Announcements

Convex Optimization (next quarter)

EE 578 Maryam Fazel

- Modeling, how to formulate real-world problems as convex optimization
- Constrained optimization (KKT, duality,)

CSE 535 Yin Tat Lee

- Algorithms (first order)
- Analysis (convergence proofs)

Statistics stuff

Stat 538 Zaid Harchaoui

- VC dimension, covering #
- What is "learnable"

(spring)
ML stuff

CS 547 Tim Althoff

- "Data science" "Big data"
- Large-scale data analysis and inference.

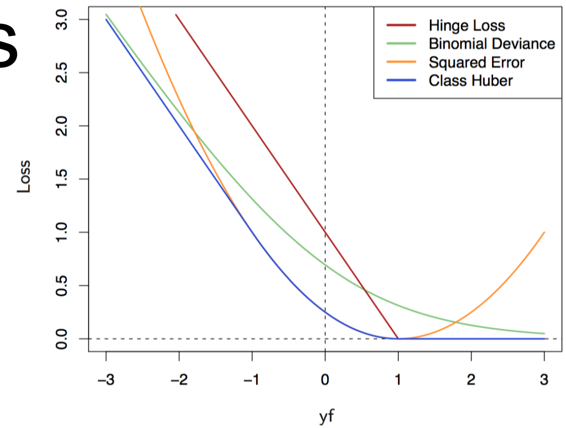
Kernels

Machine Learning – CSE546

Kevin Jamieson
University of Washington

November 6, 2018

Machine Learning Problems



- Have a bunch of iid data of the form:

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- Learning a model's parameters:

$$\sum_{i=1}^n \ell_i(w)$$

Each $\ell_i(w)$ is convex.

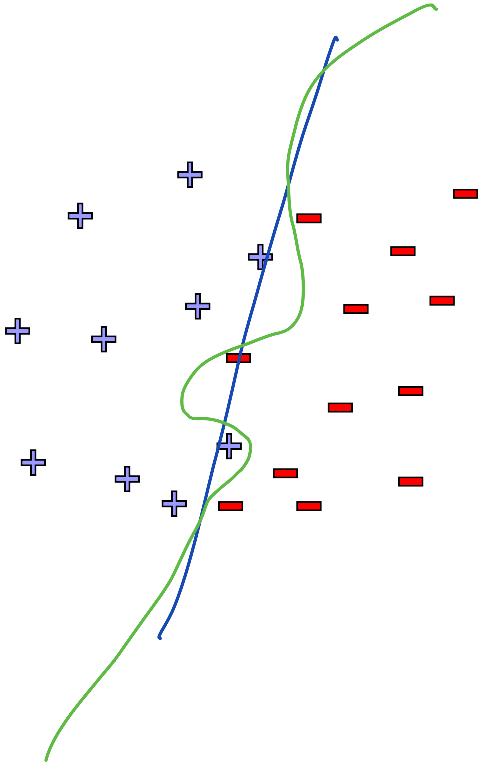
Hinge Loss: $\ell_i(w) = \max\{0, 1 - y_i \underline{x_i^T w}\}$

Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i \underline{x_i^T w}))$

Squared error Loss: $\ell_i(w) = (y_i - \underline{x_i^T w})^2$

All in terms of inner products! Even nearest neighbor can use inner products!

What if the data is not linearly separable?



Use features of features of features of features….

$$\phi(x) : \mathbb{R}^d \to \mathbb{R}^p$$

Feature space can get really large really quickly!

Dot-product of polynomials

$\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = \text{polynomials of degree}$ exactly d

$$d = 1 : \phi(u) = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \qquad \langle \phi(u), \phi(v) \rangle = u_1 v_1 + u_2 v_2$$

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$$d = 2 : \phi(u) = \begin{bmatrix} u_1^2 \\ u_2^2 \\ u_1 u_2 \\ u_2 u_1 \end{bmatrix} \qquad \langle \phi(u), \phi(v) \rangle = u_1^2 v_1^2 + u_2^2 v_2^2 + 2 u_1 u_2 v_1 v_2$$

$$= (u_1 v_1 + u_2 v_2)^2 = (u^T v)^2$$

Dot-product of polynomials

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$$= (u_1 v_1 + u_2 v_2)^2 = (u^T v)^2$$

