

EE269
Signal Processing for Machine Learning
Lecture 13

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Gaussian regression models

- ▶ $y \in \mathbb{R}$ continuous label and $x \in \mathbb{R}^d$
- ▶ training set x_1, \dots, x_n and labels y_1, \dots, y_n

$$p(y|x, w, b) = N(w^T x + b, \sigma^2)$$

- ▶ $P(w)$ prior probability of w
- ▶ infinitely many classes parametrized by w
- ▶ $\max_w P(y|x_1, \dots, x_n) = P(y|x_1, \dots, x_n, w, b)P(w)$
- ▶ independent observations: $= \prod_{i=1}^n P(y_i|x_i, w, b)P(w)$
- ▶ Maximum a Posteriori (MAP) estimate w_{MAP}

$$\begin{aligned} w_{MAP} &= \arg \max \prod_{i=1}^n P(y_i|x_i, w, b)P(w) \\ &= \arg \max \sum_{i=1}^n \log P(y_i|x_i, w, b) + \log P(w) \end{aligned}$$

Gaussian regression models

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$$w_{MAP} = \arg \max \sum_{i=1}^n \log P(y_i|x_i, w, b) + \log P(w)$$

- ▶ Gaussian prior on w : $P(w) = N(0, t^2 I)$

$$w_{MAP} = \arg \max -\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - w^T x_i - b)^2 - \frac{1}{2t^2} \|w\|_2^2$$

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- ▶ ℓ_2 regularization (Ridge regression)

Gaussian regression models

- ▶ Laplace prior $P(w) \propto e^{-\frac{|w_1|}{t}} \dots e^{-\frac{|w_d|}{t}}$

$$w_{MAP} = \arg \min_w \sum_{i=1}^n (y_i - w^T x_i - b)^2 + \frac{\sigma^2}{t} \|w\|_1$$

- ▶ ℓ_1 regularization (Lasso)

ℓ_2 regularization (Ridge regression)

$$\min_w \|Xw - y\|_2^2 + \lambda \|w\|_2^2 \quad (1)$$

ℓ_1 regularization (Lasso)

$$\min_w \|Xw - y\|_2^2 + \lambda \|w\|_1 \quad (2)$$

Exponential density $e^{-\frac{|w|}{t}}$ vs Gaussian density $e^{-\frac{w^2}{t^2}}$

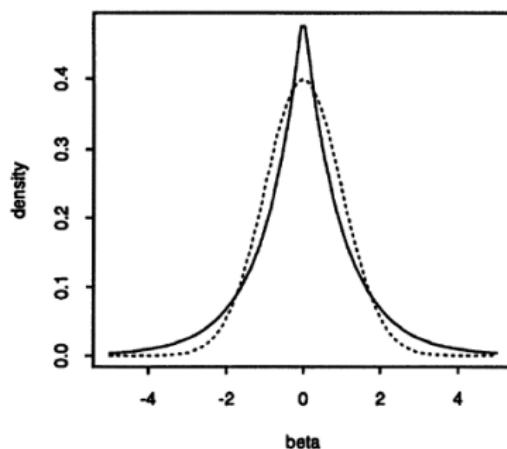


Fig. 7. Double-exponential density (—) and normal density (---): the former is the implicit prior used by the lasso; the latter by ridge regression

Least Squares Regression and Duality

- ▶ in matrix-vector notation (redefine $\lambda \leftarrow n\lambda$)

$$\min_w \frac{1}{2} \|Xw - y\|_2^2 + \frac{\lambda}{2} \|w\|_2^2$$

- ▶ equivalent constrained problem

$$\min_{z, w : Xw = z} \frac{1}{2} \|z - y\|_2^2 + \frac{\lambda}{2} \|w\|_2^2$$

- ▶ Dual problem:

$$\max_{\alpha} -\alpha^T \left(\frac{1}{2\lambda} X X^T + \frac{1}{2} I \right) \alpha + \alpha^T y$$

KKT conditions imply $w^* = \frac{1}{\lambda} X^T \alpha^*$

We can solve the dual in closed form $\alpha^* = (\frac{1}{\lambda} X X^T + I)^{-1} y$

Dual Least Squares Regression Problem

Dual problem:

$$\max_{\alpha} -\alpha^T \left(\frac{1}{2\lambda} X X^T + \frac{1}{2} I \right) \alpha + \alpha^T y$$

KKT conditions imply $w^* = \frac{1}{\lambda} X^T \alpha^*$

We can solve the dual in closed form $\alpha^* = (\frac{1}{\lambda} X X^T + I)^{-1} y$

