

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.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
Francesco Orabona: A Modern Introduction to Online Learning.
<https://arxiv.org/abs/1912.13213>

Outline

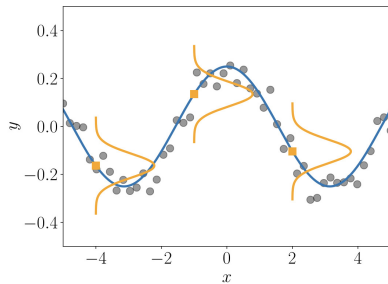
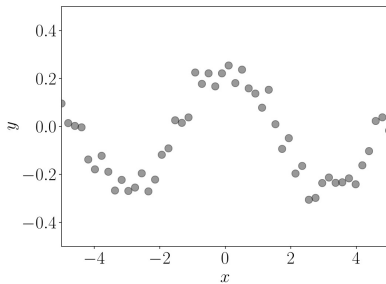
- 1 Introduction
- 2 Problem Formulation
- 3 Parameter Estimation
 - Maximum Likelihood Estimation (MLE)
 - Overfitting in Linear Regression
 - Maximum A Posteriori Estimation (MAP)
 - MAP Estimation as Regularization

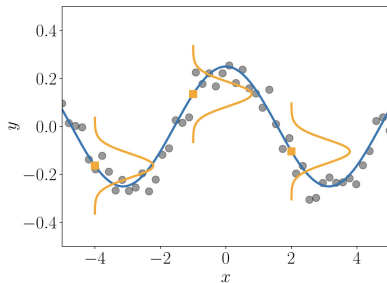
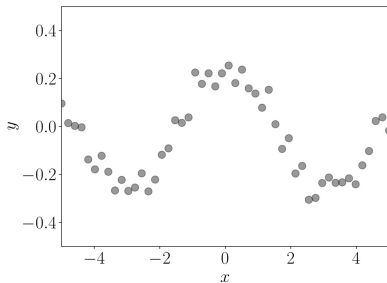
Linear Regression

Aim

Find (or Infer) a function $f : \mathbb{R}^D \mapsto \mathbb{R}$ 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.





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.
 - Equip model predictions with confidence bounds.

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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:

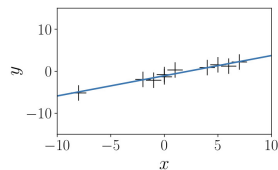
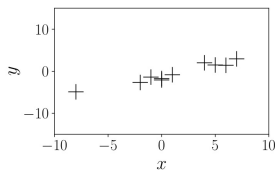
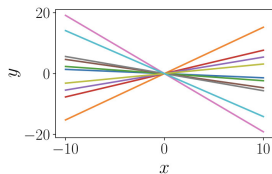
$$p(y \mid \mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y \mid \mathbf{x}^\top \boldsymbol{\theta}, \sigma^2).$$

\Longleftrightarrow

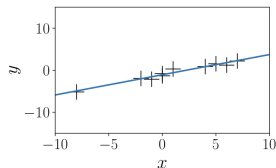
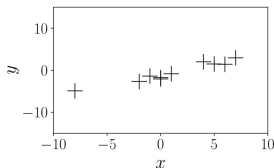
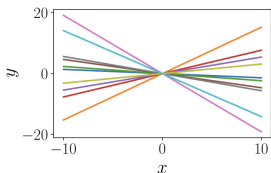
$$y = \mathbf{x}^\top \boldsymbol{\theta} + \epsilon,$$

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.



- “Linear”: linear in the parameters.
- Hence, $y = \phi^\top(\mathbf{x})\theta$ is also regarded as a linear regression (ϕ can be nonlinear) .

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The Likelihood

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

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

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 θ_{ML}

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

Note:

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

Maximum Likelihood Estimation (MLE)

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

Note:

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

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How to find the desired θ_{ML} ?

- 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 \Leftrightarrow Minimize negative log-likelihood

The negative log-likelihood

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

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

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

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

Ignoring the constant terms, we obtain

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

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

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★ We use the positive definite property of $\mathbf{X}^\top \mathbf{X}$ if $\text{rank}(\mathbf{X}) = D$.

Remark

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

MLE with Features

- Note that “linear” regression is linear in the “parameters”.
- 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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$$\Longleftrightarrow$$

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

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

Polynomial Regression

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

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

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

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

We can also define a feature matrix as

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

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

Feature Matrix for Second-Order Polynomials

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

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The negative log-likelihood can be written as

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

- Replacing \mathbf{X} by Φ .
- Both of them are independent of θ .

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- Both of them are independent of θ .
- Similarly, we have¹

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

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Estimating the Noise Variance (1/2)

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- Write down the log-likelihood:

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

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

Estimating the Noise Variance (2/2)

- The partial derivative w.r.t. σ^2 :

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

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

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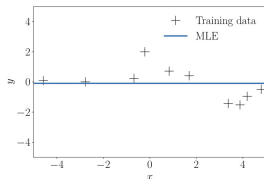
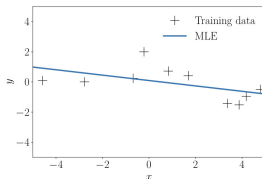
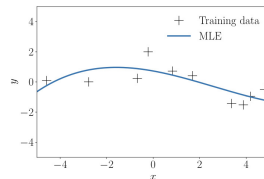
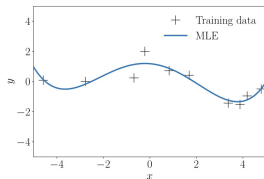
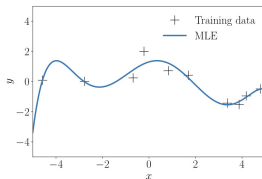
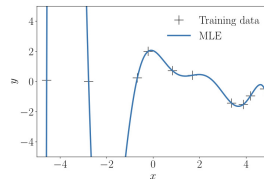
- Model selection:

Evaluating the Quality of the Model

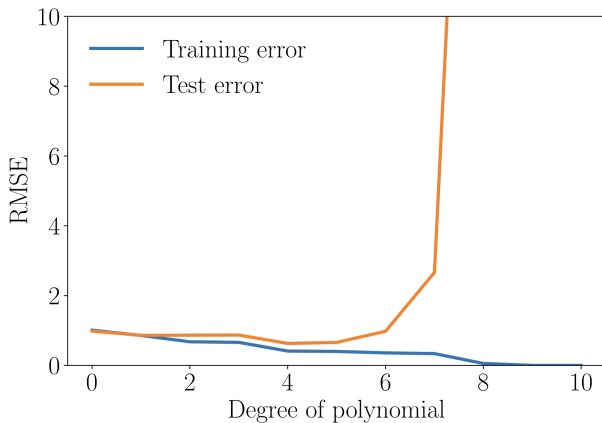
- We can evaluate the quality of the model by computing the error/loss.
- Given that σ^2 is not a free model parameter, we can ignore that term by scaling by $1/\sigma^2$ and derive a squared-error function $\|\mathbf{y} - \Phi\boldsymbol{\theta}\|^2$.
- To compare the errors of datasets with **different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

$$\sqrt{\frac{1}{N}\|\mathbf{y} - \Phi\boldsymbol{\theta}\|^2} = \sqrt{\frac{1}{N}\sum_{i=1}^N (y_i - \phi^\top(\mathbf{x}_i)\boldsymbol{\theta})^2}$$

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

(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.



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

Motivation

- MLE is prone to overfitting.
- **Experience:** The parameter values becomes relatively large when the model is overfitting.

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Motivation

- 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** $p(\theta)$ on the parameters.
- **Rough idea:** Encode the parameter values that are plausible before seeing any data.
 - For example, a Gaussian prior $p(\theta) = \mathcal{N}(\mathbf{0}, I)$.

Maximum a Posteriori Estimation (1/5)

- Once a dataset $(\mathcal{X}, \mathcal{Y})$ is available, we seek 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.

Maximum a Posteriori Estimation (2/5)

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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.

We minimize the negative log-posterior w.r.t. $\boldsymbol{\theta}$:

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

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:

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

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

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

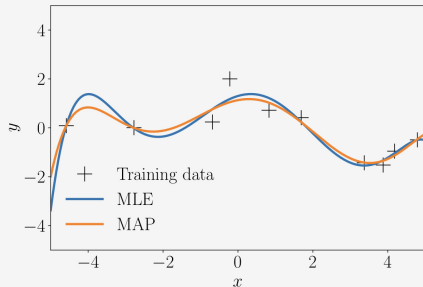
Finally, we have

Maximum a Posteriori Estimation (5/5)

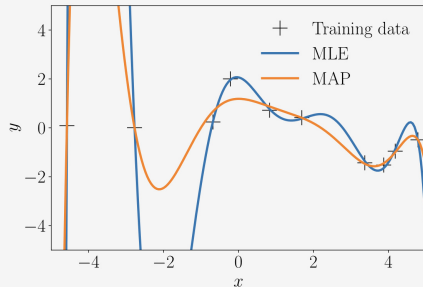
$$\begin{aligned} & \frac{1}{\sigma^2}(\boldsymbol{\theta}^\top \boldsymbol{\Phi}^\top \boldsymbol{\Phi} - \mathbf{y}^\top \boldsymbol{\Phi}) + \frac{1}{b^2} \boldsymbol{\theta}^\top = \mathbf{0}^\top \\ \Leftrightarrow & \boldsymbol{\theta}^\top \left(\frac{1}{\sigma^2} \boldsymbol{\Phi}^\top \boldsymbol{\Phi}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

Finally, we have

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



(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:

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

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 $p(\boldsymbol{\theta}) = \mathcal{N}(\mathbf{0}, b^2 \mathbf{I})$, 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

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

Minimizing the regularized least-squares loss function yields

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

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 $p(\theta) = \mathcal{N}(\mathbf{0}, b^2 I)$.

Discussions