Probabilistic View of Linear Regression

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February 16, 2020

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Probabilistic View of Linear Regression

- Example function (black solid diagonal line) and its predictive uncertainty at x = 60 (drawn as a Gaussian).

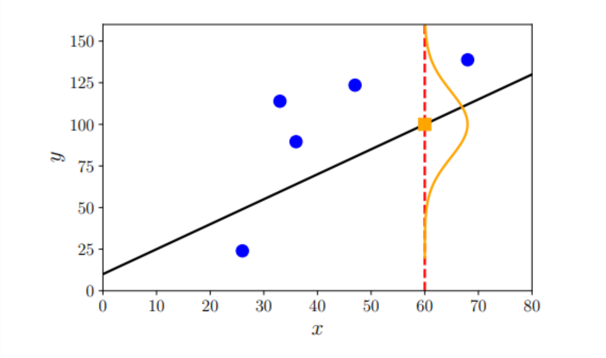

Figure 1: Probabilistic view of Linear Regression. Note that we don't have point estimates any longer.

Probabilistic View of Linear Regression

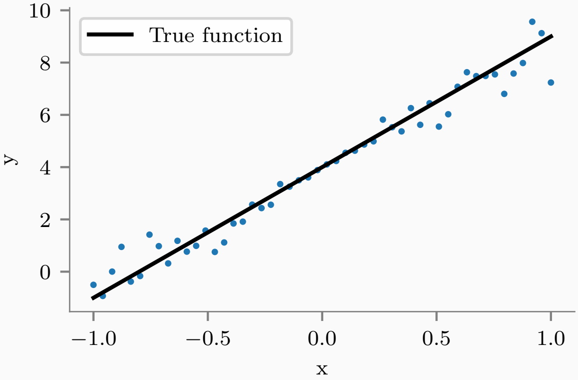

Figure 2: Dataset we will be using for this exercise

Probabilistic View of Linear Regression

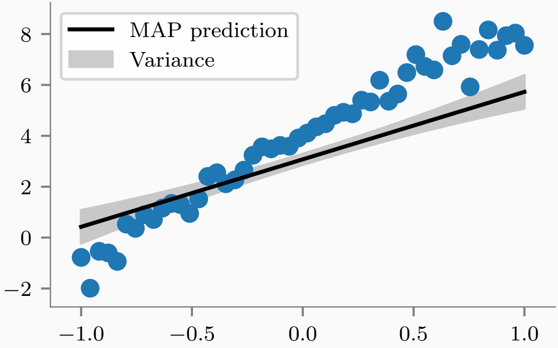

Figure 3: Sample predictions we will be making (with variance)

Probabilistic View of Linear Regression

- In this view, we consider a likelihood function

$$p(y|\mathbf{x}) = \mathcal{N}\left(y|f(\mathbf{x}), \sigma^2\right)$$

where $\mathbf{x} \in \mathbb{R}^D$ and the inputs and $y \in \mathbb{R}$ are the noisy function values, with the functional relationship between $\mathbf{x}$ and y given by

$$y = f(\mathbf{x}) + \epsilon,$$

where $\epsilon \sim \mathcal{N}(0, \sigma^2)$, is i.i.d. measurement noise with mean 0 and variance σ^2.

- Suppose we are given a training set $\mathcal{D} := \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_N)\}$, consisting of N inputs $x_n \in \mathbb{R}^D$ and corresponding targets $y_n \in \mathbb{R}$, $n = 1, 2, 3, \ldots N$. The graphical model for the same under the probabilistic viewpoint is as given below.

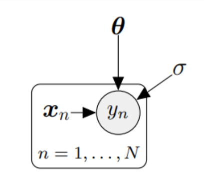

Figure 4: Probabilistic Graphical Model for Linear Regression

Parameter Estimation and MLE

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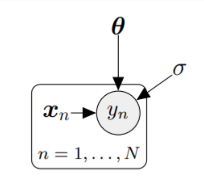

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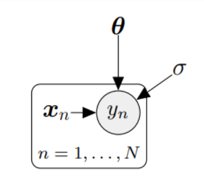

Figure 4: Probabilistic Graphical Model for Linear Regression

In the above PGM, the observed random variables are shaded and the deterministic random variables are without circles.

Parameter Estimation and MLE

- Note that y_i and y_j are conditionally independent given their respective inputs $\boldsymbol{x}_i, \boldsymbol{x}_j$ so that the likelihood factorizes according to

$$\begin{aligned} p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) &= p\left(y_1, \ldots, y_N | \boldsymbol{x}_1, \ldots, \boldsymbol{x}_N, \boldsymbol{\theta}\right) \\ &= \prod_{n=1}^{N} p\left(y_n | \boldsymbol{x}_n, \boldsymbol{\theta}\right) = \prod_{n=1}^{N} \mathcal{N}\left(y_n | \boldsymbol{x}_n^\top \boldsymbol{\theta}, \sigma^2\right) \end{aligned}$$

where $\mathcal{X} := \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$ and $\mathcal{Y} := \{y_1, y_2, \ldots, y_n\}$.

