QUY NHON UNIVERSITY DEPARTMENT OF MATHEMATICS AND STATISTICS

Linear Regression

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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

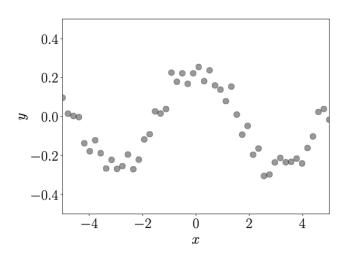


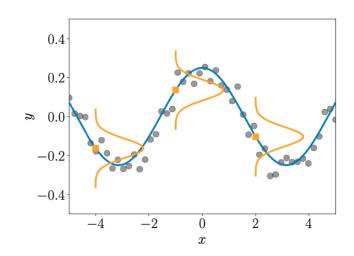
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Regression Problem





- 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)

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

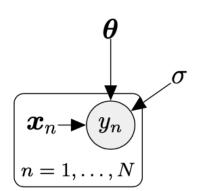
- Assume: linear regression, Gaussian noise
- $y = f(x) + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- Likelihood: for $\mathbf{x} \in \mathbb{R}^D$ and $y \in \mathbb{R}$, $p(y \mid \mathbf{x}) = \mathcal{N}(y \mid f(\mathbf{x}), \sigma^2)$
- Linear regression with the parameter $\theta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

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

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

Parameter Estimation

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



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

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

where
$$\mathcal{X} = \{x_1, \dots, x_n\}$$
 and $\mathcal{Y} = \{y_1, \dots, y_n\}$

Estimation methods: ML and MAP



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MLE (Maximum Likelihood Estimation) (1)

- $\theta_{\mathsf{ML}} = \operatorname{arg\,max}_{\boldsymbol{\theta}} p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = \operatorname{arg\,min}_{\boldsymbol{\theta}} \Big(\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) \Big)$
- For Gaussian noise with $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]^\mathsf{T}$ and $\mathbf{y} = [y_1, \dots, y_n]^\mathsf{T}$,

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

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

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

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

MLE (Maximum Likelihood Estimation) (2)

• For Gaussian noise with $\boldsymbol{X} = [\boldsymbol{x}_1, \dots, \boldsymbol{x}_n]^\mathsf{T}$ and $\boldsymbol{y} = [y_1, \dots, y_n]^\mathsf{T}$,

$$oldsymbol{ heta}_{\mathsf{ML}} = rg \min_{oldsymbol{ heta}} rac{1}{2\sigma^2} \left\| oldsymbol{y} - oldsymbol{X} oldsymbol{ heta}
ight\|^2, \quad L(oldsymbol{ heta}) = rac{1}{2\sigma^2} \left\| oldsymbol{y} - oldsymbol{X} oldsymbol{ heta}
ight\|^2$$

- ullet In case of Gaussian noise, $heta_{
 m ML}= heta$ 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 $\frac{dL}{d\theta} = 0$

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

$$\iff \theta_{\mathsf{ML}}^{\mathsf{T}} \mathbf{X}^{\mathsf{T}} \mathbf{X} = \mathbf{y}^{\mathsf{T}} \mathbf{X}$$

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

$$\iff \theta_{\mathsf{ML}} = (\mathbf{X}^{\mathsf{T}} \mathbf{X})^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{y}$$



MLE with Features

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

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

• 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 :

