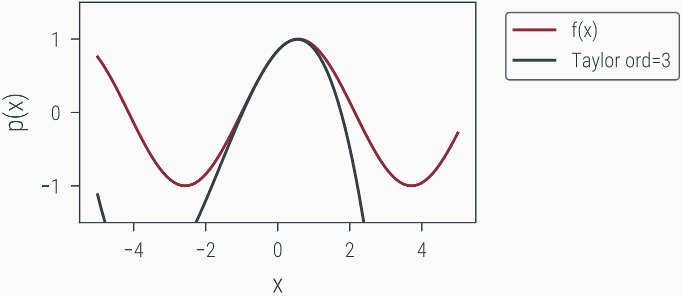
Taylor Approximation of a 1D Function

Taylor approximation at $x_0 = 0$:



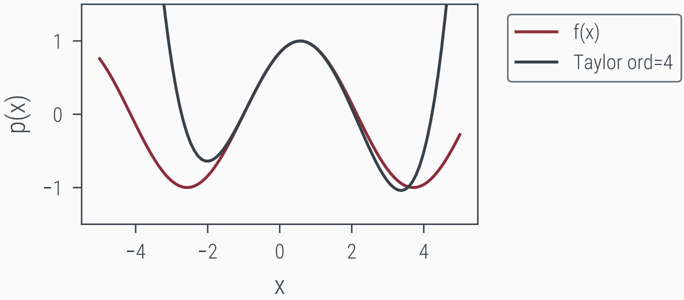
Taylor Approximation of a 1D Function

Taylor approximation at $x_0 = 0$:



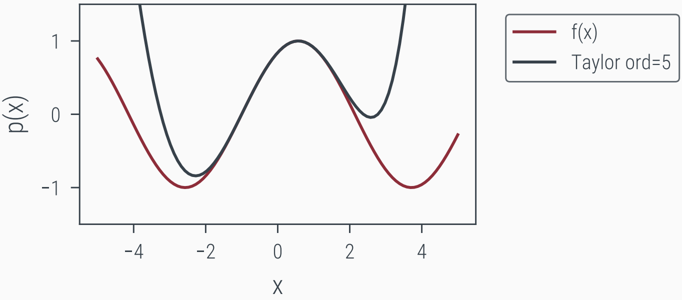
Taylor Approximation of a 1D Function

Taylor approximation at $x_0 = 0$:



Taylor Approximation of a 1D Function

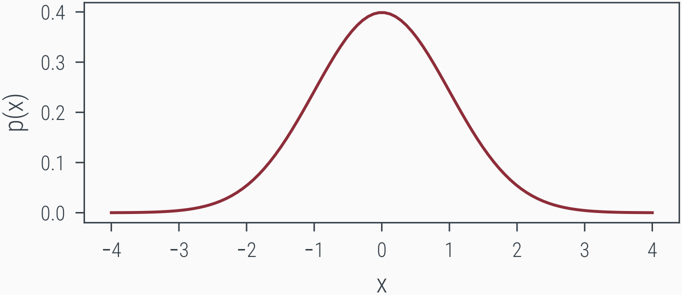
Taylor approximation at $x_0 = 0$:



Taylor Approximation of a 1D Gaussian Function

Consider the standard normal distribution: $p(x) \sim \mathcal{N}(x|0,1)$

$$p(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$$



Taylor Approximation of a 1D Gaussian Function

We will try to approximate log of the above function using Taylor series expansion around $x_0 = 0$.

Taylor Approximation of a 1D Gaussian Function

We will try to approximate log of the above function using Taylor series expansion around $x_0 = 0$.

$$f(x) = \log p(x) = \log\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{x^2}{2}$$

Taylor Approximation of a 1D Gaussian Function

We will try to approximate log of the above function using Taylor series expansion around $x_0 = 0$.

$$
\begin{aligned}
f(x) &= \log p(x) = \log\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{x^2}{2} \\
f(0) &= \log\left(\frac{1}{\sqrt{2\pi}}\right)
\end{aligned}
$$

Taylor Approximation of a 1D Gaussian Function

We will try to approximate log of the above function using Taylor series expansion around $x_0 = 0$.