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  where $\mathcal{X} := \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n\}$ and $\mathcal{Y} := \{y_1, y_2, \ldots, y_n\}$.
- The likelihood and the factors $p(y_n|\boldsymbol{x}_n, \boldsymbol{\theta})$ are Gaussian due to the noise distribution.

Prediction

- Note that once we have the optimal parameters $\boldsymbol{\theta}^* \in \mathbb{R}^D$, we can predict function values using this parameter estimate. For an arbitrary test input $\boldsymbol{x}_*$ the corresponding distribution of y_* then becomes the following:

$$p(y_*|\boldsymbol{x}_*, \boldsymbol{\theta}) = \mathcal{N}(y_*|\boldsymbol{x}_*^\top \boldsymbol{\theta}^*, \sigma^2)$$

Maximum Likelihood Estimate

- A typically widely used method to find the desired parameters $\boldsymbol{\theta}_{ML}$ is *maximum likelihood estimation*, where we find the parameters that maximize the likelihood.

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- Important Remark: The likelihood $p(\mathbf{y}|\mathbf{x}, \boldsymbol{\theta})$ is not a probability distribution in $\boldsymbol{\theta}$. It is a function of $\boldsymbol{\theta}$ and need not integrate to 1. Note that we compute likelihood for a given $\mathcal{Y}$ and $\mathcal{X}$.

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- When we write $p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta})$, we are talking about the conditional distribution of $\mathcal{Y}$, given a fixed $\mathcal{X}$ and $\boldsymbol{\theta}$. In the case of likelihood, $\boldsymbol{\theta}$ is the variable.

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- When we want to maximize likelihood, we are trying to maximize the product of several probabilities. This can lead to numerical underflow.
- Since logarithm function is monotonic, maximizing the logarithm of a function is equivalent to maximizing the function.

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$$\log p\left(y_n|\mathbf{x}_n,\boldsymbol{\theta}\right) = -\frac{1}{2\sigma^2}\left(y_n - \mathbf{x}_n^\top\boldsymbol{\theta}\right)^2 + \text{ const}$$

where the constant is independent of $\boldsymbol{\theta}$.

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and $\boldsymbol{X} := [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N] \in \mathbb{R}^{N \times D}$ and $\boldsymbol{y} := [y_1, \ldots, y_N]^\top \in \mathbb{R}^N$.

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$$\boldsymbol{\theta}_{ML} = (\boldsymbol{X}^\top\boldsymbol{X}^{-1})\boldsymbol{X}^\top\boldsymbol{y}$$

Visualising Likelihood

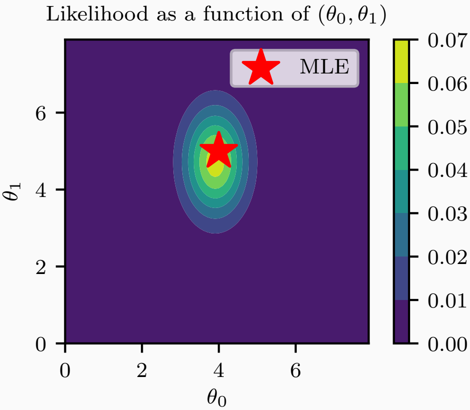

Figure 5: Likelihood (not $\mathcal{LL}$) for our data set

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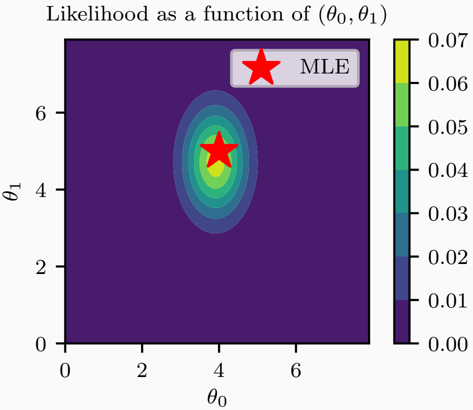

Figure 5: Likelihood (not $\mathcal{LL}$) for our data set

$$\mathcal{L}(\theta) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(y_i - \hat{y}_i)^2}{2\sigma^2}}$$

Visualising MLE fit

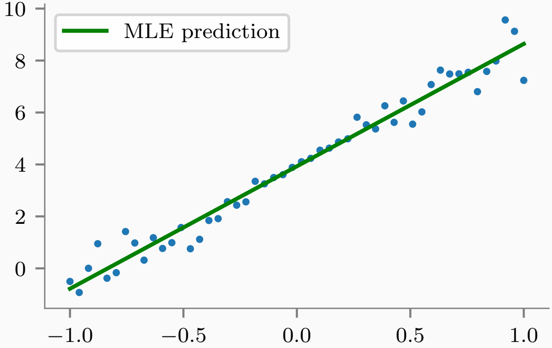

Figure 6: MLE prediction

Estimating the noise variance

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- Now :Relax this assumption and obtain a maximum likelihood estimator σ^2_{ML} for the noise variance.
- We use the same procedure as above: write down the log-likelihood, compute its derivative with respect to $\sigma^2 > 0$, set it to 0 and obtain the needed estimate.