- ▶ Given test sample x , the prediction is
 $w^{*T} x = \left(\frac{1}{\lambda} \sum_{i=1}^n x_i \alpha_i^* \right) x = \frac{1}{\lambda} \sum_{i=1}^n \langle x_i, x \rangle \alpha_i^*$
- ▶ Kernel map $x \rightarrow \Phi(x)$ and kernel matrix
 $K_{ij} = \kappa(x, y) = \langle \Phi(x), \Phi(y) \rangle$
- ▶ Dual solution $\alpha^* = (\frac{1}{\lambda} K + I)^{-1} y$
- ▶ Prediction $\hat{f}(x) = \frac{1}{\lambda} \sum_{i=1}^n \kappa(x_i, x) \alpha_i^*$

Kernel Regression Application

- ▶ polynomial kernel $\kappa(x, y) = (1 + x^T y)^4$
prediction $\hat{f}(x) = \frac{1}{\lambda} \sum_{i=1}^n \kappa(x_i, x) \alpha_i^*$

Kernel Regression Application

- ▶ Gaussian kernel $\kappa(x, y) = e^{-\frac{\|x-y\|_2^2}{2\sigma^2}}$
prediction $\hat{f}(x) = \frac{1}{\lambda} \sum_{i=1}^n \kappa(x_i, x) \alpha_i^*$

Reproducing Kernel Hilbert Space

- ▶ Mercer's Theorem: Any positive definite kernel function can be represented in terms of eigenfunctions

$$\kappa(x, y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \phi_i(y)$$

- ▶ The functions $\phi(x)$ form an orthonormal basis for a function space

$$\mathcal{H}_k = \{f : f(x) = \sum_{i=1}^{\infty} f_i \phi_i(x), \quad \sum_{i=1}^{\infty} \frac{f_i^2}{\lambda_i} < \infty\}$$

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- ▶ For two functions $f(x) = \sum_{i=1}^{\infty} f_i \phi_i(x)$ and $g(x) = \sum_{i=1}^{\infty} g_i(x) \phi_i$
- ▶ define inner product

$$\langle f, g \rangle_{\mathcal{H}} = \sum_{i=1}^{\infty} \frac{f_i g_i}{\lambda_i}$$

- ▶ reproducing property: $\langle \kappa(x, \cdot), \kappa(y, \cdot) \rangle_{\mathcal{H}} = \kappa(x, y)$

Representer Theorem in Reproducing Kernel Hilbert Space

$$(*) \quad \min_{f \in \mathcal{H}_k} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}_k}^2$$

- ▶ Representer theorem : The optimal solution must have the form $f^*(x) = \sum_{i=1}^n \alpha_i \kappa(x, x_i)$

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- ▶ Plugging in and applying reproducing property $\langle \kappa(x_i, \cdot), \kappa(x_j, \cdot) \rangle_{\mathcal{H}} = \kappa(x_i, x_j)$, we get

$$(*) = \min_{\alpha} \|K\alpha - y\|_2^2 + \lambda \alpha^T K \alpha$$

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$$(*) = \min_{\alpha} \|K\alpha - y\|_2^2 + \lambda \alpha^T K \alpha$$

- ▶ solution $\alpha^* = (K + \lambda I)^{-1} y$
- ▶ prediction $\hat{f}(x) = \sum_{i=1}^n \alpha_i^* \kappa(x, x_i)$
- ▶ same prediction rule obtained with dual ridge regression

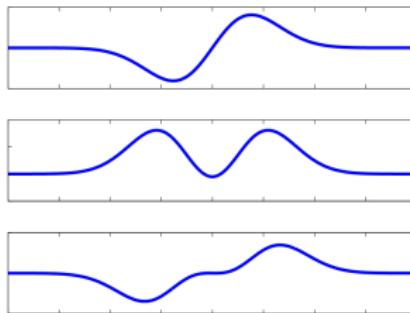
Example: Gaussian Kernel

- ▶ Gaussian kernel $\kappa(x, y) = e^{-\frac{\|x-y\|_2^2}{2\sigma^2}}$

$$\kappa(x, y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \phi_i(y)$$

$$\phi(x) \propto e^{-(c-a)x^2} H_i(x\sqrt{2c}) \text{ and } \lambda_i = b^i$$

a, b, c are functions of σ and H_k is the i th order Hermite polynomial



Example: Gaussian Kernel

- ▶ Gaussian kernel $\kappa(x, y) = e^{-\frac{\|x-y\|_2^2}{2\sigma^2}}$

$$f(x) = \sum_{i=1}^n \alpha_i \kappa(x_i, x) = \sum_{i=1}^n \sum_{j=1}^{\infty} \lambda_j \phi_j(x_i) \phi_j(x) = \sum_{j=1}^{\infty} f_j \sqrt{\lambda_j} \phi_j(x)$$

where $f_j = \sum_{i=1}^m \alpha_i \sqrt{\lambda_j} \phi_j(x_i)$

$$\min_{f \in \mathcal{H}_k} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}_k}^2$$