General d : $\phi(u) = \begin{bmatrix} u_1^d \\ u_2^d \\ u_1^{d-1} u_2 \\ u_1^{d-2} u_2^2 \\ \vdots \end{bmatrix}$ $\qquad \langle \phi(u), \phi(v) \rangle = (u^T v)^d$

Dimension of $\phi(u)$ is roughly p^d if $u \in \mathbb{R}^p$

Kernel Trick

$$\widehat{w} = \arg\min_w \sum_{i=1}^n (y_i - x_i^T w)^2 + \lambda ||w||_w^2$$

$\hat{w} \in \mathbb{R}^d, \; x_i \in \mathbb{R}^d$

There exists an $\alpha \in \mathbb{R}^n$: $\boxed{\widehat{w} = \sum_{i=1}^n \alpha_i x_i}$ Why?

Suppose not. Then $\hat{w} = \sum \alpha_i x_i + \underbrace{w_\perp}$ where $w_\perp^T x_i = 0 \;\; \forall i$

$$\left\| \sum \alpha_i x_i + w_\perp \right\|_2 = \left\| \sum \alpha_i x_i \right\| + \| w_\perp \|$$

Kernel Trick

$$\widehat{w} = \arg\min_w \sum_{i=1}^n (y_i - x_i^T w)^2 + \lambda ||w||_w^2$$

There exists an $\alpha \in \mathbb{R}^n$: $\widehat{w} = \sum_{i=1}^n \alpha_i x_i$

$K_{ij} = \phi(x_i)^T \phi(x_j)$

$$\widehat{\alpha} = \arg\min_\alpha \sum_{i=1}^n (y_i - \sum_{j=1}^n \alpha_j \boxed{\langle x_j, x_i \rangle})^2 + \lambda \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \boxed{\langle x_i, x_j \rangle}$$

Kernel Trick

$$\widehat{w} = \arg\min_w \sum_{i=1}^n (y_i - x_i^T w)^2 + \lambda ||w||_{\cancel{w}\,2}^2$$

There exists an $\alpha \in \mathbb{R}^n$: $\boxed{\widehat{w} = \sum_{i=1}^n \alpha_i x_i}$

$$\widehat{\alpha} = \arg\min_\alpha \sum_{i=1}^n (y_i - \sum_{j=1}^n \alpha_j \langle x_j, x_i \rangle)^2 + \lambda \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j \langle x_i, x_j \rangle$$

$$= \arg\min_\alpha \sum_{i=1}^n (y_i - \sum_{j=1}^n \alpha_j K(x_i, x_j))^2 + \lambda \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j K(x_i, x_j)$$

$$= \arg\min_\alpha ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

New $z \in \mathbb{R}^d$, predict

$$z^T \widehat{w} = \sum_i \alpha_i z^T x_i = \sum_i \alpha_i K(z, x_i)$$

$$K_{i,j} = \underline{K(x_i, x_j)} = \underline{\langle \phi(x_i), \phi(x_j) \rangle}$$

Why regularization?

Typically, $\mathbf{K} \succ 0$. What if $\lambda = 0$?

$$\widehat{\alpha} = \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

$\nabla = 0 \implies -K(y - K\alpha) + \lambda K \alpha = 0$

$\cancel{K} y = \cancel{K}(K + \lambda I)\alpha$

$$\boxed{\hat{\alpha} = (K + \lambda I)^{-1} y}$$

$\hat{w} = X^T \hat{\alpha}$ $\qquad \hat{y} = X\hat{w} = XX^T\hat{\alpha} = K\hat{\alpha} = K(K+\lambda I)^{-1} y$

Why regularization?

Typically, $\mathbf{K} \succ 0$. What if $\lambda = 0$?

$$\widehat{\alpha} = \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

Unregularized kernel least squares can (over) fit **any data**!

$$\widehat{\alpha} = \mathbf{K}^{-1}\mathbf{y}$$

$$K\hat{\alpha} = y$$

Common kernels

$K(x,y) = \phi(x)^T \phi(y)$

- Polynomials of degree exactly d

$$K(\mathbf{u},\mathbf{v}) = (\mathbf{u}\cdot\mathbf{v})^d$$

- Polynomials of degree up to d

$$K(\mathbf{u},\mathbf{v}) = (\mathbf{u}\cdot\mathbf{v}+1)^d$$

- Gaussian (squared exponential) kernel

$$K(\mathbf{u},\mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||_2^2}{2\sigma^2}\right)$$