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

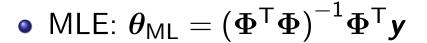
Feature Matrix and MLE

• Now, for the entire training set $\{x_1, \dots, x_N\}$,

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

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

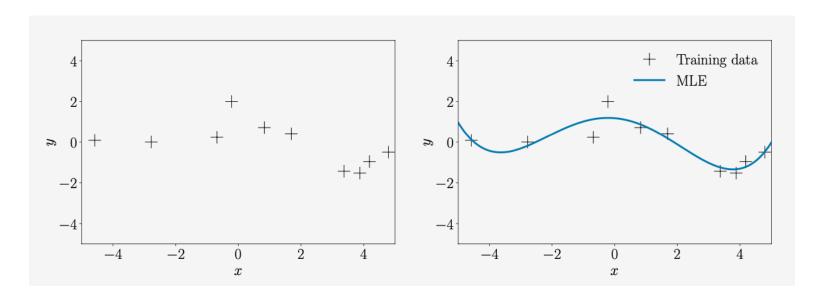
$$-\log p(\mathcal{Y} \mid \mathcal{X}, \boldsymbol{\theta}) = \frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{\Phi}\boldsymbol{\theta}\|^2 + \text{const}$$





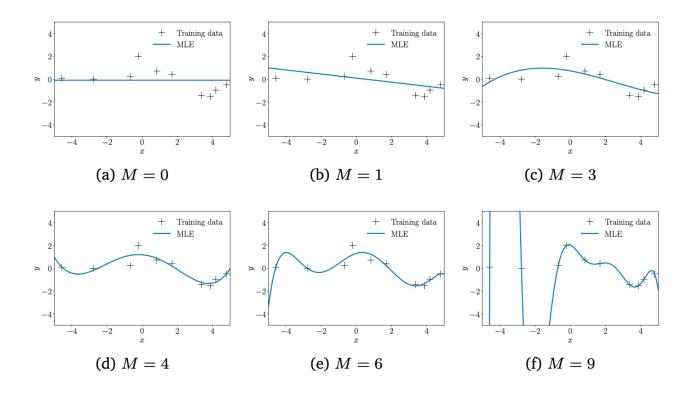
Polynomial Fit

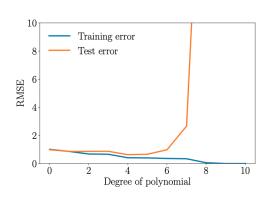
- N=10 data, where $x_n \sim \mathcal{U}[-5,5]$ and $y_n = -\sin(x_n/5) + \cos(x_n) + \epsilon$, $\epsilon \sim \mathcal{N}(0,0.2^2)$
- Fit with poloynomial with degree 4 using ML





Overfitting in Linear Regression





- 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)

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

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

Gradient

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



MAPE for Gaussian Prior (1)

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

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

$$-\log p(m{ heta}|\mathcal{X},\mathcal{Y}) = rac{1}{2\sigma^2}(m{y} - m{\Phi}m{ heta})^\mathsf{T}(m{y} - m{\Phi}m{ heta}) + rac{1}{2b^2}m{ heta}^\mathsf{T}m{ heta} + \mathsf{const}$$

Gradient

$$-rac{\mathsf{d} \log p(oldsymbol{ heta}|\mathcal{X},\mathcal{Y})}{\mathsf{d}oldsymbol{ heta}} = rac{1}{\sigma^2}(oldsymbol{ heta}^\mathsf{T}oldsymbol{\Phi}^\mathsf{T}oldsymbol{\Phi} - oldsymbol{y}^\mathsf{T}oldsymbol{\Phi}) + rac{1}{b^2}oldsymbol{ heta}^\mathsf{T}$$



MAPE for Gausssian Prior (2)

MAP vs. ML

$$m{ heta_{\mathsf{MAP}}} = \underbrace{\left(m{\Phi}^\mathsf{T} m{\Phi} + rac{\sigma^2}{b^2} m{I}
ight)}^{-1} m{\Phi}^\mathsf{T} m{y}, \quad m{ heta_{\mathsf{ML}}} = \left(m{\Phi}^\mathsf{T} m{\Phi}
ight)^{-1} m{\Phi}^\mathsf{T} m{y}$$

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



Aside: MAPE for General Gaussian Prior (3)

- Example. A (conjugate) Gaussian prior $p(\theta) \sim \mathcal{N}(m_0, S_0)$
- Negative log-posterior

