Mathematics for Machine Learning

— Linear Regression

Problem Formulation & Parameter Estimation

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Credits for the resource

- The slides are based on the textbooks:
  - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
  - *Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.*
  - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. Wiley. 2019.*
- We could partially refer to the monograph:
  Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

Outline

1. Introduction
2. Problem Formulation
3. Parameter Estimation
   - Maximum Likelihood Estimation (MLE)
   - Overfitting in Linear Regression
   - Maximum A Posteriori Estimation (MAP)
   - MAP Estimation as Regularization
4. Bayesian Linear Regression

Linear Regression

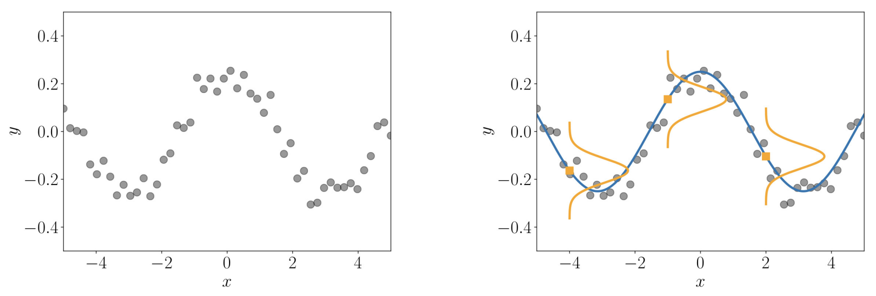
Aim

Find (or Infer) a function $f : \mathbb{R}^D \to \mathbb{R}$ which maps input $\mathbf{x} \in \mathbb{R}^D$ to the corresponding function values $f(\mathbf{x}) \in \mathbb{R}$.

- And we hope f to generalize well to unseen input.

- Training input: $\{\mathbf{x}_i\}_{i=1}^N$
- Assume the noisy observations $\{y_i\}_{i=1}^N$ for $y_i = f(\mathbf{x}_i) + \epsilon$, an i.i.d. random variable ϵ.
    - Consider zero-mean Gaussian noise throughout our discussions.

- Observe (noisy) function values $y_n = f(x_n) + \epsilon$.



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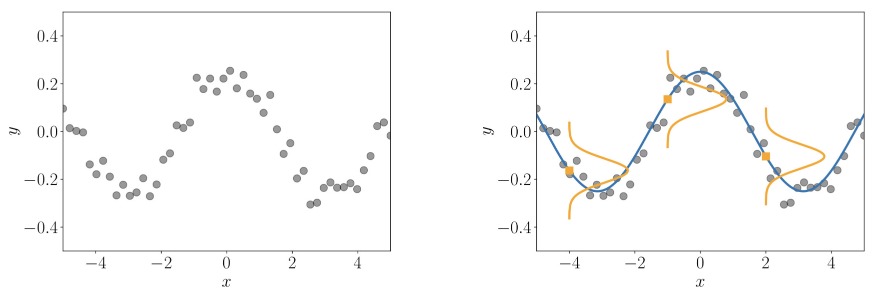


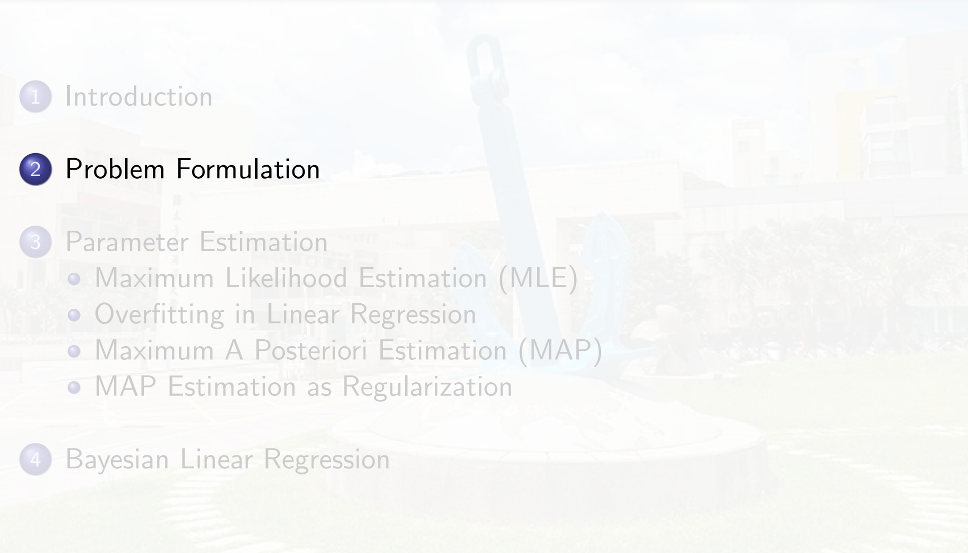
Applications of regression:

- Time series analysis, reinforcement learning, optimization, computer games, classification algorithms, etc.

Problems Involved in Regression

- Choice of the model and the parametrization.
  - Function classes, particular parametrization (e.g., degree of the polynomial)
- Finding good parameters.
  - Loss minimization w.r.t. different loss functions.
- Overfitting and model selection.
- Relationship b/w loss functions and parameter priors.
  - Probabilistic models.
- Uncertainty modeling.
  - We have limited amount of data.
  - The smaller the training set, the more important uncertainty modeling.
  - Equip model predictions with confidence bounds.