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$$\log p\left(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta},\sigma^2\right)$$
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&= \sum_{n=1}^{N} \log \mathcal{N}\left(y_n | \mathbf{x}_n^T \boldsymbol{\theta}, \sigma^2\right) \\
&= \sum_{n=1}^{N} \left(-\frac{1}{2}\log(2\pi) - \frac{1}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\left(y_n - x_n^T \boldsymbol{\theta}\right)^2 \right)
\end{aligned}
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&\log p\left(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}, \sigma^2\right) \\
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&= \sum_{n=1}^{N}\left(-\frac{1}{2} \log(2\pi) - \frac{1}{2} \log \sigma^2 - \frac{1}{2\sigma^2}\left(y_n - x_n^T \boldsymbol{\theta}\right)^2\right) \\
&= -\frac{N}{2} \log \sigma^2 - \frac{1}{2\sigma^2} \sum_{n=1}^{N}\left(y_n - x_n^T \boldsymbol{\theta}\right)^2 + \text{ const.}
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$$\frac{N}{2\sigma^2} = \frac{s}{2\sigma^4}$$

Which is the same as

$$\sigma^2_{\mathrm{ML}} = \frac{s}{N} = \frac{1}{N}\sum_{n=1}^{N}\left(y_n - x_n^T\boldsymbol{\theta}\right)^2$$

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- Answer: We place a prior $p(\boldsymbol{\theta})$ on the parameters.
- Example: Gaussian prior $p(\theta) = \mathcal{N}(0, 1)$ on a parameter which we expect to lie in the interval [-2, 2].
- Once we have a dataset $\mathcal{X}, \mathcal{Y}$, instead of maximizing the likelihood, we seek parameters to maximize the posterior distribution $p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y})$.

Visualizing Prior

We choose a prior as $\mathcal{N}_2([0\ 0]^T, \mathcal{I})$

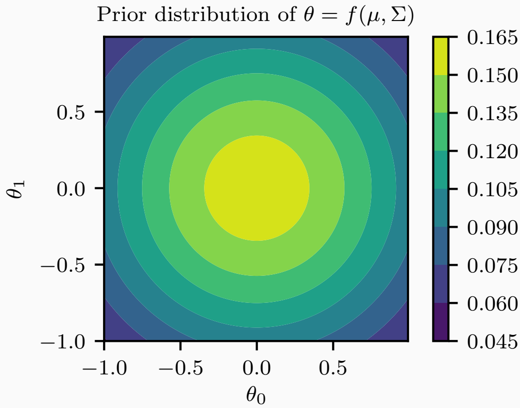

Figure 7: Prior distribution

Samples from Prior

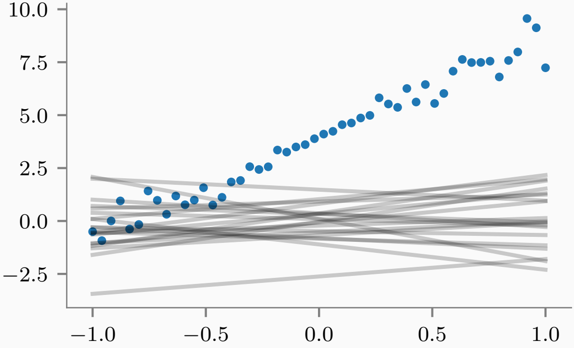

Figure 8: Samples from prior distribution

Maximum A Posteriori Estimation

- From Bayes Theorem, we have

$$p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{Y}|\mathcal{X})}$$

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- Use the prior distribution $\mathcal{N}(0, b^2 I_n)$
- Draw covariance matrix

Maximum A Posteriori Estimation

- To find the MAP estimate, we follow the same steps as for MLE, firstly by considerating the log-posterior.

$$\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \log p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) + \text{ const}$$

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- We have,

$$\boldsymbol{\theta}_{\mathrm{MAP}} \in \arg\min_{\boldsymbol{\theta}} \{-\log p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) - \log p(\boldsymbol{\theta})\}$$

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- Now computing the gradient with respect to $\boldsymbol{\theta}$, we have

$$-\frac{\mathrm{d} \log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y})}{\mathrm{d}\boldsymbol{\theta}} = -\frac{\mathrm{d} \log p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta})}{\mathrm{d}\boldsymbol{\theta}} - \frac{\mathrm{d} \log p(\boldsymbol{\theta})}{\mathrm{d}\boldsymbol{\theta}}$$

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- Using the conjugate Gaussian Prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, b^2 \boldsymbol{I})$ on the parameters $\boldsymbol{\theta}$, we get the negative log posterior as follows:

$$-\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{1}{2\sigma^2}(y - X\theta)^\top (y - X\theta) + \frac{1}{2b^2}\theta^\top \theta + \text{ const}$$

Maximum A Posteriori Estimation: Proof continued

$$-\log p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y}) = \frac{1}{2\sigma^2}(y - X\theta)^\top(y - X\theta) + \frac{1}{2b^2}\theta^\top\theta + \text{ const}$$

