Laplace Approximation

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Outline

Taylor Series Expansion
ND Taylor Series
Laplace Approximation

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

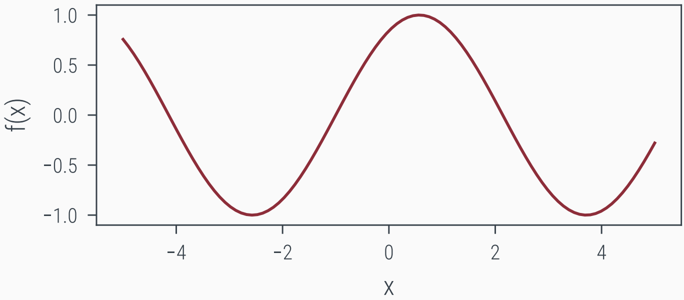
1D Taylor Series

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

Taylor Approximation of a 1D Function

Consider the following function:

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



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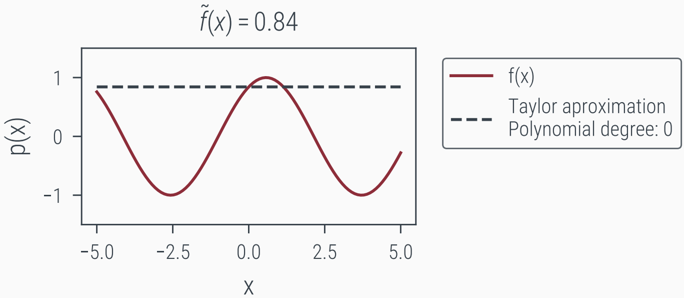

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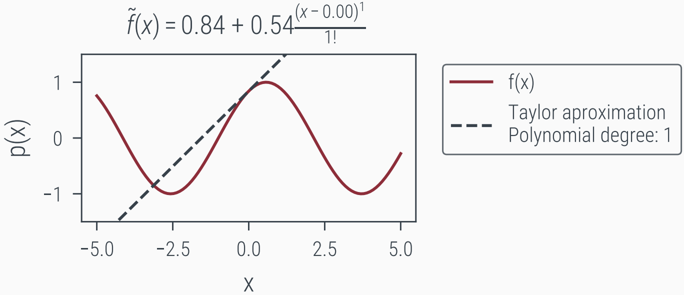

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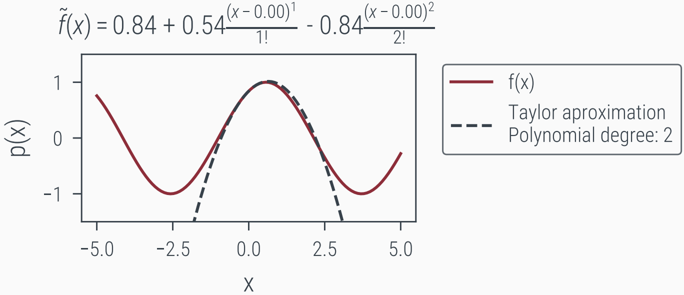

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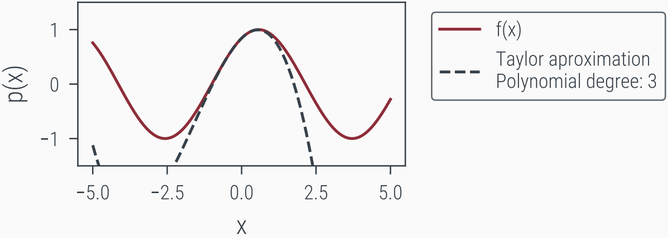
Taylor approximation at $x_0 = 0$:

$$\tilde{f}(x) = 0.84 + 0.54\frac{(x-0.00)^1}{1!} - 0.84\frac{(x-0.00)^2}{2!} - 0.54\frac{(x-0.00)^3}{3!}$$