Outline



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Problem Formulation

- Because of observing noise, we adopt a probabilistic approach to explicitly model the noise using a likelihood function.
- **Focus:** a regression problem with the likelihood function:

$$p(y \mid \mathbf{x}) = \mathcal{N}(y \mid f(\mathbf{x}), \sigma^2).$$

  - $\mathbf{x} \in \mathbb{R}^D$: inputs.
  - $y \in \mathbb{R}$: noisy function values (targets).
  - The relationship between $\mathbf{x}$ and y:

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

for $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

An Example of Linear Regression

- An example of linear regression:

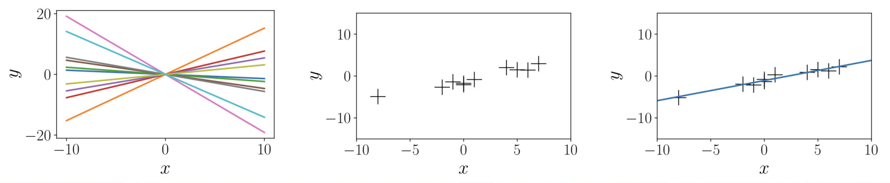
$$p(y \mid \mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y \mid \mathbf{x}^\top \boldsymbol{\theta}, \sigma^2).$$

$\iff$

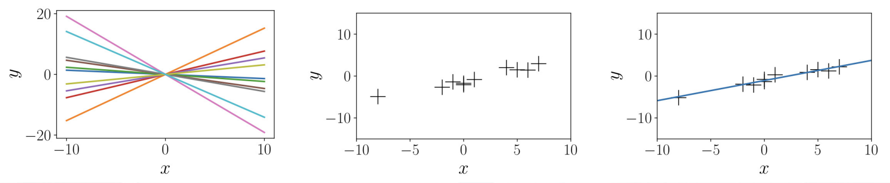
$$y = \mathbf{x}^\top \boldsymbol{\theta} + \epsilon,$$

for $\epsilon \sim \mathcal{N}(0, \sigma^2)$.

  - $\boldsymbol{\theta} \in \mathbb{R}^D$: the parameters we seek.
  - ϵ: the only source of uncertainty.



- “Linear”: linear in the parameters.
  - Parameters: describing a function by a linear combination of input features.



- “Linear”: linear in the parameters.
  - Parameters: describing a function by a linear combination of input features.
- Hence, $y = \phi^\top(\mathbf{x})\boldsymbol{\theta}$ is also regarded as a linear regression (ϕ can be nonlinear).
  - A “feature” here is a representation $\phi(\mathbf{x})$ of the input $\mathbf{x}$.

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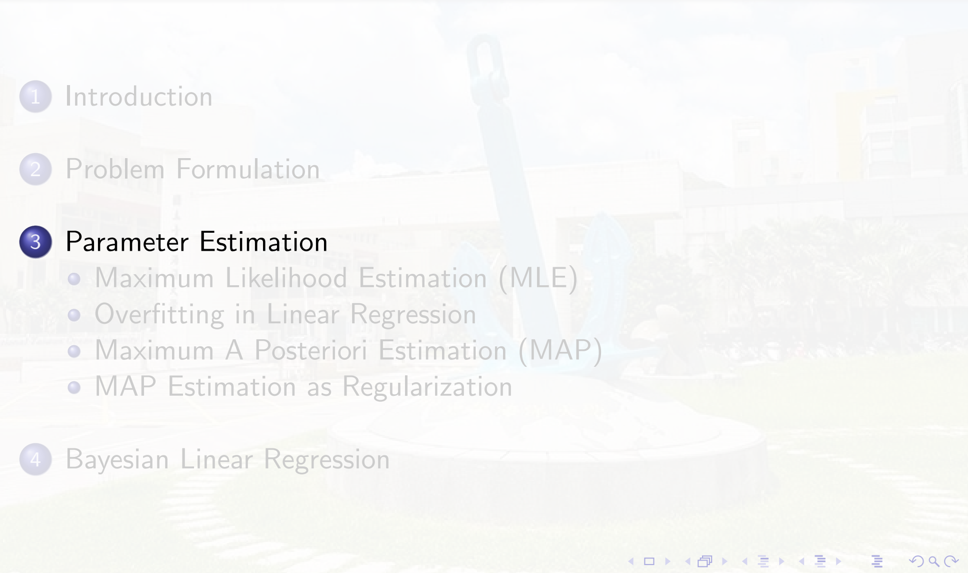

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The Likelihood

- Given a training set $\mathcal{D} := \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$, $\mathbf{x}_i \in \mathbb{R}^D$ and $y_i \in \mathbb{R}$ for $i = 1, \ldots, N$.
- By the independence of the input, the likelihood factorizes:

$$p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) \quad = \quad p(y_1, \ldots, y_N \mid \mathbf{x}_1, \ldots, \mathbf{x}_N, \boldsymbol{\theta})$$

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$$\begin{aligned} p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) &= p(y_1, \ldots, y_N \mid \mathbf{x}_1, \ldots, \mathbf{x}_N, \boldsymbol{\theta}) \\ &= \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \boldsymbol{\theta}) = \prod_{i=1}^{N} \mathcal{N}(y_i \mid \mathbf{x}_i^\top \boldsymbol{\theta}, \sigma^2). \end{aligned}$$

The likelihood and the factors $p(y_i \mid \mathbf{x}_i, \boldsymbol{\theta})$ are Gaussian due to the noise distribution.

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  The likelihood and the factors $p(y_i \mid \mathbf{x}_i, \boldsymbol{\theta})$ are Gaussian due to the noise distribution.

- **Goal:** Find optimal parameters $\boldsymbol{\theta}^* \in \mathbb{R}^D$.
- Then we can make predictions for an arbitrary test input $\mathbf{x}_*$ and get target y_* with $p(y_* \mid \mathbf{x}_*, \boldsymbol{\theta}^*) = \mathcal{N}(y_* \mid \mathbf{x}_*^\top \boldsymbol{\theta}^*, \sigma^2)$.

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Maximum Likelihood Estimation (MLE)

Find parameters $\boldsymbol{\theta}_{ML}$

$$\boldsymbol{\theta}_{ML} \in \arg\max_{\boldsymbol{\theta}} p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}).$$

Note:

- The likelihood $p(y \mid \mathbf{x}, \boldsymbol{\theta})$ is NOT a probability distribution of $\boldsymbol{\theta}$.

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Note:

- The likelihood $p(y \mid \mathbf{x}, \boldsymbol{\theta})$ is NOT a probability distribution of $\boldsymbol{\theta}$. It's a function of $\boldsymbol{\theta}$ (might not be integrable w.r.t $\boldsymbol{\theta}$).
- However, it's a normalized probability distribution in y.

How to find the desired $\boldsymbol{\theta}_{ML}$?