Here, the first term corresponds to the contribution from the log-likelihood, and the second term originates from the log-prior. The gradient of the log-posterior with respect to the parameters θ is then

$$-\frac{\mathrm{d}\log p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y})}{\mathrm{d}\theta} = \frac{1}{\sigma^2}\left(\theta^\top X^T X - y^\top X\right) + \frac{1}{b^2}\theta^\top$$

Maximum A Posteriori Estimation: Proof continued

We will find the MAP estimate θ_{MAP} by setting this gradient to 0^T and solving for θ_{MAP}. We obtain

$$\frac{1}{\sigma^2}\left(\theta^\top X^\top X - y^\top X\right) + \frac{1}{b^2}\theta^\top = \mathbf{0}^\top$$

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$$\implies \theta^\top\left(\frac{1}{\sigma^2}X^\top X + \frac{1}{b^2}I\right) - \frac{1}{\sigma^2}y^\top X = \mathbf{0}^\top$$

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\begin{aligned}
&\frac{1}{\sigma^2}\left(\theta^\top X^\top X - y^\top X\right) + \frac{1}{b^2}\theta^\top = \mathbf{0}^\top \\
&\implies \theta^\top\left(\frac{1}{\sigma^2}X^\top X + \frac{1}{b^2}I\right) - \frac{1}{\sigma^2}y^\top X = \mathbf{0}^\top \\
&\implies \theta^\top\left(X^T X + \frac{\sigma^2}{b^2}I\right) = y^\top X
\end{aligned}
$$

Maximum A Posteriori Estimation: Proof continued

We will find the MAP estimate θ_{MAP} by setting this gradient to 0^T and solving for θ_{MAP}. We obtain

$$\begin{aligned}
&\frac{1}{\sigma^2}\left(\theta^\top X^\top X - y^\top X\right) + \frac{1}{b^2}\theta^\top = \mathbf{0}^\top \\
&\implies \theta^\top\left(\frac{1}{\sigma^2}X^\top X + \frac{1}{b^2}I\right) - \frac{1}{\sigma^2}y^\top X = \mathbf{0}^\top \\
&\implies \theta^\top\left(X^T X + \frac{\sigma^2}{b^2}I\right) = y^\top X \\
&\implies \theta^\top = y^\top X\left(X^T X + \frac{\sigma^2}{b^2}I\right)^{-1}
\end{aligned}$$

$$\boldsymbol{\theta}_{MAP} = (\boldsymbol{X}^\top \boldsymbol{X} + \frac{\sigma^2}{b^2}\boldsymbol{I})^{-1}\boldsymbol{X}^\top \boldsymbol{y}$$

Maximum A Posteriori Estimation

$$\boldsymbol{\theta}_{MAP} = \left(X^\top X + \frac{\sigma^2}{b^2} I\right)^{-1} X^\top \boldsymbol{y}$$

If $\mu = \frac{\sigma^2}{b^2}$, then

$$\boldsymbol{\theta}_{MAP} = \left(X^\top X + \mu I\right)^{-1} X^\top \boldsymbol{y}$$

Optimal MAP and MLE solutions

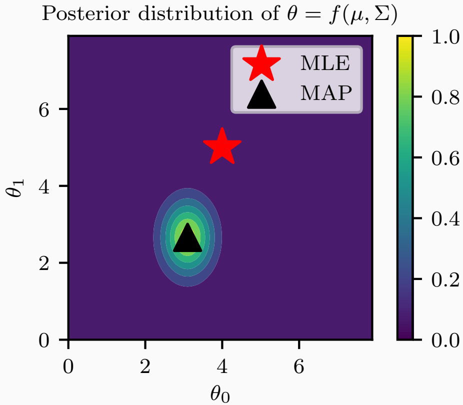

Figure 9: MAP and MLE

Maximum A Posteriori Estimation

- In the below example, we place a Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(0, I)$ on the parameters $\boldsymbol{\theta}$ and determine the MAP estimates. For the lower order polynomial the effect of the prior is not as pronounced as it is in the case of the higher order polynomial and keeps the polynomial relatively smooth in the second case.

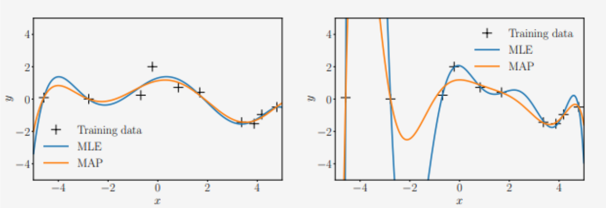

Figure 10: Polynomial Regression and MAP Estimates. Degree 6 and 8 respectively for Figures (a) and (b).

Maximum A Posteriori Estimation

- In the below example, we place a Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(0, I)$ on the parameters $\boldsymbol{\theta}$ and determine the MAP estimates. For the lower order polynomial the effect of the prior is not as pronounced as it is in the case of the higher order polynomial and the prior keeps the second polynomial relatively smooth.