- Sigmoid

$$K(\mathbf{u},\mathbf{v}) = \tanh(\eta\mathbf{u}\cdot\mathbf{v}+\nu)$$

Mercer's Theorem

- When do we have a valid Kernel K(x,x')?
- Sufficient:

  $K(x, x')$ is a valid kernel if there exists $\phi(x)$ such that $K(x, x') = \phi(x)^T \phi(x')$

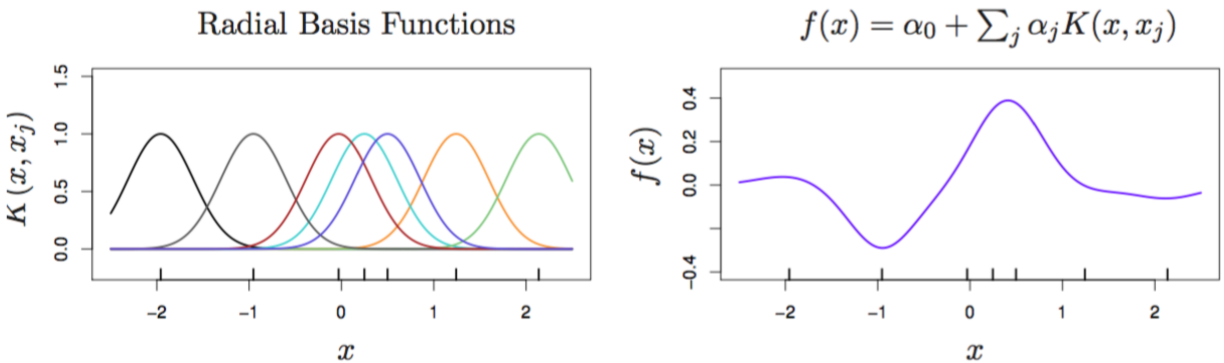
- Mercer's Theorem:

  $K(x, x')$ is a valid kernel if and only if $\mathbf{K}$ is symmetric and positive semi-definite for any pointset $(x_1, \ldots, x_n)$ where $\mathbf{K}_{i,j} = K(x_i, x_j)$.

RBF Kernel

$$K(\mathbf{u},\mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||_2^2}{2\sigma^2}\right)$$

- Note that this is like weighting "bumps" on each point like kernel smoothing but now we **learn** the weights

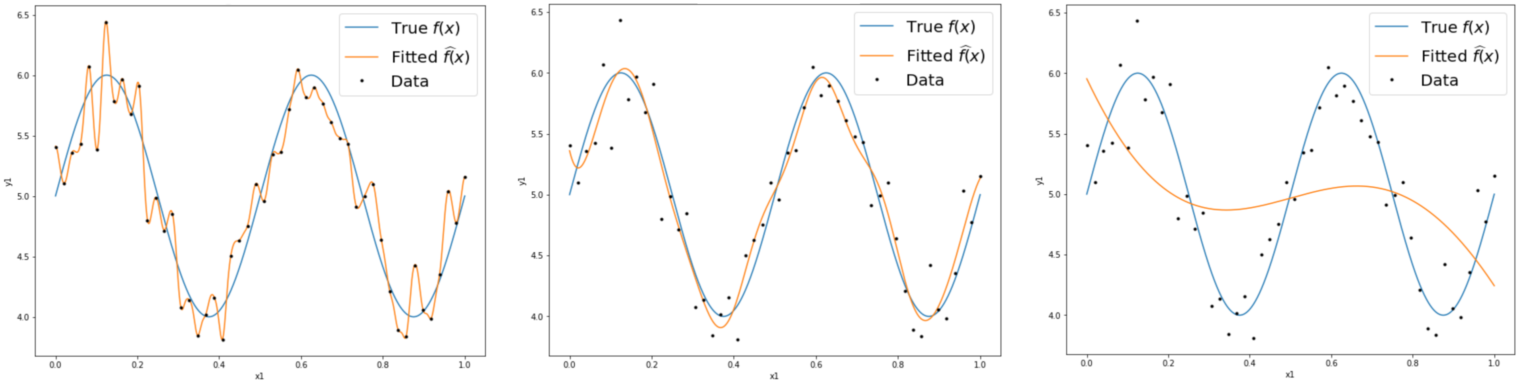


RBF Kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||_2^2}{2\sigma^2}\right)$$