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1. Perform gradient ascent (or descent).
2. For linear regression, we can directly have a closed-form solution.
3. In practice, we do not maximize the likelihood directly. Instead, we apply the negative log-likelihood.
    - It does not suffer from numerical underflow.
    - The differentiation rules become simpler.

Maximize likelihood ⇔ Minimize negative log-likelihood

The negative log-likelihood

$$-\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = -\log \prod_{i=1}^{N} p(y_i \mid \mathbf{x}_i, \boldsymbol{\theta})$$

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⋆ **Note:** the independence assumption on the training set applies here.

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$$\log p(y_i \mid \mathbf{x}_i, \boldsymbol{\theta}) = -\frac{1}{2\sigma^2}(y_i - \mathbf{x}^\top \boldsymbol{\theta})^2 + \text{constant}_{\text{indepent of } \boldsymbol{\theta}}.$$

Ignoring the constant terms, we obtain

$$\begin{aligned}\mathcal{L}(\boldsymbol{\theta}) &:= \frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - \mathbf{x}_i^\top\boldsymbol{\theta})^2 \\ &= \frac{1}{2\sigma^2}(\mathbf{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\mathbf{y} - \boldsymbol{X}\boldsymbol{\theta}) = \frac{1}{2\sigma^2}\|\mathbf{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2,\end{aligned}$$

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

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$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \mathbf{0}^\top \iff \boldsymbol{\theta}_{ML}^\top \boldsymbol{X}^\top \boldsymbol{X} = \mathbf{y}^\top \boldsymbol{X}$$

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$$\begin{aligned}\frac{\partial\mathcal{L}}{\partial\boldsymbol{\theta}} = \mathbf{0}^\top &\iff \boldsymbol{\theta}_{ML}^\top\boldsymbol{X}^\top\boldsymbol{X} = \mathbf{y}^\top\boldsymbol{X} \\ &\iff \boldsymbol{\theta}_{ML}^\top = \mathbf{y}^\top\boldsymbol{X}(\boldsymbol{X}^\top\boldsymbol{X})^{-1}\end{aligned}$$

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To get $\boldsymbol{\theta}$, we need to solve $\dfrac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \mathbf{0}^\top$:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \boldsymbol{\theta}} = \mathbf{0}^\top \quad &\iff \quad \boldsymbol{\theta}_{ML}^\top \boldsymbol{X}^\top \boldsymbol{X} = \mathbf{y}^\top \boldsymbol{X} \\ &\iff \quad \boldsymbol{\theta}_{ML}^\top = \mathbf{y}^\top \boldsymbol{X}(\boldsymbol{X}^\top \boldsymbol{X})^{-1} \\ &\iff \quad \boldsymbol{\theta}_{ML} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1}\boldsymbol{X}^\top \mathbf{y}.\end{aligned}$$

⋆ We use the positive definite property of $\boldsymbol{X}^\top \boldsymbol{X}$ if $\operatorname{rank}(\boldsymbol{X}) = D$.

Remark

- We can get a global minimum because the Hessian $\nabla^2_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = \boldsymbol{X}^\top \boldsymbol{X}$ is positive definite (for full rank $\boldsymbol{X}$?).

MLE with Features

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- We can perform an arbitrary nonlinear transformation $\phi(\mathbf{x})$ of the input $\mathbf{x}$, and then linearly combine these components.

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- The corresponding linear regression turns out to be:

$$p(y \mid \mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y \mid \phi^\top(\mathbf{x})\boldsymbol{\theta}, \sigma^2).$$

$\Longleftrightarrow$

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$\iff$

$$y = \boldsymbol{\phi}^\top(\mathbf{x})\boldsymbol{\theta} + \epsilon = \sum_{k=0}^{K-1} \theta_k \phi_k(\mathbf{x}) + \epsilon$$

- $\phi : \mathbb{R}^D \to \mathbb{R}$ is a (nonlinear) transformation of the input $\mathbf{x}$
- $\phi_k : \mathbb{R}^D \to \mathbb{R}$: the kth feature vector of ϕ.

Polynomial Regression (Example)

Consider a regression problem $y = \boldsymbol{\phi}^\top(x)\boldsymbol{\theta} + \epsilon$, for $x \in \mathbb{R}$ and $\boldsymbol{\theta} \in \mathbb{R}^K$. A polynomial transformation of x is often used as

$$\boldsymbol{\phi}(x) = \begin{bmatrix} \phi_0(x) \\ \phi_1(x) \\ \vdots \\ \phi_{K-1}(x) \end{bmatrix} = \begin{bmatrix} 1 \\ x \\ x^2 \\ \vdots \\ x^{K-1} \end{bmatrix} \in \mathbb{R}^K.$$

- We lift the original one-dimensional input space into a K-dimensional feature space.
- We can model polynomials of degree $\leq K - 1$ as $f(x) = \sum_{k=1}^{K-1} \theta_k x^k = \boldsymbol{\phi}^\top(x)\boldsymbol{\theta}$, for $\boldsymbol{\theta} = [\theta_0, \ldots, \theta_{K-1}]^\top \in \mathbb{R}^K$ which contains the linear parameters θ_k.

For $\mathbf{x}_i \in \mathbb{R}^D$

We can also define a feature matrix as

$$\mathbf{\Phi} := \begin{bmatrix} \boldsymbol{\phi}^\top(\mathbf{x}_1) \\ \vdots \\ \boldsymbol{\phi}^\top(\mathbf{x}_N) \end{bmatrix} = \begin{bmatrix} \phi_0(\mathbf{x}_1) & \cdots & \phi_{K-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \cdots & \phi_{K-1}(\mathbf{x}_2) \\ \vdots & & \vdots \\ \phi_0(\mathbf{x}_N) & \cdots & \phi_{K-1}(\mathbf{x}_N) \end{bmatrix} \in \mathbb{R}^{N\times K},$$

where $\Phi_{ij} = \phi_j(\mathbf{x}_i)$ and $\phi_j : \mathbb{R}^D \to \mathbb{R}$.