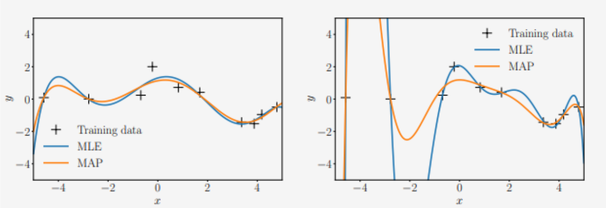

Figure 11: Polynomial Regression and MAP Estimates. Degree 6 and 8 respectively for Figures (a) and (b).

Bayesian Linear Regression

- In Bayesian Linear Regression, we consider the following model:

$$\text{Prior} \;: p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{m_0}, \boldsymbol{S}_0)$$

$$\text{Likelihood} \;: p(y|\boldsymbol{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\boldsymbol{x}^\top \boldsymbol{\theta}, \sigma^2)$$

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$$\text{Likelihood} \ : p(y|\boldsymbol{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\boldsymbol{x}^\top \boldsymbol{\theta}, \sigma^2)$$

- As a PGM, we can represent it as follows:

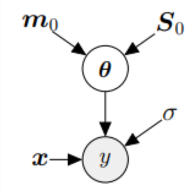

Figure 12: Graphical Model for Bayesian Linear Regression

Bayesian Linear Regression

- The full probabilistic model, i.e., the joint distribution of observed and unobserved random variables, y and $\boldsymbol{\theta}$, respectively, is

$$p(y, \boldsymbol{\theta}|\mathbf{x}) = p(y|\mathbf{x}, \boldsymbol{\theta})p(\boldsymbol{\theta})$$

Bayesian Linear Regression

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$$p(y, \boldsymbol{\theta}|\mathbf{x}) = p(y|\mathbf{x}, \boldsymbol{\theta})p(\boldsymbol{\theta})$$

- The posterior distribution in this case is given by,

$$p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{Y}|\mathcal{X})}$$

Bayesian Linear Regression

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- The denominator above is called as the marginal likelihood or evidence, which ensures that the posterior is normalized and is independent of the parameters. An alternative way of writing the denominator is,

$$p(\mathcal{Y}|\mathcal{X}) = \int p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta}$$

Parameter Posterior

- The parameter posterior can be computed in closed form as follows:

$$p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \mathcal{N}\left(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N\right)$$

$$\boldsymbol{S}_N = \left(\boldsymbol{S}_0^{-1} + \sigma^{-2}\mathsf{X}^\top \boldsymbol{X}\right)^{-1}$$

$$\boldsymbol{m}_N = \boldsymbol{S}_N\left(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{X}^\top \boldsymbol{y}\right)$$

Parameter Posterior

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$$p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y}) = \mathcal{N}\left(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N\right)$$
$$\boldsymbol{S}_N = \left(\boldsymbol{S}_0^{-1} + \sigma^{-2}\boldsymbol{X}^\top\boldsymbol{X}\right)^{-1}$$
$$\boldsymbol{m}_N = \boldsymbol{S}_N\left(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{X}^\top\boldsymbol{y}\right)$$

- The above posterior follows from:

Posterior $\quad p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y}) = \dfrac{p(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(\mathcal{Y}|\mathcal{X})}$

Likelihood $\quad p(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta}) = \mathcal{N}\left(\boldsymbol{y}|\boldsymbol{X}\boldsymbol{\theta}, \sigma^2\boldsymbol{I}\right)$

Prior $\quad p(\boldsymbol{\theta}) = \mathcal{N}\left(\boldsymbol{\theta}|\boldsymbol{m}_0, \boldsymbol{S}_0\right)$

Parameter Posterior: Continued

Instead of looking at the product of the prior and the likelihood, we can transform the problem into log-space and solve for the mean and covariance of the posterior by completing the squares.
The sum of the log-prior and the log-likelihood is

$$\log \mathcal{N}\left(\boldsymbol{y}|\boldsymbol{X}\boldsymbol{\theta}, \sigma^2 \boldsymbol{I}\right) + \log \mathcal{N}\left(\boldsymbol{\theta}|\boldsymbol{m}_0, \boldsymbol{S}_0\right)$$

Parameter Posterior: Continued

Instead of looking at the product of the prior and the likelihood, we can transform the problem into log-space and solve for the mean and covariance of the posterior by completing the squares.
The sum of the log-prior and the log-likelihood is

$$\log \mathcal{N}\left(\boldsymbol{y} | \boldsymbol{X}\boldsymbol{\theta}, \sigma^2 \boldsymbol{I}\right) + \log \mathcal{N}\left(\boldsymbol{\theta} | \boldsymbol{m}_0, \boldsymbol{S}_0\right)$$
$$= -\frac{1}{2}\left(\sigma^{-2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) + (\boldsymbol{\theta} - \boldsymbol{m}_0)^\top \boldsymbol{S}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_0)\right) + \text{ const}$$

Parameter Posterior: Continued

Instead of looking at the product of the prior and the likelihood, we can transform the problem into log-space and solve for the mean and covariance of the posterior by completing the squares.