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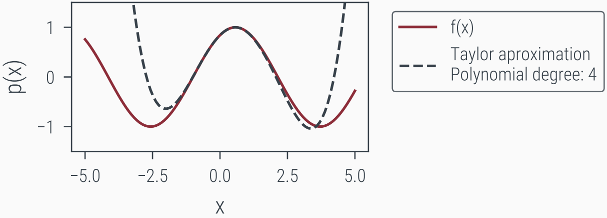

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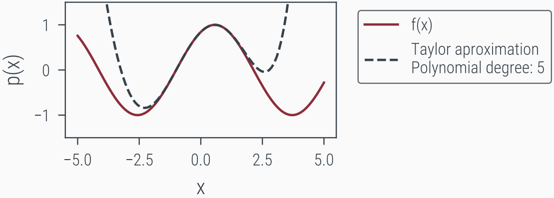

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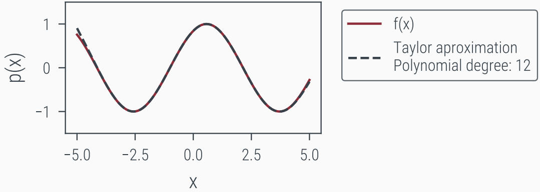
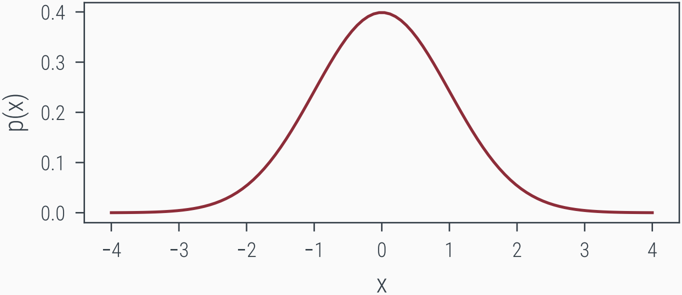


Taylor Approximation of a 1D Gaussian Function

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

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



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

ND Taylor Series

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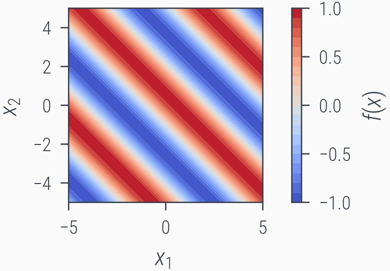
$$\tilde{f}(\boldsymbol{x}) = f(\boldsymbol{x}_0) + \nabla f(\boldsymbol{x}_0)^T(\boldsymbol{x} - \boldsymbol{x}_0) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{x}_0)^T \nabla^2 f(\boldsymbol{x}_0)(\boldsymbol{x} - \boldsymbol{x}_0) + \dots$$

Approximate a 2d function

We take the following function:

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



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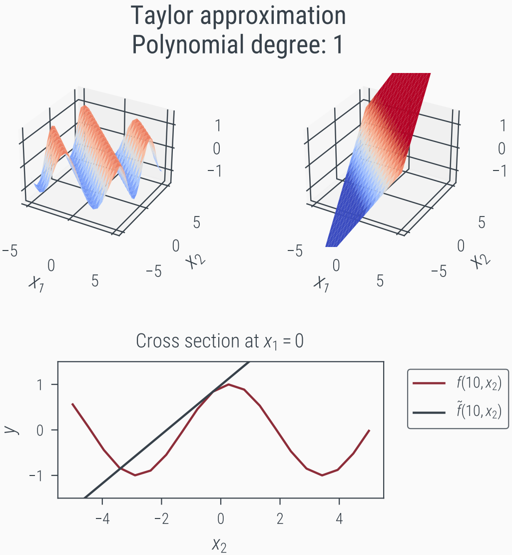