$$f(x) = \log p(x) = \log\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{x^2}{2}$$

$$f(0) = \log\left(\frac{1}{\sqrt{2\pi}}\right)$$

$$f'(0) \cdot x = -x_0 \cdot x = 0$$

Taylor Approximation of a 1D Gaussian Function

We will try to approximate log of the above function using Taylor series expansion around $x_0 = 0$.

$$f(x) = \log p(x) = \log\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{x^2}{2}$$

$$f(0) = \log\left(\frac{1}{\sqrt{2\pi}}\right)$$

$$f'(0) \cdot x = -x_0 \cdot x = 0$$

$$f''(0) \cdot \frac{x^2}{2} = -1 \cdot \frac{x^2}{2}$$

Taylor Approximation of a 1D Gaussian Function

We will try to approximate log of the above function using Taylor series expansion around $x_0 = 0$.

$$f(x) = \log p(x) = \log\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{x^2}{2}$$

$$f(0) = \log\left(\frac{1}{\sqrt{2\pi}}\right)$$

$$f'(0) \cdot x = -x_0 \cdot x = 0$$

$$f''(0) \cdot \frac{x^2}{2} = -1 \cdot \frac{x^2}{2}$$

$$\text{Taylor approximated } \tilde{f}(x) = \log\left(\frac{1}{\sqrt{2\pi}}\right) - \frac{x^2}{2}$$

ND Taylor Series

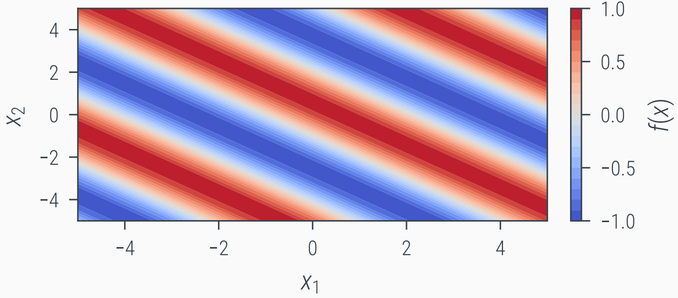
ND Taylor Series

$$f(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \nabla f(\boldsymbol{x}_0)^T(\boldsymbol{x} - \boldsymbol{x}_0) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^T \nabla^2 f(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0) + \dots$$

Approximate a 2d function

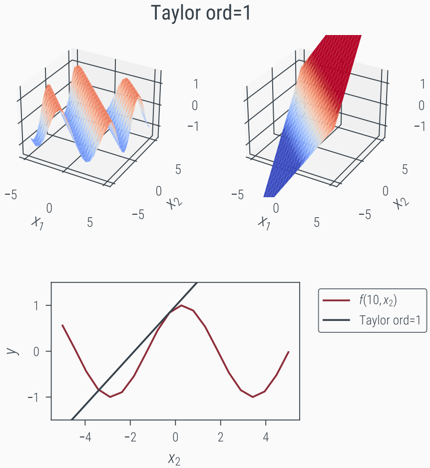
We take the following function:

$$f(x_1, x_2) = \sin(1 + x_1 + x_2)$$



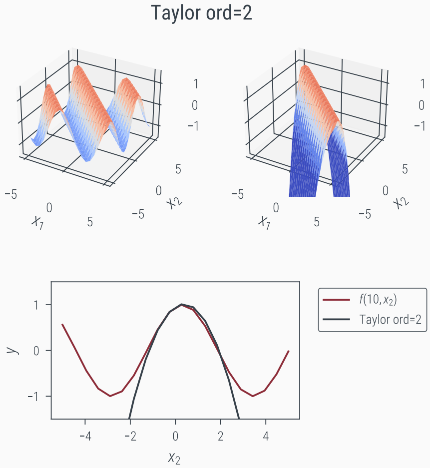
Approximate a 2d function

Taylor approximation at $x_0 = (0, 0)$:



Approximate a 2d function

Taylor approximation at $x_0 = (0, 0)$:



Laplace Approximation

Laplace Approximation

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} p(\mathcal{D}, \boldsymbol{\theta})$$

Laplace Approximation

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} p(\mathcal{D}, \boldsymbol{\theta})$$

We can rewrite this as:

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} e^{-f(\boldsymbol{\theta})}$$

$$f(\boldsymbol{\theta}) = -\log p(\mathcal{D}, \boldsymbol{\theta})$$

Laplace Approximation

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} p(\mathcal{D}, \boldsymbol{\theta})$$

We can rewrite this as:

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} e^{-f(\boldsymbol{\theta})}$$
$$f(\boldsymbol{\theta}) = -\log p(\mathcal{D}, \boldsymbol{\theta})$$

Note that $f(\boldsymbol{\theta})$ is the negative log joint which is used as a loss function to estimate $\boldsymbol{\theta}_{MAP}$.

