

Lecture 9: Linear Regression

Yi, Yung (이용)

Mathematics for Machine Learning

MONTH DAY, 2021

MONTH DAY, 2021 1 / 32

Roadmap



- Problem Formulation
- Parameter Estimation: ML
- Parameter Estimation: MAP
- Bayesian Linear Regression
- Maximum Likelihood as Orthogonal Projection

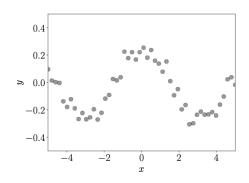


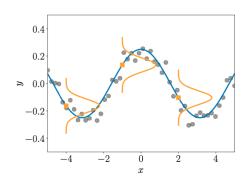
- Problem Formulation
- Parameter Estimation: ML
- Parameter Estimation: MAP
- Bayesian Linear Regression
- Maximum Likelihood as Orthogonal Projection

MONTH DAY, 2021 3 / 32

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



- · Linear regression, Gaussian noise
- Notation for simplification (this is how the textbook uses)

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

- Likelihood: for $\mathbf{x} \in \mathbb{R}^D$ and $\mathbf{y} \in \mathbb{R}$, $p(\mathbf{y} \mid \mathbf{x}) = \mathcal{N}(\mathbf{y} \mid f(\mathbf{x}), \sigma^2)$
- $y = f(\mathbf{x}) + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- Linear regression with the parameter $oldsymbol{ heta} \in \mathbb{R}^D$

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

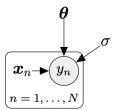
Prior with Gaussian nose: $p(y \mid \mathbf{x}) = \mathcal{N}(y \mid \mathbf{x}^{\mathsf{T}} \boldsymbol{\theta}, \sigma^2)$

MONTH DAY, 2021 5 / 32

Parameter Estimation



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



• Assuming iid of N data, 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 $\mathcal{X} = \{ \mathbf{x}_1, \dots, \mathbf{x}_n \}$ and $\mathcal{Y} = \{ y_1, \dots, y_n \}$

ML and MAP

Roadmap



- Problem Formulation
- Parameter Estimation: ML
- Parameter Estimation: MAP
- Bayesian Linear Regression
- Maximum Likelihood as Orthogonal Projection

MONTH DAY, 2021 7 / 32

MLE (Maximum Likelihood Estimation) (1)



•
$$heta_{\mathsf{ML}} = \operatorname{arg\,max}_{ heta} p(\mathcal{Y} \mid \mathcal{X}, oldsymbol{ heta}) = \operatorname{arg\,min}_{oldsymbol{ heta}} \Big(- \log p(\mathcal{Y} \mid \mathcal{X}, oldsymbol{ heta}) \Big)$$

• 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 $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_n]^\mathsf{T}$ and $\mathbf{y} = [y_1, \dots, y_n]^\mathsf{T}$, $\theta_\mathsf{ML} = \arg\min_{\mathbf{0}} \frac{1}{2\sigma^2} \|\mathbf{y} \mathbf{X}\boldsymbol{\theta}\|^2$, $L(\boldsymbol{\theta}) = \frac{1}{2\sigma^2} \|\mathbf{y} \mathbf{X}\boldsymbol{\theta}\|^2$
- In this special case of Gaussian noise, finding MLE is equivalent to finding heta that minimizes the empirical risk with squared loss function
 - Models as functions = Model as probabilistic models
- We find θ such that $\frac{dL}{d\theta} = 0$

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

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

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

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

MONTH DAY, 2021 9 / 32

MLE with Features



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

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

• 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 :

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

MONTH DAY, 2021 10 / 32

Feature Matrix and MLE



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

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

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

$$-\log p(\mathcal{Y}\mid\mathcal{X},oldsymbol{ heta}) = rac{1}{2\sigma^2}\left\|oldsymbol{y} - oldsymbol{\Phi}oldsymbol{ heta}
ight\|^2 + \mathsf{const}$$

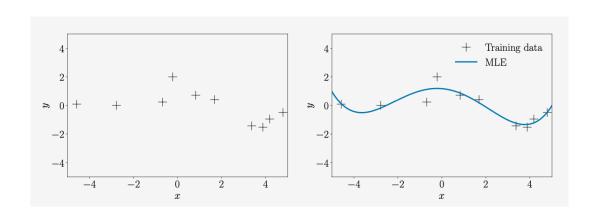
• MLE: $oldsymbol{ heta}_{\mathsf{ML}} = \left(oldsymbol{\Phi}^\mathsf{T} oldsymbol{\Phi}
ight)^{-1} oldsymbol{\Phi}^\mathsf{T} oldsymbol{y}$