The sum of the log-prior and the log-likelihood is

$$\log \mathcal{N}\left(\boldsymbol{y}|\boldsymbol{X\theta}, \sigma^2 \boldsymbol{I}\right) + \log \mathcal{N}\left(\boldsymbol{\theta}|\boldsymbol{m}_0, \boldsymbol{S}_0\right)$$

$$= -\frac{1}{2}\left(\sigma^{-2}(\boldsymbol{y} - \boldsymbol{X\theta})^\top(\boldsymbol{y} - \boldsymbol{X\theta}) + (\boldsymbol{\theta} - \boldsymbol{m}_0)^\top \boldsymbol{S}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_0)\right) + \text{ const}$$

where the constant contains terms independent of θ. We will ignore the constant in the following. We now factorize the above equation

Parameter Posterior: Continued

$$-\frac{1}{2}\left(\sigma^{-2}\boldsymbol{y}^\top\boldsymbol{y} - 2\sigma^{-2}\boldsymbol{y}^\top\boldsymbol{X}\theta + \boldsymbol{\theta}^\top\sigma^{-2}\mathbf{X}^\top\boldsymbol{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top\boldsymbol{S}_0^{-1}\boldsymbol{\theta}\right.$$
$$\left.-2\boldsymbol{m}_0^\top\boldsymbol{S}_0^{-1}\theta + \boldsymbol{m}_0^\top\boldsymbol{S}_0^{-1}\boldsymbol{m}_0\right)$$

Parameter Posterior: Continued

$$-\frac{1}{2}\left(\sigma^{-2}\boldsymbol{y}^\top\boldsymbol{y} - 2\sigma^{-2}y^\top X\theta + \boldsymbol{\theta}^\top\sigma^{-2}\mathsf{X}^\top\boldsymbol{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top\boldsymbol{S}_0^{-1}\boldsymbol{\theta}\right.$$
$$\left.-2m_0^\top S_0^{-1}\theta + \boldsymbol{m}_0^\top\boldsymbol{S}_0^{-1}\boldsymbol{m}_0\right)$$
$$= -\frac{1}{2}\left(\boldsymbol{\theta}^\top\left(\sigma^{-2}\mathsf{X}^\top\mathsf{X} + \boldsymbol{S}_0^{-1}\right)\boldsymbol{\theta} - 2(\sigma^{-2}X^\top y + S_0^{-1}m_0)^\top\theta\right) + \text{ const}$$

Parameter Posterior: Continued

$$
\begin{aligned}
&-\tfrac{1}{2}\left(\sigma^{-2}\boldsymbol{y}^\top\boldsymbol{y} - 2\sigma^{-2}y^\top X\theta + \boldsymbol{\theta}^\top\sigma^{-2}\mathbf{X}^\top X\boldsymbol{\theta} + \boldsymbol{\theta}^\top \boldsymbol{S}_0^{-1}\boldsymbol{\theta}\right. \\
&\left.-2m_0^\top S_0^{-1}\theta + \boldsymbol{m}_0^\top \boldsymbol{S}_0^{-1}\boldsymbol{m}_0\right) \\
&= -\tfrac{1}{2}\left(\boldsymbol{\theta}^\top\left(\sigma^{-2}\mathbf{X}^\top\mathbf{X} + \boldsymbol{S}_0^{-1}\right)\boldsymbol{\theta} - 2(\sigma^{-2}X^\top y + S_0^{-1}m_0)^\top\theta\right) + \text{ const}
\end{aligned}
$$

where the constant contains the black terms which are independent of θ. The orange terms are terms that are linear in θ, and the blue terms are the ones that are quadratic in θ.

Parameter Posterior: Continued

$$
\begin{aligned}
&-\tfrac{1}{2}\left(\sigma^{-2}\boldsymbol{y}^\top\boldsymbol{y} - 2\sigma^{-2}y^\top X\theta + \boldsymbol{\theta}^\top\sigma^{-2}\mathsf{X}^\top \boldsymbol{X}\boldsymbol{\theta} + \boldsymbol{\theta}^\top\boldsymbol{S}_0^{-1}\boldsymbol{\theta}\right. \\
&\left.-2m_0^\top S_0^{-1}\theta + \boldsymbol{m}_0^\top\boldsymbol{S}_0^{-1}\boldsymbol{m}_0\right) \\
&= -\tfrac{1}{2}\left(\boldsymbol{\theta}^\top\left(\sigma^{-2}\mathsf{X}^\top\mathsf{X} + \boldsymbol{S}_0^{-1}\right)\boldsymbol{\theta} - 2(\sigma^{-2}X^\top y + S_0^{-1}m_0)^\top\theta\right) + \text{ const}
\end{aligned}
$$

where the constant contains the black terms which are independent of θ. The orange terms are terms that are linear in θ, and the blue terms are the ones that are quadratic in θ.