The bandwidth sigma has an enormous effect on fit:

$\sigma = 10^{-2}$ $\lambda = 10^{-4}$ $\sigma = 10^{-1}$ $\lambda = 10^{-4}$ $\sigma = 10^{-0}$ $\lambda = 10^{-4}$



$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

RBF Kernel

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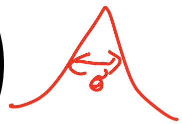

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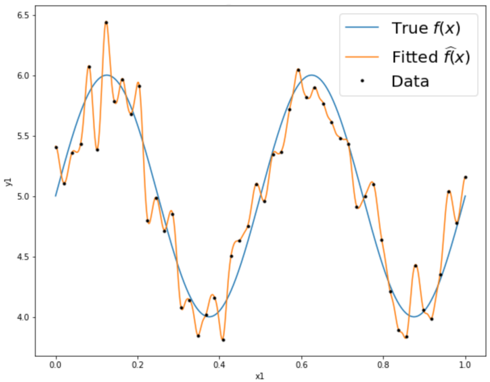
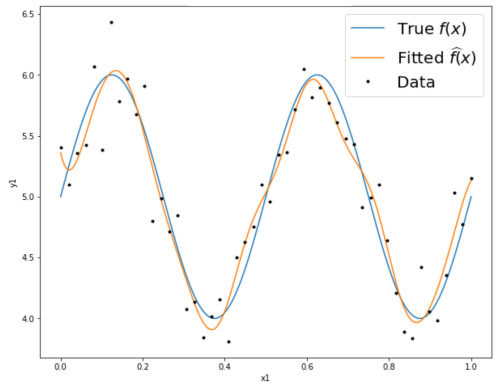
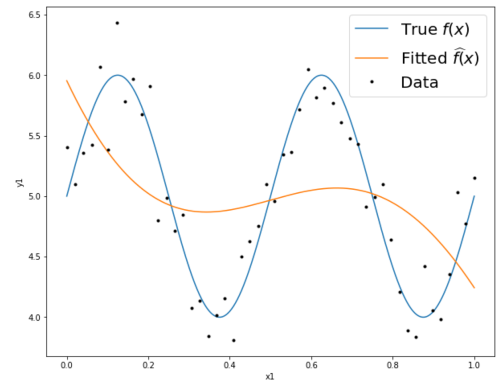


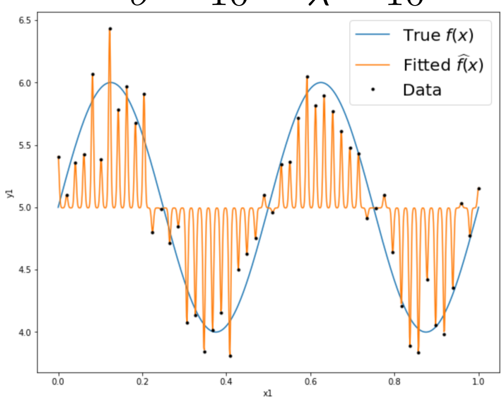
$\sigma = 10^{-1} \quad \lambda = 10^{-4}$



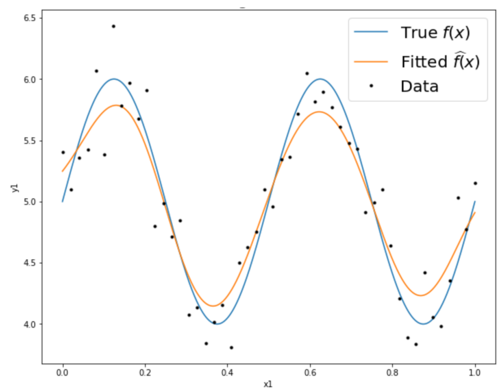
$\sigma = 10^{-0} \quad \lambda = 10^{-4}$



$\sigma = 10^{-3} \quad \lambda = 10^{-4}$



$\sigma = 10^{-1} \quad \lambda = 10^{-0}$



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RBF Kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||_2^2}{2\sigma^2}\right)$$

Basis representation in 1d?

$$\boxed{[\phi(x)]_i = \frac{1}{\sqrt{i!}} e^{-\frac{x^2}{2}} x^i \quad \text{for } i = 0, 1, \ldots}$$

$$\phi(x)^T \phi(x') = \sum_{i=0}^{\infty} \left(\frac{1}{\sqrt{i!}} e^{-\frac{x^2}{2}} x^i\right) \left(\frac{1}{\sqrt{i!}} e^{-\frac{(x')^2}{2}} (x')^i\right)$$

$$= e^{-\frac{x^2 + (x')^2}{2}} \sum_{i=0}^{\infty} \frac{1}{i!} (xx')^i$$

$$= e^{-|x-x'|^2/2}$$

$$\hat{\alpha} = (K + \lambda I)^{-1} y$$

If n is very large, allocating an n-by-n matrix is tough. Can we truncate the above sum to approximate the kernel?