MONTH DAY, 2021 11 / 32

Polynomial Fit

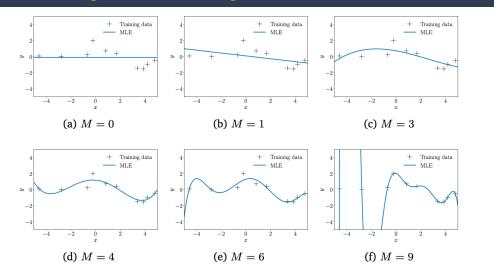


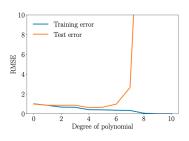
- N=10 data, where $x_n \sim \mathcal{U}[-5,5]$ and $y_n=-\sin(x_n/5)+\cos(x_n)+\epsilon$, $\epsilon \sim \mathcal{N}(0,0.2^2)$
- Fit with poloynomial with degree 4 using ML



Overfitting in Linear Regression







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

MONTH DAY, 2021 13 / 32

Roadmap



- Problem Formulation
- Parameter Estimation: ML
- Parameter Estimation: MAP
- Bayesian Linear Regression
- Maximum Likelihood as Orthogonal Projection

MAPE (Maximum A Posteriori Estimation)



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

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

Gradient

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

MONTH DAY, 2021 15 / 32

MAPE for Gaussian Prior (1)



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

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

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

Gradient

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

MAPE for Gaussian 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

MONTH DAY, 2021 17 / 32

Aside: MAPE for General Gausssian 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 $p(\boldsymbol{\theta}) \sim \mathcal{N}(\mathbf{m}_0, \mathbf{S}_0)$:
$$-\log p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{Y}) = \frac{1}{2\sigma^2}(\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta})^{\mathsf{T}}(\mathbf{y} - \boldsymbol{\Phi}\boldsymbol{\theta}) + \frac{1}{2}(\boldsymbol{\theta} - \mathbf{m}_0)^{\mathsf{T}}\mathbf{S}_0^{-1}(\boldsymbol{\theta} - \mathbf{m}_0) + \text{const}$$

• 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)

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

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

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

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

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

MONTH DAY, 2021 19 / 32

Roadmap



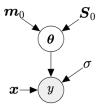
- Problem Formulation
- Parameter Estimation: ML
- Parameter Estimation: MAP
- Bayesian Linear Regression
- Maximum Likelihood as Orthogonal Projection

Bayesian Linear Regression



- Earlier, ML and MAP. Now, fully Bayesian
- Model

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



 Goal: For an input x_{*}, we want to compute the following posterior predictive distribution of y_{*}:

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

 \circ (*): parameter posterior distribution that needs to be computed

MONTH DAY, 2021 21 / 32

Parameter Posterior Distribution (1)



Parameter posterior distribution

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

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

(Proof of 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)



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

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

- cyan color: quadratic term, orange color: linear term
- $p(\theta|\mathcal{X},\mathcal{Y}) \propto \exp($ quadratic in θ $) \implies$ 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 .

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

Thus,

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

MONTH DAY, 2021 23 / 32

Posterior Predictions (1)



• Posterior predictive distribution

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

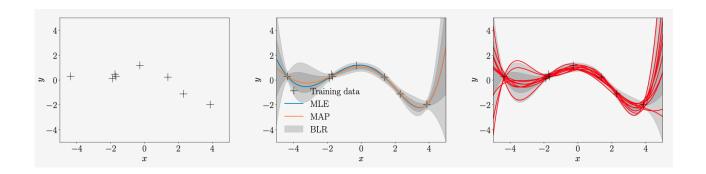
$$= \int \mathcal{N} \Big(y_*|\phi^{\mathsf{T}}(\mathbf{x}_*)\boldsymbol{\theta}, \sigma^2 \Big) \mathcal{N} \Big(\boldsymbol{\theta}|\mathbf{m}_N, \mathbf{S}_N \Big) d\boldsymbol{\theta}$$

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

• The mean $\phi^{\mathsf{T}}(\mathbf{x}_*)\mathbf{m}_{\mathsf{N}}$ coincides with the MAP estimate

Posterior Predictions (2)





• BLR: Bayesian Linear Regression

MONTH DAY, 2021 25 / 32

Computing Marginal Likelihood



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

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

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

Roadmap



- Problem Formulation
- Parameter Estimation: ML
- Parameter Estimation: MAP
- Bayesian Linear Regression
- Maximum Likelihood as Orthogonal Projection

MONTH DAY, 2021 27 / 32

ML as Orthogonal Projection



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

 \circ Orthogonal projection of $oldsymbol{y}$ onto the one-dimensional subspace spanned by $oldsymbol{X}$

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

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

 $\circ~$ Orthogonal projection of $\textbf{\emph{y}}$ onto the K-dimensional subspace spanned by columns of Φ

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)
 - \circ 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
 - \circ K-layer deep neural nets: $\mathbf{x}_{k+1} = f_k(\mathbf{x}_k), f_k(\mathbf{x}_k) = \sigma_k(\mathbf{A}_k\mathbf{x}_k + \mathbf{b}_k)$

MONTH DAY, 2021 29 / 32

Summary and Other Issues (2)



- Gaussian process
 - \circ 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
 - \circ When N << D (small training data)
 - Prior that enforces sparsity, e.g., Laplace prior
 - \circ A linear regression with teh Laplace prior = linear regression with LASSO (L1 regularization)



Questions?

MONTH DAY, 2021 31 / 32

Review Questions



1)