Parameter Posterior: Continued

We find that this equation is quadratic in θ. The fact that the unnormalized log-posterior distribution is a (negative) quadratic form implies that the posterior is Gaussian, i.e

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$$p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \exp(\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y})) \propto \exp(\log p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) + \log p(\boldsymbol{\theta}))$$

Parameter Posterior: Continued

We find that this equation is quadratic in θ. The fact that the unnormalized log-posterior distribution is a (negative) quadratic form implies that the posterior is Gaussian, i.e

$$p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y}) = \exp(\log p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y})) \propto \exp(\log p(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}))$$

$$\propto \exp\left(-\frac{1}{2}\left(\boldsymbol{\theta}^\top\left(\sigma^{-2}\mathbf{X}^\top\mathbf{X} + \mathbf{S}_0^{-1}\right)\boldsymbol{\theta} - 2\left(\sigma^{-2}X^\top y + S_0^{-1}m_0\right)^\top\theta\right)\right)$$

Parameter Posterior: Continued

The remaining task is it to bring this (unnormalized) Gaussian into the form that is proportional to $\mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N)$, i.e., we need to identify the mean m_N and the covariance matrix S_N . To do this, we use the concept of completing the squares. The desired log-posterior is

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$$\log \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N) = -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_N)^\top \boldsymbol{S}_N^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_N) + \text{ const}$$

Parameter Posterior: Continued

The remaining task is it to bring this (unnormalized) Gaussian into the form that is proportional to $\mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N)$, i.e., we need to identify the mean m_N and the covariance matrix S_N . To do this, we use the concept of completing the squares. The desired log-posterior is

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$$= -\frac{1}{2}\left(\boldsymbol{\theta}^\top \boldsymbol{S}_N^{-1}\boldsymbol{\theta} - 2m_N^\top \boldsymbol{S}_N^{-1}\boldsymbol{\theta} + \boldsymbol{m}_N^\top \boldsymbol{S}_N^{-1}\boldsymbol{m}_N\right)$$

Parameter Posterior: Continued

The remaining task is it to bring this (unnormalized) Gaussian into the form that is proportional to $\mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N)$, i.e., we need to identify the mean m_N and the covariance matrix S_N . To do this, we use the concept of completing the squares. The desired log-posterior is

$$\log \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_N, \boldsymbol{S}_N) = -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_N)^\top \boldsymbol{S}_N^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_N) + \text{ const}$$
$$= -\frac{1}{2}\left(\boldsymbol{\theta}^\top \boldsymbol{S}_N^{-1}\boldsymbol{\theta} - 2m_N^\top \boldsymbol{S}_N^{-1}\boldsymbol{\theta} + \boldsymbol{m}_N^\top \boldsymbol{S}_N^{-1}\boldsymbol{m}_N\right)$$

Here, we factorized the quadratic form $(\boldsymbol{\theta} - \boldsymbol{m}_N)^\top \boldsymbol{S}_N^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_N)$ into a term that is quadratic in θ alone (blue), a term that is linear in θ (orange), and a constant term (black). This allows us now to find S_N and m_N by matching the colored expressions

Parameter Posterior: Continued

$$S_N^{-1} = X^\top \sigma^{-2} I X + S_0^{-1}$$

Parameter Posterior: Continued

$$S_N^{-1} = X^\top \sigma^{-2} I X + S_0^{-1}$$
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Parameter Posterior: Continued

$$S_N^{-1} = X^\top \sigma^{-2} I X + S_0^{-1}$$
$$S_N = \left(\sigma^{-2} X^\top X + S_0^{-1}\right)^{-1}$$

$$m_N^\top S_N^{-1} = \left(\sigma^{-2} X^\top y + S_0^{-1} m_0\right)^\top$$

Parameter Posterior: Continued

$$S_N^{-1} = X^\top \sigma^{-2} I X + S_0^{-1}$$
$$S_N = \left(\sigma^{-2} X^\top X + S_0^{-1}\right)^{-1}$$

$$m_N^\top S_N^{-1} = \left(\sigma^{-2} X^\top y + S_0^{-1} m_0\right)^\top$$
$$m_N = S_N \left(\sigma^{-2} X^\top y + S_0^{-1} m_0\right)$$

Samples from Posterior

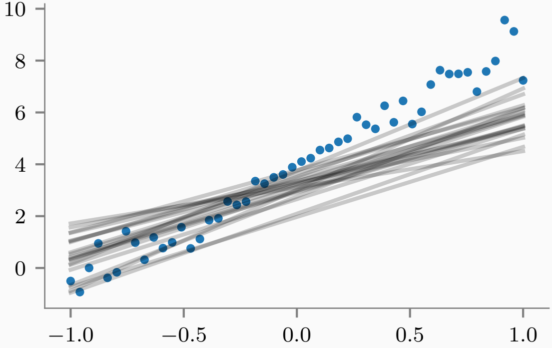


Figure 13: MAP and MLE

Posterior Predictions

- The predictive distribution of y_*, at a test input $\boldsymbol{x}_*$ using the parameter prior $p(\boldsymbol{\theta})$ is computed as follows.

$$
\begin{aligned}
p\left(y_* | \mathcal{X}, \mathcal{Y}, \boldsymbol{x}_*\right) &= \int p\left(y_* | \boldsymbol{x}_*, \boldsymbol{\theta}\right) p(\boldsymbol{\theta} | \mathcal{X}, \mathcal{Y}) \mathrm{d}\boldsymbol{\theta} \\
&= \int \mathcal{N}\left(y_* | \boldsymbol{x}_*^\top \boldsymbol{\theta}, \sigma^2\right) \mathcal{N}\left(\boldsymbol{\theta} | \boldsymbol{m}_N, \boldsymbol{S}_N\right) \mathrm{d}\boldsymbol{\theta} \\
&= \mathcal{N}\left(y_* | \boldsymbol{x}_*^\top \boldsymbol{m}_N, \boldsymbol{x}_*^\top \boldsymbol{S}_N \boldsymbol{x}_* + \sigma^2\right)
\end{aligned}
$$

Fully Bayesian Predictions

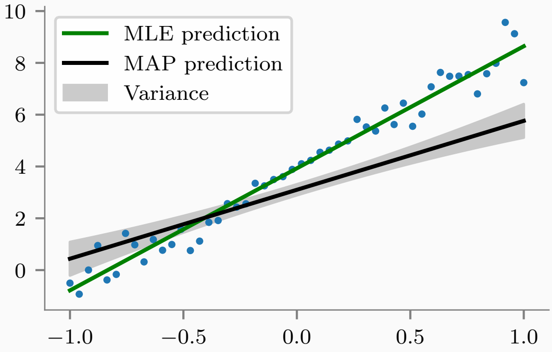
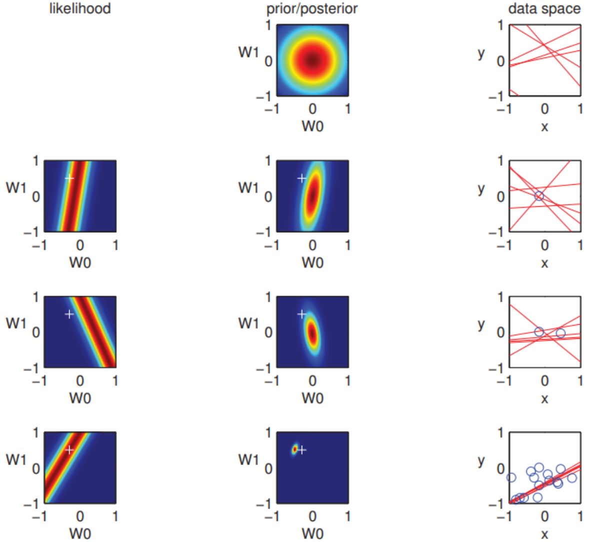


Figure 14: MAP, MLE and Fully Bayesian

Summary



Bayesian Linear Regression Analysis

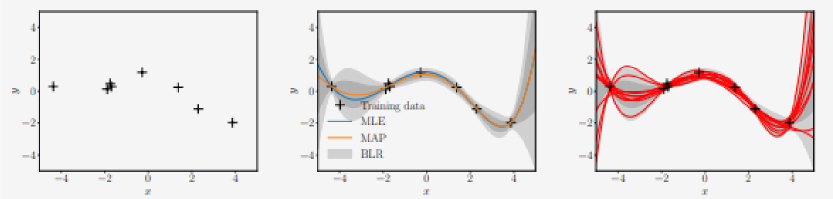
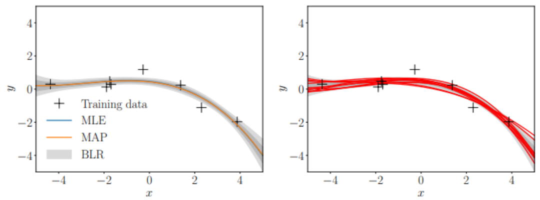
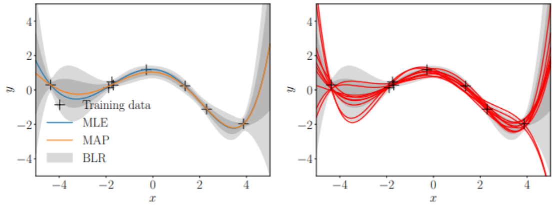


Figure 15: Bayesian linear regression and posterior over functions. (a) training data; (b) posterior distribution over functions; different shades correspond to different confidence intervals (c) Samples from the posterior over functions.

Bayesian Linear Regression Analysis

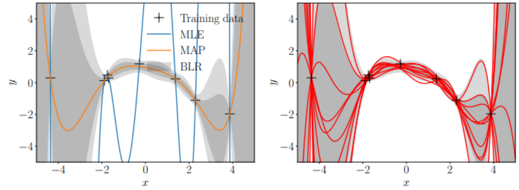


(a) Posterior distribution for polynomials of degree $M = 3$ (left) and samples from the posterior over functions (right).



(b) Posterior distribution for polynomials of degree $M = 5$ (left) and samples from the posterior over functions (right).

Bayesian Linear Regression Analysis



(c) Posterior distribution for polynomials of degree $M = 7$ (left) and samples from the posterior over functions (right).

Figure 16: Left panels: The mean of the Bayesian linear regression model coincides with the MAP estimate. The predictive uncertainty is the sum of the noise term and the posterior parameter uncertainty, which depends on the location of the test input. Right panels: sampled functions from the posterior distribution.