RBF kernel and random features

$$2\cos(\alpha)\cos(\beta) = \cos(\alpha+\beta) + \cos(\alpha-\beta)$$

$$e^{jz} = \cos(z) + j\sin(z)$$

Recall HW1 where we used the feature map:

$$\phi(x) = \begin{bmatrix} \sqrt{2}\cos(w_1^T x + b_1) \\ \vdots \\ \sqrt{2}\cos(w_p^T x + b_p) \end{bmatrix} \qquad \begin{array}{l} w_k \sim \mathcal{N}(0, 2\gamma\, I) \\ b_k \sim \text{uniform}(0,\pi) \end{array}$$

$$\mathbb{E}[\frac{1}{p}\phi(x)^T\phi(y)] = \frac{1}{p}\sum_{k=1}^{p}\mathbb{E}[2\cos(w_k^T x + b_k)\cos(w_k^T y + b_k)]$$

$$= \mathbb{E}_{w,b}[2\cos(w^T x + b)\cos(w^T y + b)]$$

$$= \mathbb{E}_{w,b}\left[\cancel{\cos(w^T(x+y)+2b)} + \cos(w^T(x-y))\right]$$

$$=$$

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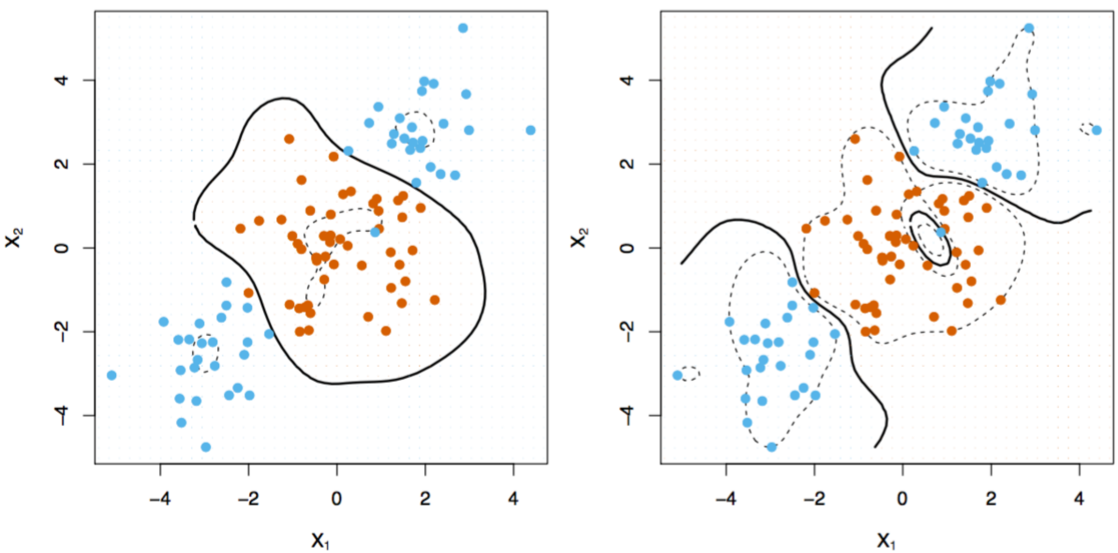
$$\begin{aligned} \mathbb{E}[\frac{1}{p}\phi(x)^T\phi(y)] &= \frac{1}{p}\sum_{k=1}^{p} \mathbb{E}[2\cos(w_k^T x + b_k)\cos(w_k^T y + b_k)] \\ &= \mathbb{E}_{w,b}[2\cos(w^T x + b)\cos(w^T y + b)] \\ &= e^{-\gamma\|x-y\|_2^2} \end{aligned}$$

[Rahimi, Recht NIPS 2007]
"NIPS Test of Time Award, 2018"

RBF Classification

$$\widehat{w} = \min_{b,w} \sum_{i=1}^{n} \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2$$

$$\min_{\alpha,b} \sum_{i=1}^{n} \max\{0, 1 - y_i(b + \sum_{j=1}^{n} \alpha_j \langle x_i, x_j \rangle)\} + \lambda \sum_{i,j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$



Wait, infinite dimensions?