Example

Feature Matrix for Second-Order Polynomials

$$\boldsymbol{\Phi} := \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_N & x_N^2 \end{bmatrix}.$$

With the feature matrix $\mathbf{\Phi}$:

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The negative log-likelihood can be written as

$$-\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = \frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{\Phi}\boldsymbol{\theta})^\top(\mathbf{y} - \mathbf{\Phi}\boldsymbol{\theta}) + \text{constant}.$$

- Replacing $\boldsymbol{X}$ by $\mathbf{\Phi}$.
- Both of them are independent of $\boldsymbol{\theta}$.

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- Replacing $\boldsymbol{X}$ by $\boldsymbol{\Phi}$.
- Both of them are independent of $\boldsymbol{\theta}$.
- Similarly, we have[1]

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

[1] Requring rank($\boldsymbol{\Phi}$) = K

Estimating the Noise Variance (1/2)

- We can also use the principle of MLE to obtain that for σ^2_{ML} for the noise variance.

Estimating the Noise Variance (1/2)

- We can also use the principle of MLE to obtain that for σ^2_{ML} for the noise variance.
- Write down the log-likelihood:

$$\begin{aligned}
\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}, \sigma^2) &= \sum_{i=1}^{N} \log \mathcal{N}(y_i \mid \boldsymbol{\phi}^\top(\mathbf{x}_i)\boldsymbol{\theta}, \sigma^2) \\
&= \sum_{i=1}^{N} \left(-\frac{1}{2}\log(2\pi) - \frac{1}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(y_i - \boldsymbol{\phi}^\top(\mathbf{x}_i)\boldsymbol{\theta})^2 \right) \\
&= -\frac{N}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\sum_{i=1}^{N}(y_i - \boldsymbol{\phi}^\top(\mathbf{x}_i)\boldsymbol{\theta})^2 + \text{constant}
\end{aligned}$$

Estimating the Noise Variance (1/2)

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Let $s := \sum_{i=1}^{N}(y_i - \boldsymbol{\phi}^\top(\mathbf{x}_i)\boldsymbol{\theta})^2$.

Estimating the Noise Variance (2/2)

- The partial derivative w.r.t. σ^2:

$$\frac{\partial \log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}, \sigma^2)}{\partial \sigma^2} = -\frac{N}{2\sigma^2} + \frac{1}{\sigma^4} s = 0$$

$$\iff \quad \frac{N}{2\sigma^2} = \frac{s}{2\sigma^4}.$$

Thus,

$$\sigma^2_{ML} = \frac{s}{N} = \frac{1}{N} \sum_{i=1}^{N} (y_i - \phi^\top(\mathbf{x}_i)\boldsymbol{\theta})^2.$$

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Evaluating the Quality of the Model

- We can evaluate the quality of the model by computing the error/loss.
- Given that σ^2 is not a free model parameter, we can ignore that term by scaling by $1/\sigma^2$ and derive a squared-error function $\|\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2$.

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- To compare the errors of datasets with different sizes and the same scale, we often use the root-mean squared error (RMSE):

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- Given that σ^2 is not a free model parameter, we can ignore that term by scaling by $1/\sigma^2$ and derive a squared-error function $\|\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2$.
- To compare the errors of datasets with different sizes and the same scale, we often use the root-mean squared error (RMSE):

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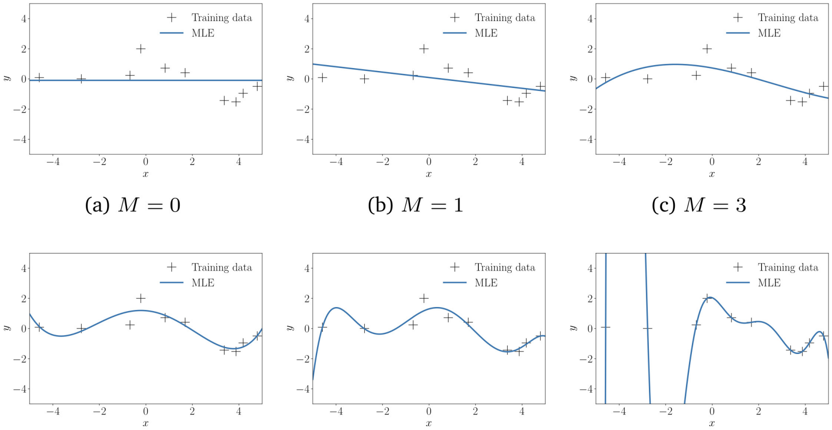
- Model selection: determine the best degree of the polynomial.
  - Brute-force searching and enumerate all reasonable polynomial degrees M.

Overfitting in Linear Regression

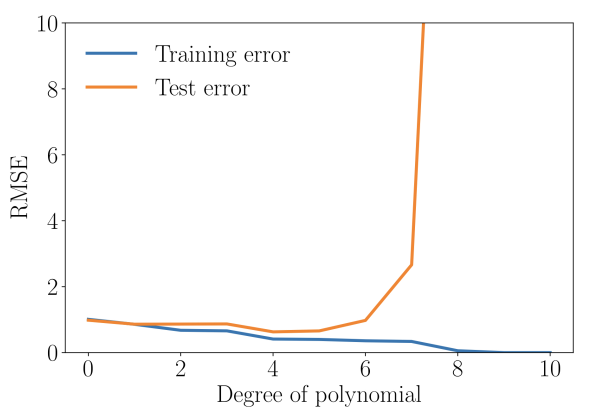


(a) $M = 0$ (b) $M = 1$ (c) $M = 3$

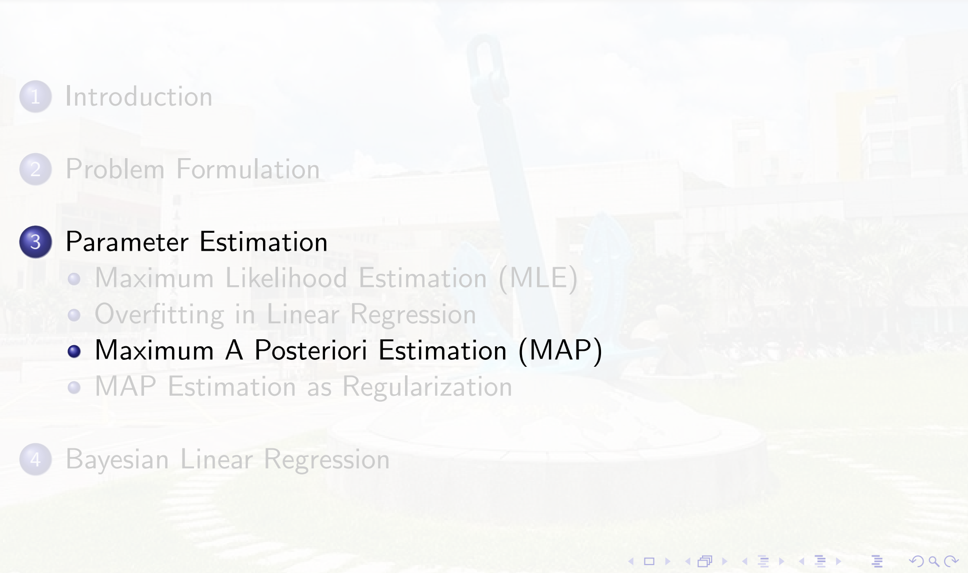
(d) $M = 4$ (e) $M = 6$ (f) $M = 9$

Goal: a good generalization by making *accurate* predictions for new unseen data.

- A separate test set comprising 200 data points generated using exactly the same procedure used to generate the training set.



Outline



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2. Problem Formulation
3. **Parameter Estimation**
   - Maximum Likelihood Estimation (MLE)
   - Overfitting in Linear Regression
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- MLE is prone to overfitting.
- **Experience:** The parameter values becomes relatively large when the model is overfitting.
- To mitigate the effect of huge parameter values, we place a prior distribution $p(\boldsymbol{\theta})$ on the parameters.
- **Rough idea:** Encode the parameter values that are plausible before seeing any data.
    - For example, a Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, \boldsymbol{I})$.

Maximum a Posteriori Estimation (1/5)

- Once a dataset $(\mathcal{X}, \mathcal{Y})$ is available, we week parameters that maximize the posterior distribution $p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y})$ instead of maximizing the likelihood.

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

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  - The prior will have an effect on the parameter vector.
  - $\boldsymbol{\theta}_{MAP}$: the maximizer of the above posterior (i.e., the MAP estimate).

Maximum a Posteriori Estimation (2/5)

The log-transformation of the posterior:

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

The constant is independent of $\boldsymbol{\theta}$.

We can see that the MAP estimate is a compromise between the prior and the data-dependent likelihood.

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We minimize the negative log-posterior w.r.t. θ:

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

Maximum a Posteriori Estimation (3/5)

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

The gradient:

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

Assume the Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, b^2\boldsymbol{I})$. We have

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

Maximum a Posteriori Estimation (4/5)

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

Hence, the gradient of the log-posterior w.r.t. $\boldsymbol{\theta}$ is

$$-\frac{\mathrm{d}\log p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y})}{\mathrm{d}\boldsymbol{\theta}} = \frac{1}{\sigma^2}(\boldsymbol{\theta}^\top\boldsymbol{\Phi}^\top\boldsymbol{\Phi} - \mathbf{y}^\top\boldsymbol{\Phi}) + \frac{1}{b^2}\boldsymbol{\theta}^\top.$$

Setting the gradient to $\mathbf{0}^\top$ to get $\boldsymbol{\theta}_{MAP}$:

Maximum a Posteriori Estimation (5/5)

$$\begin{aligned}
& \frac{1}{\sigma^2}(\boldsymbol{\theta}^\top \boldsymbol{\Phi}^\top \boldsymbol{\Phi} - \mathbf{y}^\top \boldsymbol{\Phi}) + \frac{1}{b^2}\boldsymbol{\theta}^\top = \mathbf{0}^\top \\
\iff \quad & \boldsymbol{\theta}^\top \left(\frac{1}{\sigma^2}\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \frac{1}{b^2}\boldsymbol{I} \right) - \frac{1}{\sigma^2}\mathbf{y}^\top \boldsymbol{\Phi} = \mathbf{0}^\top \\
\iff \quad & \boldsymbol{\theta}^\top \left(\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \frac{\sigma^2}{b^2}\boldsymbol{I} \right) = \mathbf{y}^\top \boldsymbol{\Phi} \\
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\end{aligned}$$

Finally, we have

Maximum a Posteriori Estimation (5/5)

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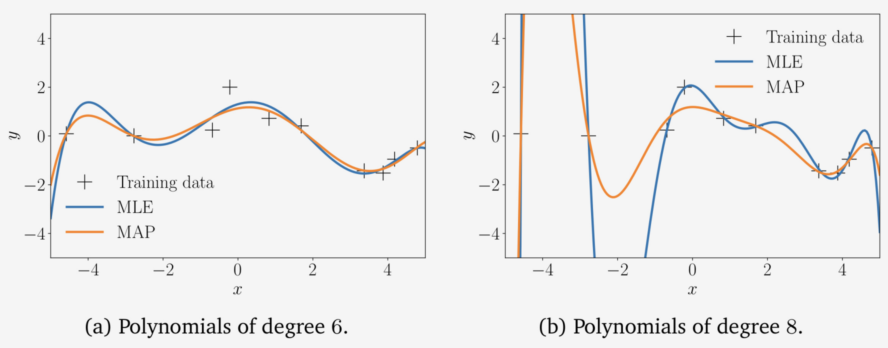

(a) Polynomials of degree 6.

(b) Polynomials of degree 8.

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Motivation (I)

- Mitigate the effect of overfitting by penalizing the amplitude of the parameters by means of regularization.
- Consider the regularized least squares:

$$\underbrace{\|\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2}_{\text{for fitting data}} + \underbrace{\lambda\|\boldsymbol{\theta}\|_2^2}_{\text{regularizer}}$$

  for the regularization parameter $\lambda \geq 0$.
  - The 2-norm $\|\cdot\|_2$ can be replaced by other types of norm.

Motivation (II)

- The regularizer $\lambda\|\boldsymbol{\theta}\|_2^2$ can be seen as a negative log-Gaussian prior.
- The Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, b^2\boldsymbol{I})$, so the negative log-Gaussian prior is

$$-\log p(\boldsymbol{\theta}) = \frac{1}{2b^2}\|\boldsymbol{\theta}\|_2^2 + \text{constant}$$

hence we have $\lambda = \frac{1}{2b^2}$.

Minimizing the regularized least-squares loss function yields

$$\boldsymbol{\theta}_{RLS} = (\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \lambda \boldsymbol{I})^{-1} \boldsymbol{\Phi}^\top \mathbf{y}.$$

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This is identical to the MAP estimate for $\lambda = \frac{\sigma^2}{b^2}$.

- σ^2: the noise variance
- b^2: the variance of the Gaussian prior $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, b^2 \boldsymbol{I})$.

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From MAP to Bayesian Linear Regression

- So far we have used point estimates of the parameters $\boldsymbol{\theta}$:
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- **Bayesian linear regression:**
  - Treat $\boldsymbol{\theta}$ as a random variable.
  - Use Bayes' rule to obtain the posterior distribution $p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y})$.
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  - Make predictions by integrating over all plausible parameter values.
- This will give us not only a prediction, but also a measure of uncertainty.

Bayesian Linear Regression Model (1/2)

- Recall the feature-based linear regression model

$$y = \boldsymbol{\phi}^\top(\mathbf{x})\boldsymbol{\theta} + \epsilon, \qquad \epsilon \sim \mathcal{N}(0, \sigma^2).$$

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  where
  - $\boldsymbol{\Phi} \in \mathbb{R}^{N \times K}$: feature matrix, i-th row $\boldsymbol{\phi}^\top(\mathbf{x}_i)$,
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- The likelihood is Gaussian:

$$p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = \mathcal{N}(\mathbf{y} \mid \boldsymbol{\Phi}\boldsymbol{\theta},\, \sigma^2 \boldsymbol{I}_N).$$

Bayesian Linear Regression Model (2/2)

- We place a Gaussian prior on the parameter vector $\boldsymbol{\theta}$:

$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} \mid \mathbf{m}_0, \boldsymbol{S}_0),$$

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- This prior encodes our a priori beliefs about likely parameter values.
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- Because both prior and likelihood are Gaussian, the posterior will also be Gaussian (Exercise).

Remark: Product of Gaussian Densities

- Consider two D-dimensional Gaussians in **the same variable x**:

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A}) \ \text{ and } \ \mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}).$$

- Their product is proportional to another Gaussian:

$$\mathcal{N}(\mathbf{x} \mid \mathbf{a}, \boldsymbol{A})\, \mathcal{N}(\mathbf{x} \mid \mathbf{b}, \boldsymbol{B}) = \rho \mathcal{N}(\mathbf{x} \mid \mathbf{c}, \boldsymbol{C}),$$

  where

$$\boldsymbol{C} = (\boldsymbol{A}^{-1} + \boldsymbol{B}^{-1})^{-1}, \quad \mathbf{c} = \boldsymbol{C}(\boldsymbol{A}^{-1}\mathbf{a} + \boldsymbol{B}^{-1}\mathbf{b}),$$

  and the scaling constant ρ is

$$\rho = (2\pi)^{-D/2} \det(\boldsymbol{A} + \boldsymbol{B})^{-1/2} \exp\Big(-\tfrac{1}{2}(\mathbf{a} - \mathbf{b})^\top (\boldsymbol{A} + \boldsymbol{B})^{-1} (\mathbf{a} - \mathbf{b})\Big).$$

- The constant ρ can itself be written as a Gaussian density with "inflated" covariance $\boldsymbol{A} + \boldsymbol{B}$:

$$\rho = \mathcal{N}(\mathbf{a} \mid \mathbf{b}, \boldsymbol{A} + \boldsymbol{B}) = \mathcal{N}(\mathbf{b} \mid \mathbf{a}, \boldsymbol{A} + \boldsymbol{B}).$$

Posterior over Parameters (1/2)

- By Bayes' rule,

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

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- Ignoring the normalizing constant, the posterior is proportional to

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- The exponent is a quadratic function of $\boldsymbol{\theta}$ ⇒ the posterior is Gaussian.

Posterior over Parameters (2/2)

Posterior of $\boldsymbol{\theta}$ (proof skipped)

The posterior is

$$p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y}) = \mathcal{N}(\boldsymbol{\theta} \mid \mathbf{m}_N, \boldsymbol{S}_N),$$

where the posterior covariance and mean are given by

$$\boldsymbol{S}_N^{-1} = \boldsymbol{S}_0^{-1} + \frac{1}{\sigma^2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi},$$

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- $\boldsymbol{S}_N$: the prior uncertainty $\boldsymbol{S}_0$ + information from the data.
- $\mathbf{m}_N$: a precision-weighted average of prior mean and data evidence.

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- Fewer data or very noisy data (large σ^2) $\Rightarrow$ posterior is closer to the prior.
- For a Gaussian posterior, the MAP estimate and the posterior mean coincide, but
  - MAP uses only the mode $\boldsymbol{\theta}_{\text{MAP}}$,
  - Bayesian prediction uses the *full posterior* $p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y})$.

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- It reflects what we expect *before* seeing any training data.

Posterior Predictive Distribution (1/2)

- After observing the dataset $\mathcal{D}$, we use the posterior to make predictions:

$$p(y_* \mid \mathbf{x}_*, \mathcal{X}, \mathcal{Y}) = \int p(y_* \mid \mathbf{x}_*, \boldsymbol{\theta})\, p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y})\, \mathrm{d}\boldsymbol{\theta}.$$

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- Again, both distributions inside the integral are Gaussian ⇒ the posterior predictive is Gaussian.

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- After observing the dataset $\mathcal{D}$, we use the posterior to make predictions:

$$p(y_* \mid \mathbf{x}_*, \mathcal{X}, \mathcal{Y}) = \int p(y_* \mid \mathbf{x}_*, \boldsymbol{\theta})\, p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y})\, \mathrm{d}\boldsymbol{\theta}.$$

- Again, both distributions inside the integral are Gaussian ⇒ the posterior predictive is Gaussian.
- Intuitively:
  - we average predictions over all plausible parameter values,
  - weighted by how probable they are under the posterior.

Posterior Predictive Distribution (2/2)

Posterior predictive of y_*

The predictive distribution at a new input $\mathbf{x}_*$ is

$$p(y_* \mid \mathbf{x}_*, \mathcal{X}, \mathcal{Y}) = \mathcal{N}\left(y_* \mid \mu_*(\mathbf{x}_*), \sigma_*^2(\mathbf{x}_*)\right),$$

with mean

$$\mu_*(\mathbf{x}_*) = \phi^\top(\mathbf{x}_*)\mathbf{m}_N,$$

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- The first term in σ_*^2 quantifies parameter uncertainty.
- The second term σ^2 is the measurement noise.

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- This is very useful for model assessment and decision making.

Example: Polynomial Regression Revisited

- Recall the polynomial feature maps

$$\phi(x) = [1, x, x^2, \ldots, x^{K-1}]^\top.$$

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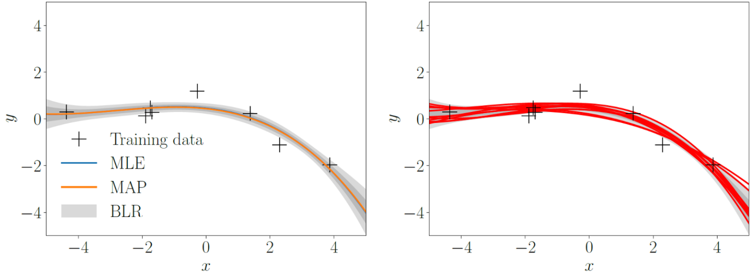
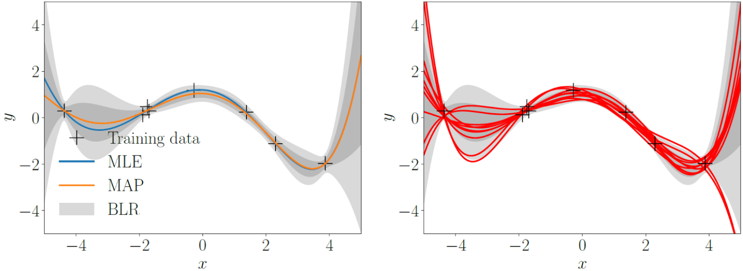
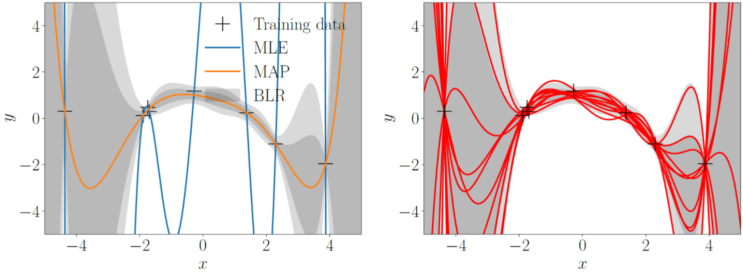
- In contrast, Bayesian linear regression
  - produces a distribution over curves,
  - with narrow uncertainty bands where data are dense,
  - and wide bands where there are few or no observations.
- This behaviour matches the qualitative picture in the textbook for Bayesian linear regression.



(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).



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

Marginal Likelihood (1/2)

- The marginal likelihood (or model evidence) is

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- In Bayesian linear regression, the integral can be computed in closed form.

Marginal Likelihood (2/2)

Closed-form marginal likelihood

Using Gaussian identities, we obtain

$$p(\mathcal{Y} \mid \mathcal{X}) = \mathcal{N}\Big(\mathbf{y} \mid \boldsymbol{\Phi}\mathbf{m}_0,\ \boldsymbol{\Phi}\boldsymbol{S}_0\boldsymbol{\Phi}^\top + \sigma^2\boldsymbol{I}_N\Big)\,.$$

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- Different model choices (e.g., different polynomial degrees) lead to different marginal likelihoods.
- The marginal likelihood automatically trades off data fit (i.e., likelihood) and model complexity (i.e., prior).

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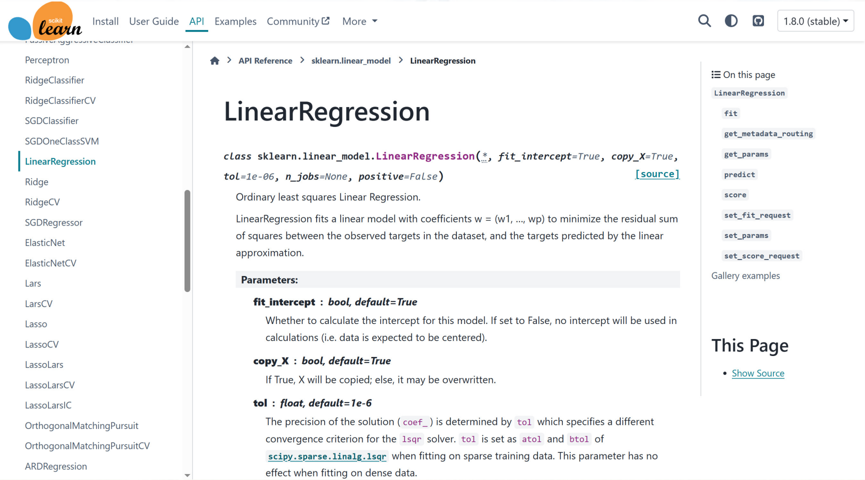
  - variance $\sigma_*^2(\mathbf{x}_*) = \phi^\top(\mathbf{x}_*)\boldsymbol{S}_N\phi(\mathbf{x}_*) + \sigma^2$.
- Bayesian linear regression improves over MLE and MAP by
  - quantifying parameter and predictive uncertainty,
  - enabling principled model comparison via the marginal likelihood.

LinearRegression — scikit-learn [link]



LinearRegression

class sklearn.linear_model.LinearRegression(**, fit_intercept=True, copy_X=True, tol=1e-06, n_jobs=None, positive=False*) [source]

Ordinary least squares Linear Regression.

LinearRegression fits a linear model with coefficients w = (w1, ..., wp) to minimize the residual sum of squares between the observed targets in the dataset, and the targets predicted by the linear approximation.

Parameters:

fit_intercept : ***bool, default=True***

Whether to calculate the intercept for this model. If set to False, no intercept will be used in calculations (i.e. data is expected to be centered).

copy_X : ***bool, default=True***

If True, X will be copied; else, it may be overwritten.

tol : ***float, default=1e-6***

The precision of the solution (`coef_`) is determined by `tol` which specifies a different convergence criterion for the `lsqr` solver. `tol` is set as `atol` and `btol` of `scipy.sparse.linalg.lsqr` when fitting on sparse training data. This parameter has no effect when fitting on dense data.

Discussions

Theorem 9.1 (Parameter Posterior)

Consider the linear regression model with Gaussian noise

$$\mathbf{y} \mid \boldsymbol{\theta}, \mathcal{X} \sim \mathcal{N}(\boldsymbol{\Phi}\boldsymbol{\theta}, \sigma^2 \boldsymbol{I}),$$

and Gaussian prior on the parameters

$$\boldsymbol{\theta} \sim \mathcal{N}(\boldsymbol{m}_0, \boldsymbol{S}_0),$$

where $\boldsymbol{\Phi}$ is the design matrix, $\boldsymbol{m}_0$ the prior mean and $\boldsymbol{S}_0$ the prior covariance.

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Theorem 9.1 (Parameter Posterior)

The posterior over parameters is Gaussian:

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

$$\text{with} \quad \boldsymbol{S}_N = \left(\boldsymbol{S}_0^{-1} + \sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\right)^{-1}, \qquad \boldsymbol{m}_N = \boldsymbol{S}_N\left(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{\Phi}^\top\mathbf{y}\right),$$

where the subscript N indicates dependence on the full training set.

Proof of Theorem 9.1 (1/3)

- By Bayes' rule, up to a normalizing constant,

$$p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y}) \; \propto \; p(\mathbf{y} \mid \mathcal{X}, \boldsymbol{\theta}) \, p(\boldsymbol{\theta}).$$

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$$p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} \mid \boldsymbol{m}_0, \boldsymbol{S}_0).$$

- Work in log-space (and drop constants independent of $\boldsymbol{\theta}$):

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

$$\log p(\boldsymbol{\theta}) = -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_0)^\top \boldsymbol{S}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_0) + \text{const}.$$

Proof of Theorem 9.1 (2/3) – completing the squares

- Summing the two log terms (still ignoring constants):

$$\begin{aligned}\log p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y}) = &-\frac{1}{2\sigma^2}(\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\top(\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) \\ &- \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_0)^\top \boldsymbol{S}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_0) + \text{const.}\end{aligned}$$

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- Expand the quadratic terms in $\boldsymbol{\theta}$:

$$(\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\top(\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) = \mathbf{y}^\top\mathbf{y} - 2\mathbf{y}^\top\boldsymbol{\Phi}\boldsymbol{\theta} + \boldsymbol{\theta}^\top\boldsymbol{\Phi}^\top\boldsymbol{\Phi}\boldsymbol{\theta},$$

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- Collect all terms that depend on $\boldsymbol{\theta}$:

$$\log p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y}) = -\frac{1}{2}\Big[\boldsymbol{\theta}^\top\big(\sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi} + \boldsymbol{S}_0^{-1}\big)\boldsymbol{\theta} \\ - 2\big(\sigma^{-2}\boldsymbol{\Phi}^\top\mathbf{y} + \boldsymbol{S}_0^{-1}\boldsymbol{m}_0\big)^\top\boldsymbol{\theta}\Big] + \text{const.}$$

Proof of Theorem 9.1 (3/3)

- A multivariate Gaussian $\mathcal{N}(\boldsymbol{\theta} \mid \boldsymbol{m}_N, \boldsymbol{S}_N)$ has log-density (up to an additive constant)

$$\begin{aligned}\log \mathcal{N}(\boldsymbol{\theta} \mid \boldsymbol{m}_N, \boldsymbol{S}_N) &= -\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_N)^\top \boldsymbol{S}_N^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_N) + \text{const} \\ &= -\frac{1}{2}\left[\boldsymbol{\theta}^\top \boldsymbol{S}_N^{-1}\boldsymbol{\theta} - 2\boldsymbol{m}_N^\top \boldsymbol{S}_N^{-1}\boldsymbol{\theta}\right] + \text{const.}\end{aligned}$$

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- Compare this with the quadratic form obtained on the previous slide:

$$\boldsymbol{\theta}^\top\left(\sigma^{-2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi} + \boldsymbol{S}_0^{-1}\right)\boldsymbol{\theta} \quad \text{and} \quad \left(\sigma^{-2}\boldsymbol{\Phi}^\top\mathbf{y} + \boldsymbol{S}_0^{-1}\boldsymbol{m}_0\right)^\top\boldsymbol{\theta}.$$

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- Matching the coefficients of the quadratic and linear terms in $\boldsymbol{\theta}$ gives

$$\boldsymbol{S}_N^{-1} = \sigma^{-2}\boldsymbol{\Phi}^\top \boldsymbol{\Phi} + \boldsymbol{S}_0^{-1} \quad \Longrightarrow \quad \boldsymbol{S}_N = (\boldsymbol{S}_0^{-1} + \sigma^{-2}\boldsymbol{\Phi}^\top \boldsymbol{\Phi})^{-1},$$

$$\boldsymbol{m}_N^\top \boldsymbol{S}_N^{-1} = \big(\sigma^{-2}\boldsymbol{\Phi}^\top \mathbf{y} + \boldsymbol{S}_0^{-1}\boldsymbol{m}_0\big)^\top \quad \Longrightarrow \quad \boldsymbol{m}_N = \boldsymbol{S}_N\big(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{\Phi}^\top \mathbf{y}\big).$$