Example: Gaussian Kernel

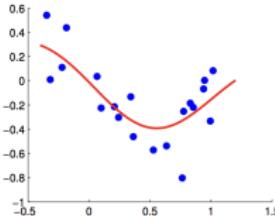
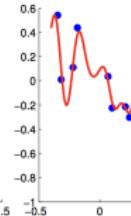
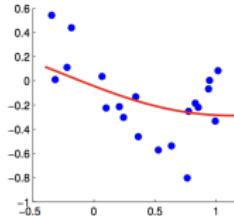
- ▶ Gaussian kernel $\kappa(x, y) = e^{-\frac{\|x-y\|_2^2}{2\sigma^2}}$

$$f(x) = \sum_{i=1}^n \alpha_i \kappa(x_i, x) = \sum_{i=1}^n \sum_{j=1}^{\infty} \lambda_j \phi_j(x_i) \phi_j(x) = \sum_{j=1}^{\infty} f_j \sqrt{\lambda_j} \phi_j(x)$$

where $f_j = \sum_{i=1}^m \alpha_i \sqrt{\lambda_j} \phi_j(x_i)$

$$\min_{f \in \mathcal{H}_k} \sum_{i=1}^n (f(x_i) - y_i)^2 + \lambda \|f\|_{\mathcal{H}_k}^2$$

- ▶ For a function $h(x) = \sum_{i=1}^{\infty} h_i \phi_i(x)$
- ▶ $\|h\|_{\mathcal{H}_k}^2 = \langle h, h \rangle_{\mathcal{H}_k} = \sum_{i=1}^{\infty} \frac{h_i^2}{\lambda_i}$ enforces smoothness by penalizing rough eigenfunctions (small λ_i).



Example: Sobolev Kernel (one dimensional signals)

$$\mathcal{H}_k = \{f : [0, 1] \rightarrow \mathbb{R} \mid f(0) = 0, \text{abs. continuous, } \int_{-\infty}^{\infty} |f'(t)|^2 dt < \infty\}$$

- ▶ absolutely continuous $\triangleq f'(t)$ exists almost everywhere,
- ▶ \mathcal{H}_k is a Reproducing Kernel Hilbert Space with kernel $\kappa(x, y) = \min(x, y)$

Sobolev Kernel vs Polynomial Kernel

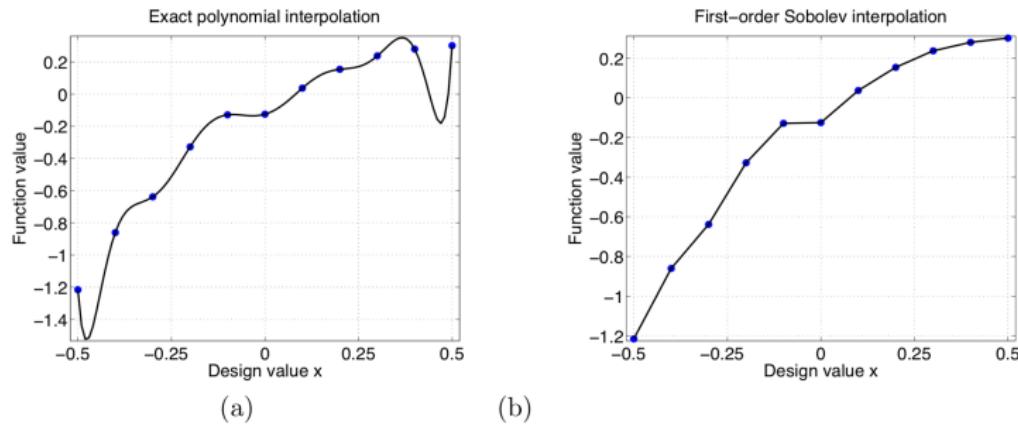


Figure 12-1. Exact interpolation of $n = 11$ equally sampled function values using RKHS methods.
(a) Polynomial kernel $\mathcal{K}(x, z) = (1 + x z)^{15}$. (b) First-order Sobolev kernel $\mathcal{K}(x, z) = 1 + \min\{x, z\}$.

Example: Sinc Kernel (one dimensional signals)

- ▶ Paley-Wiener space
- ▶ $\kappa(x, y) \triangleq \text{sinc}(\alpha(x - y)) = \frac{\sin(\alpha(x - y))}{\alpha(x - y)}$

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- ▶ $f(t)$: bandlimited functions

Example: Sinc Kernel (one dimensional signals)

- ▶ Paley-Wiener space
- ▶ $\kappa(x, y) \triangleq \text{sinc}(\alpha(x - y)) = \frac{\sin(\alpha(x-y))}{\alpha(x-y)}$
- ▶ $f(t)$: bandlimited functions
- ▶ related to Shannon-Whittaker interpolation formula
uniform samples $x[n] = x(nT)$
- ▶ bandlimited interpolation

$$x(t) = \sum_n x[n] \text{sinc}\left(\frac{t - nT}{T}\right)$$