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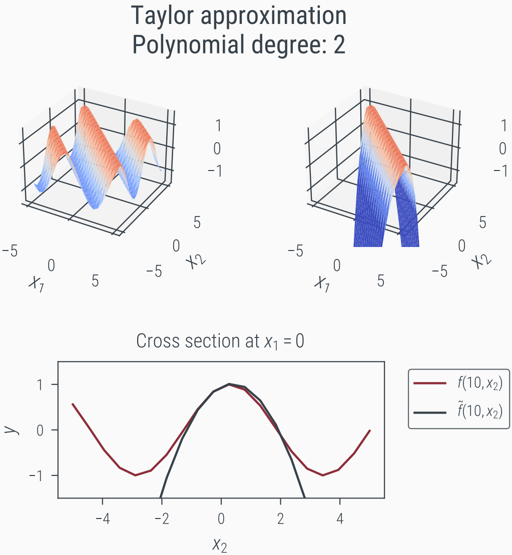

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We can rewrite this as:

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

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- In other words, if our approximation is bad where we have low probability mass, it doesn't matter much.
- Thus, we approximate $f(\boldsymbol{\theta})$ as $\tilde{f}(\boldsymbol{\theta})$ around $\boldsymbol{\theta}_{MAP}$ using Taylor series expansion up to second derivative:

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

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where $\nabla^2 f(\boldsymbol{\theta}_{MAP})$ is the Hessian matrix of $f(\boldsymbol{\theta})$ evaluated at $\boldsymbol{\theta}_{MAP}$.

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Plugging this back to the posterior equation:

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

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$$
p(\boldsymbol{\theta}|\mathcal{D}) \approx \mathcal{N}\left(\boldsymbol{\theta}|\boldsymbol{\theta}_{MAP}, \left(\nabla^2 f(\boldsymbol{\theta}_{MAP})\right)^{-1}\right)
$$

$$
Z = p(\mathcal{D}, \boldsymbol{\theta}_{MAP}) \cdot (2\pi)^{D/2} \cdot |\nabla^2 f(\boldsymbol{\theta}_{MAP})|^{-\frac{1}{2}}
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Pros and Cons of Laplace Approximation

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- 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.

Beta-Bernoulli Coin Toss

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- $h = \theta$
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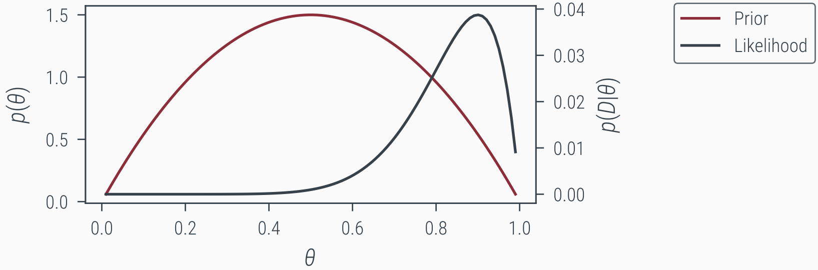
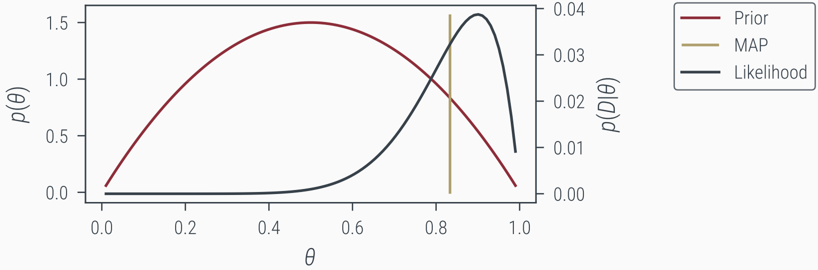


Beta-Bernoulli Coin Toss

MAP estimate:



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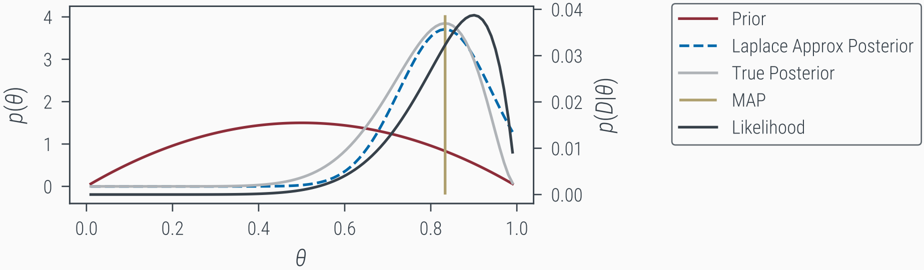
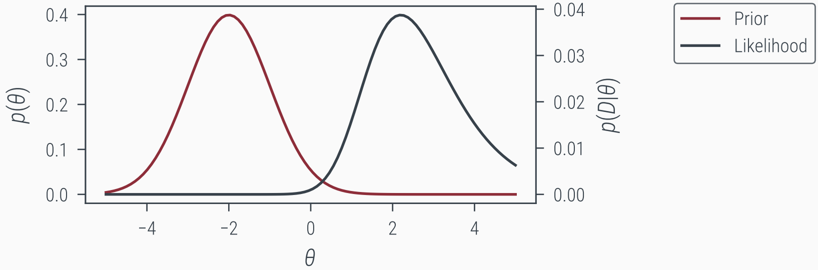


Normal Prior for Coin Toss

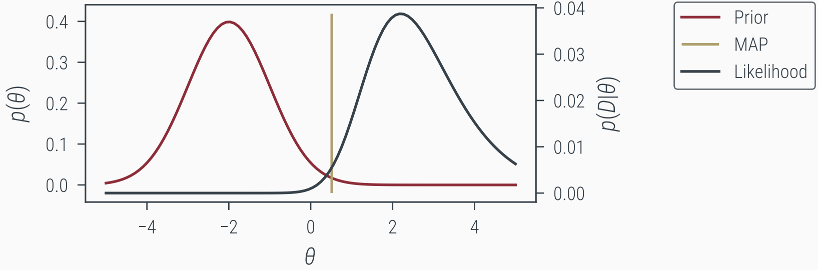
Consider the following coin toss experiment scenario:

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



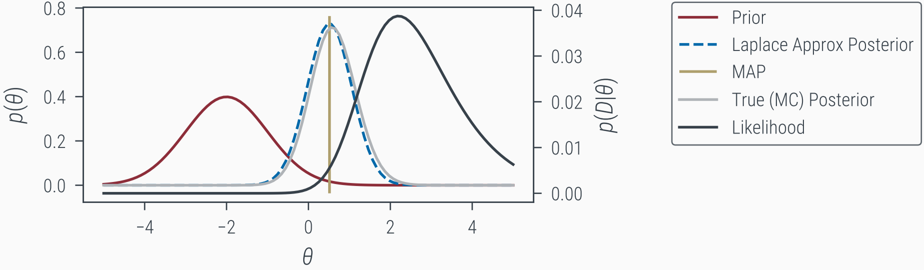
Normal Prior for Coin Toss

First, we find the MAP estimate.



Normal Prior for Coin Toss

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



We got True (MC) Posterior by a Monte Carlo estimation of the evidence.

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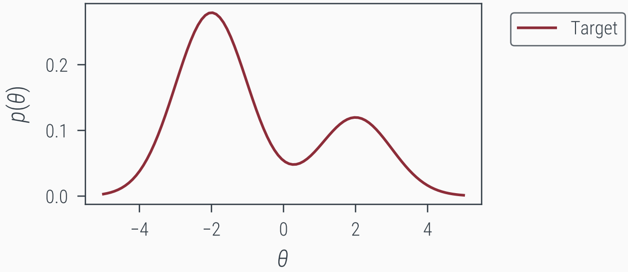

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