Laplace Approximation

- Highest mass is concentrated around $\boldsymbol{\theta}_{MAP}$ and hence it makes sense to get Taylor approximation around that point.

Laplace Approximation

- Highest mass is concentrated around $\boldsymbol{\theta}_{MAP}$ and hence it makes sense to get Taylor approximation around that point.
- In other words, if our approximation is bad where we have low probability mass, it doesn't matter much.

Laplace Approximation

- Highest mass is concentrated around $\boldsymbol{\theta}_{MAP}$ and hence it makes sense to get Taylor approximation around that point.
- In other words, if our approximation is bad where we have low probability mass, it doesn't matter much.
- Thus, we expand $f(\boldsymbol{\theta})$ around $\boldsymbol{\theta}_{MAP}$ using Taylor series expansion up to second derivative:

$$
\begin{aligned}
f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_{MAP}) &+ \nabla f(\boldsymbol{\theta}_{MAP})^T(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP}) \\
&+ \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})
\end{aligned}
$$

Laplace Approximation

$$f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_{MAP}) + \nabla f(\boldsymbol{\theta}_{MAP})^T(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})$$
$$+ \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})$$

Laplace Approximation

$$
\begin{aligned}
f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_{MAP}) &+ \nabla f(\boldsymbol{\theta}_{MAP})^T(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP}) \\
&+ \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})
\end{aligned}
$$

Since, $\boldsymbol{\theta}_{MAP}$ is minima of $f(\boldsymbol{\theta})$, $\nabla f(\boldsymbol{\theta}_{MAP}) = 0$.

Laplace Approximation

$$
\begin{aligned}
f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_{MAP}) + \nabla f(\boldsymbol{\theta}_{MAP})^T(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP}) \\
+ \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})
\end{aligned}
$$

Since, $\boldsymbol{\theta}_{MAP}$ is minima of $f(\boldsymbol{\theta})$, $\nabla f(\boldsymbol{\theta}_{MAP}) = 0$.

$$
f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_{MAP}) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})
$$

Laplace Approximation

$$
\begin{aligned}
f(\boldsymbol{\theta}) \approx f(\boldsymbol{\theta}_{MAP}) + \nabla f(\boldsymbol{\theta}_{MAP})^T(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP}) \\
+ \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})
\end{aligned}
$$

Since, $\boldsymbol{\theta}_{MAP}$ is minima of $f(\boldsymbol{\theta})$, $\nabla f(\boldsymbol{\theta}_{MAP}) = 0$.

$$
\begin{aligned}
f(\boldsymbol{\theta}) &\approx f(\boldsymbol{\theta}_{MAP}) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T \nabla^2 f(\boldsymbol{\theta}_{MAP})(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP}) \\
&= f(\boldsymbol{\theta}_{MAP}) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})^T H(\boldsymbol{\theta} - \boldsymbol{\theta}_{MAP})
\end{aligned}
$$

where H is the Hessian matrix of $f(\boldsymbol{\theta})$ evaluated at $\boldsymbol{\theta}_{MAP}$.

Laplace Approximation

Plugging this back to the posterior equation:

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} e^{-f(\boldsymbol{\theta})}$$

Laplace Approximation

Plugging this back to the posterior equation:

$$
\begin{aligned}
p(\boldsymbol{\theta}|\mathcal{D}) &= \frac{1}{Z} e^{-f(\boldsymbol{\theta})} \\
&\approx \frac{1}{Z} e^{-f(\boldsymbol{\theta}_{MAP})} e^{-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})^T H(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})}
\end{aligned}
$$

