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

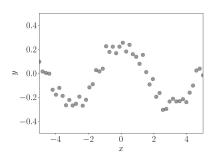
- Introduction
- Problem Formulation
- Parameter Estimation
 - Maximum Likelihood Estimation (MLE)
 - Overfitting in Linear Regression
 - Maximum A Posteriori Estimation (MAP)
 - MAP Estimation as Regularization

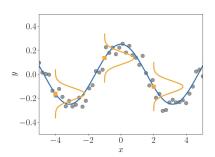
Linear Regression

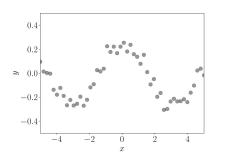
Aim

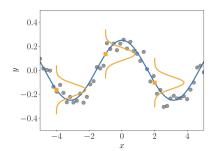
Find (or Infer) a function $f: \mathbb{R}^D \to \mathbb{R}$ which maps input $\mathbf{x} \in \mathbb{R}^D$ to the corresponding function values $f(\mathbf{x}) \in \mathbb{R}$.

- And we hope f to generalize well to unseen input.
- Training input: $\{x_i\}_{i=1}^N$
- 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

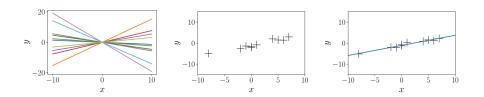
• An example of linear regression:

$$p(y \mid \mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y \mid \mathbf{x}^{\mathsf{T}} \boldsymbol{\theta}, \sigma^{2}).$$
$$v = \mathbf{x}^{\mathsf{T}} \boldsymbol{\theta} + \epsilon.$$

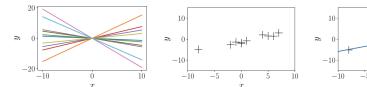
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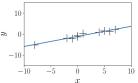
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.

- $\theta \in \mathbb{R}^D$: the parameters we seek.
- ullet 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:

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

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 $\theta^* \in \mathbb{R}^D$.
- 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 $heta_{ML}$

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

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.

ML Math - Linear Regression
Parameter Estimation
Maximum Likelihood Estimation (MLE)

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- Perform gradient ascent (or descent).
- For linear regression, we can directly have a closed-form solution.
- 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

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

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

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

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

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

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

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

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

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

Polynomial Regression (Example)

Consider a regression problem $y = \phi^{\top}(x)\theta + \epsilon$, for $x \in \mathbb{R}$ and $\theta \in \mathbb{R}^K$. A polynomial transformation of 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 $f(x) = \sum_{k=1}^{K-1} \theta_k x^k = \phi^\top(x) \theta$, for $\theta = [\theta_0, \dots, \theta_{K-1}]^\top \in \mathbb{R}^K$ which contains the linear parameters θ_k .

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

We can also define a feature matrix as

$$oldsymbol{\Phi} := \left[egin{array}{c} oldsymbol{\phi}^ op(\mathbf{x}_1) & oldsymbol{\phi}^ op(\mathbf{x}_1) & \cdots & \phi_{K-1}(\mathbf{x}_1) \ \phi_0(\mathbf{x}_2) & \cdots & \phi_{K-1}(\mathbf{x}_2) \ dots & dots & dots \ \phi_0(\mathbf{x}_N) & \cdots & \phi_{K-1}(\mathbf{x}_N) \end{array}
ight] \in \mathbb{R}^{N imes K},$$

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

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Feature Matrix for Second-Order Polynomials

$$\mathbf{\Phi} := \left[egin{array}{cccc} 1 & x_1 & x_1^2 \ 1 & x_2 & x_2^2 \ dots & dots & dots \ 1 & x_N & x_N^2 \end{array}
ight].$$

With the feature matrix Φ :

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The negative log-likelihood can be written as

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

- ullet Replacing $oldsymbol{\mathcal{X}}$ by $oldsymbol{\Phi}$.
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- Similarly, we have¹

$$oldsymbol{ heta}_{ extit{ML}} = (oldsymbol{\Phi}^ op oldsymbol{\Phi})^{-1} oldsymbol{\Phi}^ op \mathbf{y}.$$

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Estimating the Noise Variance (1/2)

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

Estimating the Noise Variance (1/2)

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- Write down the log-likelihood:

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

Estimating the Noise Variance (1/2)

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

4 11 2 4 4 12 2 4 12 2 2 9 9 9

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

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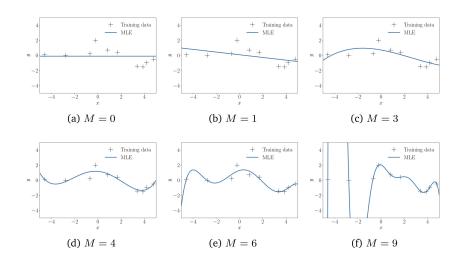
• Model selection:

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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):

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

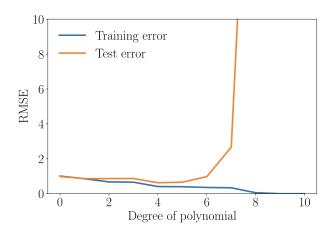
- Model selection: determine the best degree of the polynomial.
 - Brute-force searching and enumerate all reasonable polynomial degrees M.

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

ML Math - Linear Regression
Parameter Estimation
Overfitting in Linear Regression



Outline

- Introduction
- Problem Formulation
- 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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- 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 $p(\theta) = \mathcal{N}(\mathbf{0}, \mathbf{I})$.

Maximum a Posteriori Estimation (1/5)

• Once a dataset $(\mathcal{X}, \mathcal{Y})$ is available, we week parameters that maximize the posterior distribution $p(\theta \mid \mathcal{X}, \mathcal{Y})$ 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.
- θ_{MAP} : the maximizer of the above posterior (i.e., the MAP estimate).

Maximum a Posteriori Estimation (2/5)

The log-transformation of the posterior:

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

The constant is independent of θ .

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 θ .

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. θ :

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

Maximum a Posteriori Estimation (3/5)

$$m{ heta_{MAP}} \in rg\min_{m{ heta}} \{-\log p(\mathcal{Y} \mid \mathcal{X}, m{ heta}) - \log p(m{ heta})\}.$$

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

$$-\log p(oldsymbol{ heta} \mid \mathcal{X}, \mathcal{Y}) = rac{1}{2\sigma^2} (\mathbf{y} - \Phioldsymbol{ heta})^ op (\mathbf{y} - \Phioldsymbol{ heta}) + rac{1}{2b^2} oldsymbol{ heta}^ op oldsymbol{ heta} + ext{constant}$$

Maximum a Posteriori Estimation (4/5)

$$-\log p(m{ heta} \mid \mathcal{X}, \mathcal{Y}) = rac{1}{2\sigma^2} (\mathbf{y} - \mathbf{\Phi}m{ heta})^ op (\mathbf{y} - \mathbf{\Phi}m{ heta}) + rac{1}{2b^2} m{ heta}^ op m{ heta} + ext{constant}$$

Hence, the gradient of the log-posterior w.r.t. heta 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 θ_{MAP} :

Maximum a Posteriori Estimation (5/5)

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

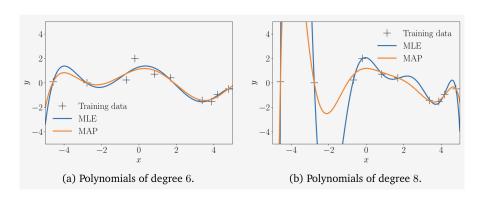
Finally, we have

Maximum a Posteriori Estimation (5/5)

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

Finally, we have

$$oldsymbol{ heta}_{MAP} = \left(oldsymbol{\Phi}^ op oldsymbol{\Phi} + rac{\sigma^2}{b^2} oldsymbol{I}
ight)^{-1} oldsymbol{\Phi}^ op \mathbf{y}.$$



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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:

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

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 $p(\theta) = \mathcal{N}(\mathbf{0}, b^2 \mathbf{I})$, so the negative log-Gaussian prior is

$$-\log p(oldsymbol{ heta}) = rac{1}{2b^2} \|oldsymbol{ heta}\|_2^2 + \mathsf{constant}$$

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

ML Math - Linear Regression
Parameter Estimation
MAP Estimation as Regularization

Minimizing the regularized least-squares loss function yields

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

Minimizing the regularized least-squares loss function yields

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

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

Discussions