Negative-log posterior for
$$f(\mathbf{x}) = \phi^{\mathsf{T}}(\mathbf{x})\boldsymbol{\theta} + \mathcal{N}(0,\sigma^2)$$
 and $p(\boldsymbol{\theta}) \sim \mathcal{N}(\mathbf{x})$

Negative-log posterior for
$$f(\mathbf{x}) = \phi^{\mathsf{T}}(\mathbf{x})\boldsymbol{\theta} + \mathcal{N}(0,\sigma^2)$$
 and $p(\boldsymbol{\theta}) \sim \mathcal{N}(\mathbf{r})$ an

 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)

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

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

$$-\log p(heta) = rac{1}{2b^2} heta^\mathsf{T} heta + \mathsf{const}$$

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

$$oldsymbol{ heta}_{\mathsf{RLS}} = \left(oldsymbol{\Phi}^\mathsf{T}oldsymbol{\Phi} + \lambda oldsymbol{I}
ight)^{-1}oldsymbol{\Phi}^\mathsf{T}oldsymbol{y}$$



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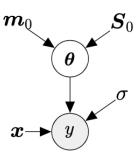


Bayesian Linear Regression

Earlier, ML and MAP. Now, fully Bayesian

Model

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



 \bullet Goal: For an input x_* , we want to compute the following posterior predictive distribution 1 of y_* :

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

• (*): 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

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

$$\mathbf{S}_N = (\mathbf{S}_0^{-1} + \sigma^2 \mathbf{\Phi}^\mathsf{T} \mathbf{\Phi})^{-1}, \quad \mathbf{m}_N = \mathbf{S}_N (\mathbf{S}_0^{-1} \mathbf{m}_0 + \sigma^{-2} \mathbf{\Phi}^\mathsf{T} \mathbf{y})$$

(Proof Sketch)

From the negative-log posterior for general Gaussian prior,

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



Parameter Posterior Distribution (2)

$$= \frac{1}{2} \left(\sigma^{-2} \mathbf{y}^{\mathsf{T}} \mathbf{y} - 2 \sigma^{-2} \mathbf{y}^{\mathsf{T}} \mathbf{\Phi} \theta + \theta^{\mathsf{T}} \sigma^{-2} \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} \theta + \theta^{\mathsf{T}} \mathbf{S}_{0}^{-1} \theta - 2 \mathbf{m}_{0}^{\mathsf{T}} \mathbf{S}_{0}^{-1} \theta + \mathbf{m}_{0}^{\mathsf{T}} \mathbf{S}_{0}^{-1} \theta \right)$$

$$= \frac{1}{2} \left(\theta^{\mathsf{T}} (\sigma^{-2} \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} + \mathbf{S}_{0}^{-1}) \theta - 2 (\sigma^{-2} \mathbf{\Phi}^{\mathsf{T}} \mathbf{y} + \mathbf{S}_{0}^{-1} \mathbf{m}_{0})^{\mathsf{T}} \theta \right) + \text{const}$$

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

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

$$= \frac{1}{2}(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{S}_{N}^{-1}\boldsymbol{\theta} - 2\boldsymbol{m}_{N}^{\mathsf{T}}\boldsymbol{S}_{N}^{-1}\boldsymbol{\theta} + \boldsymbol{m}_{N}^{\mathsf{T}}\boldsymbol{S}_{N}^{-1}\boldsymbol{m}_{N}) + \text{const}$$

• Thus, $\mathbf{S}_N^{-1} = \sigma^{-2} \mathbf{\Phi}^{\mathsf{T}} \mathbf{\Phi} + \mathbf{S}_0^{-1}$ and $\mathbf{m}_N^{\mathsf{T}} \mathbf{S}_N^{-1} = (\sigma^{-2} \mathbf{\Phi}^{\mathsf{T}} \mathbf{y} + \mathbf{S}_0^{-1} \mathbf{m}_0)^{\mathsf{T}}$



Posterior Predictions (1)

Posterior predictive distribution

L6(5)

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

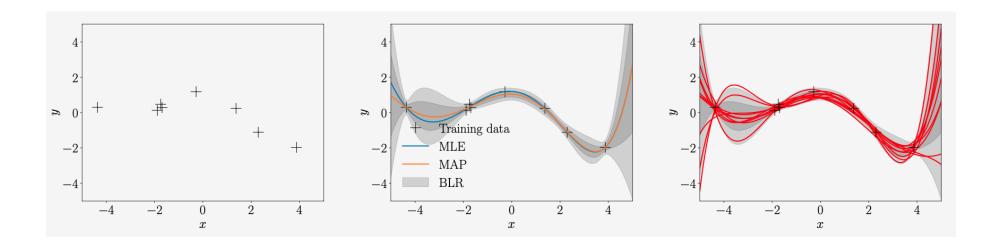
$$= \int \mathcal{N}(y_*|\phi^{\mathsf{T}}(\mathbf{x}_*)\boldsymbol{\theta}, \sigma^2) \mathcal{N}(\boldsymbol{\theta}|\mathbf{m}_N, \mathbf{S}_N) d\boldsymbol{\theta}$$

$$= \mathcal{N}(y_*|\phi^{\mathsf{T}}(\mathbf{x}_*)\mathbf{m}_N, \phi^{\mathsf{T}}(\mathbf{x}_*)\mathbf{S}_N \phi(\mathbf{x}_*) + \sigma^2)$$

• The mean $\phi^{\mathsf{T}}(\mathbf{x}_*)\mathbf{m}_N$ 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: $p(\mathcal{Y}|\mathcal{X}) = \int p(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$
- Recall that the marginal likelihood is important for model selection via Bayes factor:

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

$$\begin{split} \rho(\mathcal{Y}|\mathcal{X}) &= \int \rho(\mathcal{Y}|\mathcal{X}, \boldsymbol{\theta}) \rho(\boldsymbol{\theta}) d\boldsymbol{\theta} = \int \mathcal{N}(\boldsymbol{y}|\boldsymbol{\Phi}\boldsymbol{\theta}, \sigma^2 \boldsymbol{I}) \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{m}_0, \boldsymbol{S}_0) d\boldsymbol{\theta} \\ &= \mathcal{N}(\boldsymbol{y} \mid \boldsymbol{\Phi}\boldsymbol{m}_0, \boldsymbol{\Phi}\boldsymbol{S}_0 \boldsymbol{\Phi}^\mathsf{T} + \sigma^2 \boldsymbol{I}) \end{split}$$





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ML as Orthogonal Projection

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

$$oldsymbol{X}oldsymbol{ heta}_{\mathsf{ML}} = rac{oldsymbol{X}oldsymbol{X}^{\mathsf{T}}}{oldsymbol{X}^{\mathsf{T}}oldsymbol{X}}oldsymbol{y}$$

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

$$oldsymbol{\Phi}oldsymbol{ heta}_\mathsf{ML} = rac{oldsymbol{\Phi}oldsymbol{\Phi}^\mathsf{T}}{oldsymbol{\Phi}^\mathsf{T}oldsymbol{\Phi}} oldsymbol{y}$$

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

Summary and Other Issues (1)

- 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)
 - ullet No longer linear in heta
 - Logistic regression: $\sigma(f)=\frac{1}{1+\exp(-f)}\in [0,1]$ (interpreted as the probability of becoming 1)
 - Building blocks of (deep) feedforward neural nets
 - $\mathbf{y} = \sigma(\mathbf{A}\mathbf{x} + \mathbf{b})$. **A**: weight matrix, **b**: bias vector
 - K-layer deep neural nets: $\mathbf{x}_{k+1} = f_k(\mathbf{x}_k), f_k(\mathbf{x}_k) = \sigma_k(\mathbf{A}_k\mathbf{x}_k + \mathbf{b}_k)$



Summary and Other Issues (2)

- Gaussian process
 - ullet A distribution over parameters o 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)



THANKS FOR YOUR ATTENTION



Discussions