Laplace Approximation

Plugging this back to the posterior equation:

$$\begin{aligned} p(\boldsymbol{\theta}|\mathcal{D}) &= \frac{1}{Z} e^{-f(\boldsymbol{\theta})} \\ &\approx \frac{1}{Z} e^{-f(\boldsymbol{\theta}_{MAP})} e^{-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})^T H(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})} \\ &\sim \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}_{MAP}, H^{-1}) \end{aligned}$$

Laplace Approximation

Plugging this back to the posterior equation:

$$\begin{aligned} p(\boldsymbol{\theta}|\mathcal{D}) &= \frac{1}{Z} e^{-f(\boldsymbol{\theta})} \\ &\approx \frac{1}{Z} e^{-f(\boldsymbol{\theta}_{MAP})} e^{-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})^T H (\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})} \\ &\sim \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}_{MAP}, H^{-1}) \\ Z &= p(\mathcal{D}, \boldsymbol{\theta}_{MAP}) \cdot (2\pi)^{D/2} \cdot |H|^{-\frac{1}{2}} \end{aligned}$$

Laplace Approximation

Plugging this back to the posterior equation:

$$
\begin{aligned}
p(\boldsymbol{\theta}|\mathcal{D}) &= \frac{1}{Z} e^{-f(\boldsymbol{\theta})} \\
&\approx \frac{1}{Z} e^{-f(\boldsymbol{\theta}_{MAP})} e^{-\frac{1}{2}(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})^T H(\boldsymbol{\theta}-\boldsymbol{\theta}_{MAP})} \\
&\sim \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}_{MAP}, H^{-1}) \\
Z &= p(\mathcal{D}, \boldsymbol{\theta}_{MAP}) \cdot (2\pi)^{D/2} \cdot |H|^{-\frac{1}{2}}
\end{aligned}
$$

Note that this result is not specific to Bayesian inference and can be used to approximate any intractable function.

Pros and Cons of Laplace Approximation

- Pros:
  - Simple to implement
  - Computationally efficient
  - Can be used to approximate any intractable function

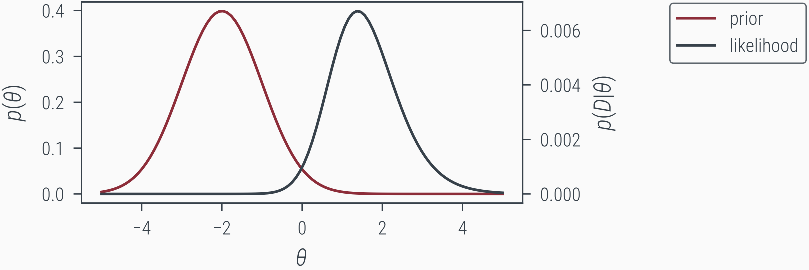
Pros and Cons of Laplace Approximation

- Pros:
  - Simple to implement
  - Computationally efficient
  - Can be used to approximate any intractable function
- Cons:
  - It can give bad approximation when posterior is not unimodal
  - Gaussian assumption can be too restrictive at times
  - Hessian matrix inversion can be numerically unstable and expensive. A diagonal or block-wise approximation can be applied to resolve this. Checkout Laplace-Redux for more details.

Normal Prior for Coin Toss

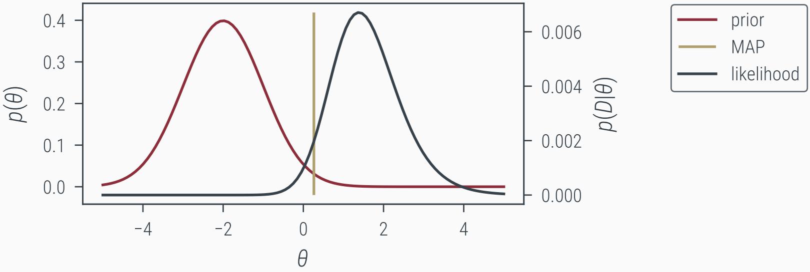
Consider the following coin toss experiment scenario:

- $\mathcal{D} = \{1, 1, 1, 1, 1, 1, 1, 0, 0\}$
- $p(\theta) = \mathcal{N}(\theta | -2, 1)$
- $h = \sigma(\theta)$
- $p(y|\theta) = h^y (1-h)^{1-y}$



Normal Prior for Coin Toss

First, we find the MAP estimate.



Normal Prior for Coin Toss

Now, according to the Laplace Approximation, the posterior is: