Lecture 9: Linear Regression

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Mathematics for Machine Learning
https://yung-web.github.io/home/courses/mathml.html
KAIST EE

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Warm-Up

Please watch this tutorial video by Luis Serrano on PCA.

https://www.youtube.com/watch?v=wYPUhge9w5c

Roadmap

(1) Problem Formulation

(2) Parameter Estimation: ML

(3) Parameter Estimation: MAP

(4) Bayesian Linear Regression

(5) Maximum Likelihood as Orthogonal Projection

Roadmap

(1) Problem Formulation

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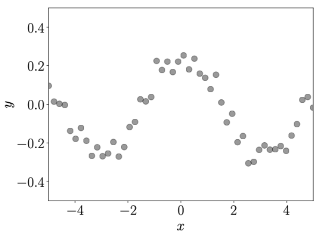
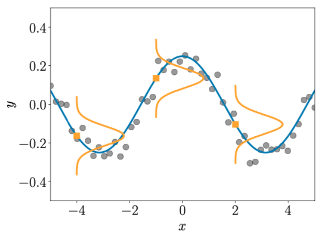
Regression Problem





- For some input values x_n, we observe noisy function values $y_n = f(x_n) + \epsilon$
- Goal: infer the function f that generalizes well to function values at new inputs
- Applications: time-series analysis, control and robotics, image recognition, etc.

Formulation

Notation for simplification (this is how the textbook uses)

$p(y|\mathbf{x}) = p_{Y|\mathbf{X}}(y|\mathbf{x}), \quad Y \sim \mathcal{N}(\mu, \sigma^2) \xrightarrow{\text{simplifies}} \mathcal{N}(y \mid f(\mathbf{x}), \sigma^2)$

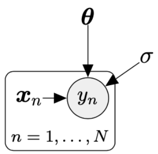
- Assume: linear regression, Gaussian noise
- $y = f(\mathbf{x}) + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- Likelihood: for $\mathbf{x} \in \mathbb{R}^D$ and $y \in \mathbb{R}$, $p(y \mid \mathbf{x}) = \mathcal{N}(y \mid f(\mathbf{x}), \sigma^2)$
- Linear regression with the parameter $\boldsymbol{\theta} \in \mathbb{R}^D$, i.e., $f(\mathbf{x}) = \mathbf{x}^\mathsf{T}\boldsymbol{\theta}$

$$p(y \mid \mathbf{x}) = \mathcal{N}(y \mid \mathbf{x}^\mathsf{T}\boldsymbol{\theta}, \sigma^2) \iff y = \mathbf{x}^\mathsf{T}\boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

Prior with Gaussian nose: $p(y \mid \mathbf{x}) = \mathcal{N}(y \mid \mathbf{x}^\mathsf{T}\boldsymbol{\theta}, \sigma^2)$

Parameter Estimation

- Training set $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$



- Assuming iid N data samples, the likelihood is factorized into:

$$p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = \prod_{n=1}^{N} p(y_n \mid \mathbf{x}_n, \boldsymbol{\theta}) = \prod_{n=1}^{N} \mathcal{N}(y_n \mid \mathbf{x}_n^\mathsf{T}, \sigma^2),$$

where $\mathcal{X} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ and $\mathcal{Y} = \{y_1, \ldots, y_n\}$

- Estimation methods: ML and MAP

Roadmap

(1) Problem Formulation
(2) Parameter Estimation: ML
(3) Parameter Estimation: MAP
(4) Bayesian Linear Regression
(5) Maximum Likelihood as Orthogonal Projection

MLE (Maximum Likelihood Estimation) (1)

- $\theta_{\text{ML}} = \arg\max_{\theta} p(\mathcal{Y} \mid \mathcal{X}, \theta) = \arg\min_{\theta} \left(-\log p(\mathcal{Y} \mid \mathcal{X}, \theta) \right)$
- For Gaussian noise with $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^\top$ and $\boldsymbol{y} = [y_1, \ldots, y_n]^\top$,

$$-\log p(\mathcal{Y} \mid \mathcal{X}, \theta) = -\log \prod_{n=1}^{N} p(y_n \mid \boldsymbol{x}_n, \theta) = -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n, \theta)$$

$$= \frac{1}{2\sigma^2} \sum_{n=1}^{N} (y_n - \boldsymbol{x}_n^\top \theta)^2 + \text{ const} = \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{X}\theta\|^2 + \text{ const}$$

Negative-log likelihood for $f(\boldsymbol{x}) = \boldsymbol{x}^\top \theta + \mathcal{N}(0, \sigma^2)$:

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

MLE (Maximum Likelihood Estimation) (2)

- For Gaussian noise with $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n]^\top$ and $\boldsymbol{y} = [y_1, \ldots, y_n]^\top$,

$$\theta_{\text{ML}} = \arg\min_{\theta} \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{X}\theta\|^2, \quad L(\theta) = \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{X}\theta\|^2$$

- In case of Gaussian noise, $\theta_{\text{ML}} = \theta$ that minimizes the empirical risk with the squared loss function
  - Models as functions = Model as probabilistic models

MLE (Maximum Likelihood Estimation) (3)

- We find θ such that $\frac{dL}{d\theta} = 0$

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

$$\iff \theta_{\text{ML}}^\top \boldsymbol{X}^\top \boldsymbol{X} = \boldsymbol{y}^\top \boldsymbol{X}$$

$$\iff \theta_{\text{ML}}^\top = \boldsymbol{y}^\top \boldsymbol{X} (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \quad (\boldsymbol{X}^\top \boldsymbol{X} \text{ is positive definite if } \text{rk}(\boldsymbol{X}) = D)$$

$$\iff \theta_{\text{ML}} = (\boldsymbol{X}^\top \boldsymbol{X})^{-1} \boldsymbol{X}^\top \boldsymbol{y}$$

MLE with Features

- Linear regression: Linear in terms of the parameters
  - $\phi(\boldsymbol{x})^\top \theta$ is also fine, where $\phi(\boldsymbol{x})$ can be non-linear (we will cover this later)
  - $\phi(\boldsymbol{x})$ are the features
- Linear regression with the parameter $\theta \in \mathbb{R}^K$, $\phi(\boldsymbol{x}) : \mathbb{R}^D \mapsto \mathbb{R}^K$:

$$p(y \mid \boldsymbol{x}) = \mathcal{N}(y \mid \phi(\boldsymbol{x})^\top \theta, \sigma^2) \iff y = \phi(\boldsymbol{x})^\top \theta + \epsilon = \sum_{k=0}^{K-1} \theta_k \phi_k(\boldsymbol{x}) + \epsilon$$

- Example. Polynomial regression. For $x \in \mathbb{R}$ and $\theta \in \mathbb{R}^K$, we lift the original 1-D input into K-D feature space with monomials x^k:

$$\phi(x) = \begin{pmatrix} \phi_0(x) \\ \vdots \\ \phi_{K-1}(x) \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ x^{K-1} \end{pmatrix} \in \mathbb{R}^K \quad \Longrightarrow \quad f(x) = \sum_{k=0}^{K-1} \theta_k x^k$$

Feature Matrix and MLE

- Now, for the entire training set $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$,

$$\boldsymbol{\Phi} := \begin{pmatrix} \phi^{\mathsf{T}}(\boldsymbol{x}_1) \\ \vdots \\ \phi^{\mathsf{T}}(\boldsymbol{x}_N) \end{pmatrix} = \begin{pmatrix} \phi_0(\boldsymbol{x}_1) & \cdots & \phi_{K-1}(\boldsymbol{x}_1) \\ \vdots & \cdots & \vdots \\ \phi_0(\boldsymbol{x}_N) & \cdots & \phi_{K-1}(\boldsymbol{x}_N) \end{pmatrix} \in \mathbb{R}^{N \times K}, \ \boldsymbol{\Phi}_{ij} = \phi_j(\boldsymbol{x}_i), \ \phi_j : \mathbb{R}^D \mapsto \mathbb{R}$$

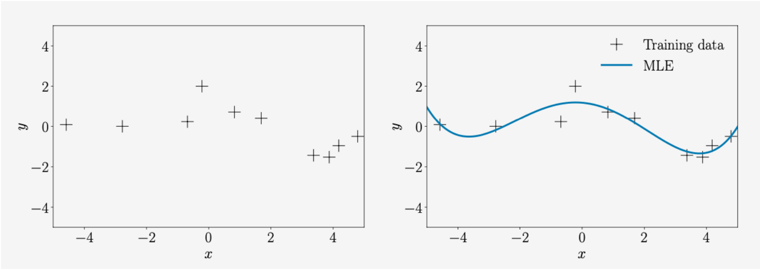
- Negative log-likelihood: Similarly to the case of $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\theta}$,
  - $p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{y} \mid \boldsymbol{\Phi}\boldsymbol{\theta}, \sigma^2 \boldsymbol{I})$
  - Negative-log likelihood for $f(\boldsymbol{x}) = \phi^{\mathsf{T}}(\boldsymbol{x})\boldsymbol{\theta} + \mathcal{N}(0, \sigma^2)$:

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

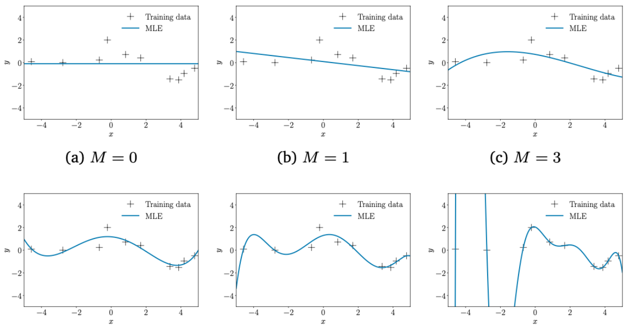
- MLE: $\boldsymbol{\theta}_{\text{ML}} = (\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{y}$

Polynomial Fit

- $N = 10$ data, where $x_n \sim \mathcal{U}[-5, 5]$ and $y_n = -\sin(x_n/5) + \cos(x_n) + \epsilon$, $\epsilon \sim \mathcal{N}(0, 0.2^2)$
- Fit with poloynomial with degree 4 using ML

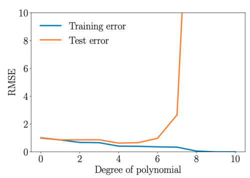


Overfitting in Linear Regression



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

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



- Higher polynomial degree is better (training error always decreases)
- Test error increases after some polynomial degree

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MAPE (Maximum A Posteriori Estimation)

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- MLE: prone to overfitting, where the magnitude of the parameters becomes large.
- a prior distribution $p(\boldsymbol{\theta})$ helps: what $\boldsymbol{\theta}$ is plausible
- MAPE and Bayes' theorem

$$p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y}) = \frac{p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) p(\boldsymbol{\theta})}{p(\mathcal{Y} \mid \mathcal{X})} \implies \boldsymbol{\theta}_{\mathrm{MAP}} \in \arg\min_{\boldsymbol{\theta}} \Big(-\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) - \log p(\boldsymbol{\theta}) \Big)$$

- Gradient

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

MAPE for Gausssian Prior (1)

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- Example. A (conjugate) Gaussian prior $p(\boldsymbol{\theta}) \sim \mathcal{N}(0, b^2 \boldsymbol{I})$
  - For Gaussian likelihood, Gaussian prior $\implies$ Gaussian posterior L6(6)
- Negative log-posterior

> Negative-log posterior for $f(\boldsymbol{x}) = \phi^{\mathsf{T}}(\boldsymbol{x})\boldsymbol{\theta} + \mathcal{N}(0, \sigma^2)$ and $p(\boldsymbol{\theta}) \sim \mathcal{N}(0, b^2 \boldsymbol{I})$:
>
> $$-\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^{\mathsf{T}}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) + \frac{1}{2b^2}\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{\theta} + \text{const}$$

- Gradient

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

MAPE for Gausssian Prior (2)

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- MAP vs. ML

$$\boldsymbol{\theta}_{\mathrm{MAP}} = \underbrace{\left(\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{\Phi} + \frac{\sigma^2}{b^2}\boldsymbol{I}\right)}_{(*)}^{-1} \boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{y}, \quad \boldsymbol{\theta}_{\mathrm{ML}} = (\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{y}$$

- The term $\frac{\sigma^2}{b^2}\boldsymbol{I}$
  - Ensures that $(*)$ is symmetric, strictly positive definite
  - Role of regularizer

Aside: MAPE for General Gausssian Prior (3)

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- Example. A (conjugate) Gaussian prior $p(\boldsymbol{\theta}) \sim \mathcal{N}(\boldsymbol{m}_0, \boldsymbol{S}_0)$
- Negative log-posterior

> Negative-log posterior for $f(\boldsymbol{x}) = \phi^{\mathsf{T}}(\boldsymbol{x})\boldsymbol{\theta} + \mathcal{N}(0, \sigma^2)$ and $p(\boldsymbol{\theta}) \sim \mathcal{N}(\boldsymbol{m}_0, \boldsymbol{S}_0)$:
>
> $$-\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^{\mathsf{T}}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_0)^{\mathsf{T}}\boldsymbol{S}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_0) + \text{const}$$

- We will use this later for computing the parameter posterior distribution in Bayesian linear regression.

Regularization: MAPE vs. Explicit Regularizer

- Explicit regularizer in regularized least squares (RLS)

$$\|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2 + \lambda \|\boldsymbol{\theta}\|^2$$

- MAPE wth Gaussian prior $p(\boldsymbol{\theta}) \sim \mathcal{N}(0, b^2\boldsymbol{I})$
  - Negative log-Gaussian prior

$$-\log p(\boldsymbol{\theta}) = \frac{1}{2b^2}\boldsymbol{\theta}^\mathsf{T}\boldsymbol{\theta} + \text{const}$$

  - $\lambda = 1/2b^2$ is the regularization term
- Not surprising that we have

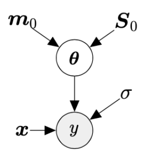
$$\boldsymbol{\theta}_{\text{RLS}} = \left(\boldsymbol{\Phi}^\mathsf{T}\boldsymbol{\Phi} + \lambda\boldsymbol{I}\right)^{-1}\boldsymbol{\Phi}^\mathsf{T}\boldsymbol{y}$$

Roadmap

Bayesian Linear Regression

- Earlier, ML and MAP. Now, fully Bayesian L8(4)
- Model

prior	$p(\boldsymbol{\theta}) \sim \mathcal{N}(\boldsymbol{m}_0, \boldsymbol{S}_0)$
likelihood	$p(y\|\boldsymbol{x}, \boldsymbol{\theta}) \sim \mathcal{N}\left(y \mid \phi^\mathsf{T}(\boldsymbol{x})\boldsymbol{\theta}, \sigma^2\right)$
joint	$p(y, \boldsymbol{\theta}\|\boldsymbol{x}) = p(y \mid \boldsymbol{x}, \boldsymbol{\theta})p(\boldsymbol{\theta})$



- Goal: For an input $\boldsymbol{x}_*$, we want to compute the following posterior predictive distribution[1] of y_*:

$$p(y_*|x_*, \mathcal{X}, \mathcal{Y}) = \int \overbrace{p(y_*|\boldsymbol{x}_*, \boldsymbol{\theta})}^{\text{likelihood}}\overbrace{p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y})}^{(*)}\,\mathrm{d}\boldsymbol{\theta}$$

  - $(*)$: parameter posterior distribution that needs to be computed

[1] Chapter 9.3.4 For ease of understanding, I've slightly changed the organization of these lecture slides from that of the textbook.

Parameter Posterior Distribution (1)

- Parameter posterior distribution Chapter 9.3.3

$$p(\boldsymbol{\theta} \mid \mathcal{X}, \mathcal{Y}) = \mathcal{N}(\boldsymbol{\theta} \mid \boldsymbol{m}_N, \boldsymbol{S}_N), \quad \text{where}$$
$$\boldsymbol{S}_N = \left(\boldsymbol{S}_0^{-1} + \sigma^2\boldsymbol{\Phi}^\mathsf{T}\boldsymbol{\Phi}\right)^{-1}, \quad \boldsymbol{m}_N = \boldsymbol{S}_N\left(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{\Phi}^\mathsf{T}\boldsymbol{y}\right)$$

(Proof Sketch)

- From the negative-log posterior for general Gaussian prior,

$$-\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^\mathsf{T}(\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{m}_0)^\mathsf{T}\boldsymbol{S}_0^{-1}(\boldsymbol{\theta} - \boldsymbol{m}_0) + \text{const}$$

Parameter Posterior Distribution (2)

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

- cyan color: quadratic term, orange color: linear term
- $p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y}) \propto \exp($ quadratic in $\boldsymbol{\theta}$ $) \implies$ Gaussian distribution
- Assume that $p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y}) = \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_N,\boldsymbol{S}_N)$, and find $\boldsymbol{m}_N$ and $\boldsymbol{S}_N$.

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

- Thus, $\boldsymbol{S}_N^{-1} = \sigma^{-2}\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi} + \boldsymbol{S}_0^{-1}$ and $\boldsymbol{m}_N^{\top}\boldsymbol{S}_N^{-1} = (\sigma^{-2}\boldsymbol{\Phi}^{\top}\boldsymbol{y} + \boldsymbol{S}_0^{-1}\boldsymbol{m}_0)^{\top}$

Posterior Predictions (1)

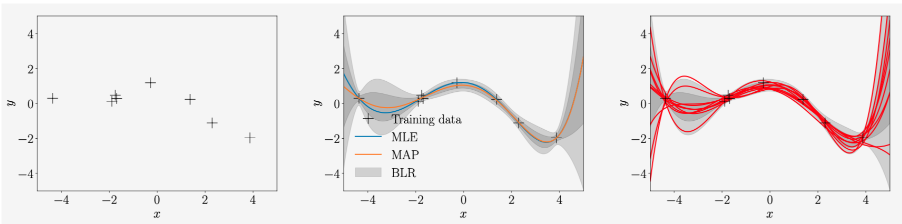
L6(5)

- Posterior predictive distribution

$$p(y_*|x_*,\mathcal{X},\mathcal{Y}) = \int p(y_*|\boldsymbol{x}_*,\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathcal{X},\mathcal{Y})\mathrm{d}\boldsymbol{\theta}$$
$$= \int \mathcal{N}\Big(y_*|\phi^{\top}(\boldsymbol{x}_*)\boldsymbol{\theta},\sigma^2\Big)\mathcal{N}\Big(\boldsymbol{\theta}|\boldsymbol{m}_N,\boldsymbol{S}_N\Big)\mathrm{d}\boldsymbol{\theta}$$
$$= \mathcal{N}\Big(y_*|\phi^{\top}(\boldsymbol{x}_*)\boldsymbol{m}_N, \phi^{\top}(\boldsymbol{x}_*)\boldsymbol{S}_N\phi(\boldsymbol{x}_*) + \sigma^2\Big)$$

- The mean $\phi^{\top}(\boldsymbol{x}_*)\boldsymbol{m}_N$ coincides with the MAP estimate

Posterior Predictions (2)



- BLR: Bayesian Linear Regression

Computing Marginal Likelihood

- Likelihood: $p(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta})$, Marginal likelihood: $p(\mathcal{Y}|\mathcal{X}) = \int p(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}$
- Recall that the marginal likelihood is important for model selection via Bayes factor:

$$(\text{Posterior odds}) = \frac{\mathbb{P}(M_1 \mid \mathcal{D})}{\mathbb{P}(M_2 \mid \mathcal{D})} = \frac{\frac{\mathbb{P}(\mathcal{D}|M_1)\mathbb{P}(M_1)}{\mathbb{P}(\mathcal{D})}}{\frac{\mathbb{P}(\mathcal{D}|M_2)\mathbb{P}(M_2)}{\mathbb{P}(\mathcal{D})}} = \underbrace{\frac{\mathbb{P}(M_1)}{\mathbb{P}(M_2)}}_{\text{Prior odds}}\underbrace{\frac{\mathbb{P}(\mathcal{D} \mid M_1)}{\mathbb{P}(\mathcal{D} \mid M_2)}}_{\text{Bayes factor}}$$

$$p(\mathcal{Y}|\mathcal{X}) = \int p(\mathcal{Y}|\mathcal{X},\boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta} = \int \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{\theta},\sigma^2\boldsymbol{I})\mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_0,\boldsymbol{S}_0)\,\mathrm{d}\boldsymbol{\theta}$$
$$= \mathcal{N}(\boldsymbol{y} \mid \boldsymbol{\Phi}\boldsymbol{m}_0, \boldsymbol{\Phi}\boldsymbol{S}_0\boldsymbol{\Phi}^{\top} + \sigma^2\boldsymbol{I})$$

Roadmap

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ML as Orthogonal Projection

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- For $f(\boldsymbol{x}) = \boldsymbol{x}^{\mathsf{T}}\boldsymbol{\theta} + \mathcal{N}(0, \sigma^2)$, $\boldsymbol{\theta}_{\mathrm{ML}} = (\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{y} = \dfrac{\boldsymbol{X}^{\mathsf{T}}\boldsymbol{y}}{\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}} \in \mathbb{R}$

$$\boldsymbol{X}\boldsymbol{\theta}_{\mathrm{ML}} = \frac{\boldsymbol{X}\boldsymbol{X}^{\mathsf{T}}}{\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}}\boldsymbol{y}$$

  - Orthogonal projection of $\boldsymbol{y}$ onto the one-dimensional subspace spanned by $\boldsymbol{X}$
- For $f(\boldsymbol{x}) = \phi^{\mathsf{T}}(\boldsymbol{x})\boldsymbol{\theta} + \mathcal{N}(0, \sigma^2)$, $\boldsymbol{\theta}_{\mathrm{ML}} = (\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{\Phi})^{-1}\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{y} = \dfrac{\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{y}}{\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{\Phi}} \in \mathbb{R}$

$$\boldsymbol{\Phi}\boldsymbol{\theta}_{\mathrm{ML}} = \frac{\boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathsf{T}}}{\boldsymbol{\Phi}^{\mathsf{T}}\boldsymbol{\Phi}}\boldsymbol{y}$$

  - Orthogonal projection of $\boldsymbol{y}$ onto the K-dimensional subspace spanned by columns of $\boldsymbol{\Phi}$

Summary and Other Issues (1)

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- Linear regression for Gaussian likelihood and conjugate Gaussian priors. Nice analytical results and closed forms
- Other forms of likelihoods for other applications (e.g., classification)
- GLM (generalized linear model): $y = \sigma \circ f$ (σ: activation function)
  - No longer linear in $\boldsymbol{\theta}$
  - Logistic regression: $\sigma(f) = \dfrac{1}{1 + \exp(-f)} \in [0, 1]$ (interpreted as the probability of becoming 1)
  - Building blocks of (deep) feedforward neural nets
  - $\boldsymbol{y} = \sigma(\boldsymbol{A}\boldsymbol{x} + \boldsymbol{b})$. $\boldsymbol{A}$: weight matrix, $\boldsymbol{b}$: bias vector
  - K-layer deep neural nets: $\boldsymbol{x}_{k+1} = f_k(\boldsymbol{x}_k)$, $f_k(\boldsymbol{x}_k) = \sigma_k(\boldsymbol{A}_k\boldsymbol{x}_k + \boldsymbol{b}_k)$

Summary and Other Issues (2)

KAIST EE

- Gaussian process
  - A distribution over parameters $\rightarrow$ a distribution over functions
  - Gaussian process: distribution over functions without detouring via parameters
  - Closely related to BLR and support vector regression, also interpreted as Bayesian neural network with a single hidden layer and the infinite number of units
- Gaussian likelihood, but non-Gaussian prior
  - When $N \ll D$ (small training data)
  - Prior that enforces sparsity, e.g., Laplace prior
  - A linear regression with the Laplace prior = linear regression with LASSO (L1 regularization)

Questions?

1)