- Isn't everything separable there? How are we not overfitting?

- Regularization! Fat shattering (R/margin)^2

String Kernels

Example from Efron and Hastie, 2016

Amino acid sequences of different lengths:

x1

IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQTVQGGTV
ERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDY**LQE**FLGVMNTEWI

x2

PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAER**LQE**NLQAYRTFHVLLA
RLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADGMLFEKK
LWGLKV**LQE**LSQWTVRSIHDLRFISSHQTGIP

All subsequences of length 3 (of possible 20 amino acids) $20^3 = 8{,}000$

$$h^3_{\mathrm{LQE}}(x_1) = 1 \text{ and } h^3_{\mathrm{LQE}}(x_2) = 2.$$

Principal Component Analysis

Machine Learning – CSE546

Kevin Jamieson
University of Washington

November 6, 2018

Linear projections

dn

Given $x_1, \dots, x_n \in \mathbb{R}^d$, for $q \ll d$ find a compressed representation with $\lambda_1, \dots, \lambda_n \in \mathbb{R}^q$ such that $x_i \approx \mu + \mathbf{V}_q \lambda_i$ and $\mathbf{V}_q^T \mathbf{V}_q = I$

qn

$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^{n} \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

Linear projections

Given $x_1, \dots, x_n \in \mathbb{R}^d$, for $q \ll d$ find a compressed representation with $\lambda_1, \dots, \lambda_n \in \mathbb{R}^q$ such that $x_i \approx \mu + \mathbf{V}_q \lambda_i$ and $\mathbf{V}_q^T \mathbf{V}_q = I$

$$\min_{\mu, \mathbf{V}_q, \{\lambda_i\}_i} \sum_{i=1}^{n} \|x_i - \mu - \mathbf{V}_q \lambda_i\|_2^2$$

Fix $\mathbf{V}_q$ and solve for μ, λ_i:

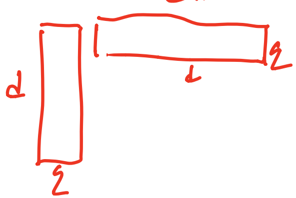
$$\mu = \bar{x} = \tfrac{1}{n} \textstyle\sum_{i=1}^n x_i$$

$$\lambda_i = \mathbf{V}_q^T (x_i - \bar{x})$$

Which gives us:

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \underbrace{\mathbf{V}_q \mathbf{V}_q^T}_{d \times d} (x_i - \bar{x})||^2.$$

$\mathbf{V}_q \mathbf{V}_q^T$ is a *projection matrix* that minimizes error in basis of size q



Linear projections

$$\sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2$$

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$$= \sum_i ||x_i - \bar{x}||_2^2 - 2(x_i - \bar{x})^T V_q V_q^T (x_i - \bar{x})$$

$$+ (x_i - \bar{x})^T V_q \underbrace{\cancel{V_q^T V_q}}_{I} V_q^T (x_i - \bar{x})$$

$$= \sum_i ||x_i - \bar{x}||_2^2 - (x_i - \bar{x}) V_q V_q^T (x_i - \bar{x})$$

$$= \sum_i Tr\left((x_i - \bar{x})(x_i - \bar{x})\right) - Tr\left(V_q^T (x_i - \bar{x})(x_i - \bar{x})^T V_q\right))$$

$$= Tr(\Sigma) - Tr(V_q^T \Sigma V_q)$$

Linear projections

$$\sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2$$

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2 = \min_{\mathbf{V}_q} Tr(\Sigma) - Tr(\mathbf{V}_q^T \Sigma \mathbf{V}_q)$$

Eigenvalue decomposition of $\sum = UDU^T$

$$q = 1 \qquad \max_{||v||_2 = 1} v_1^T \Sigma v_1 = \max_{||v||_2=1} \sum_{j=1}^{d} \underbrace{(v_1^T u_j)^2}_{} D_{j,j} = \max_j D_{j,j}$$

$$v_1 = u_1$$

Linear projections

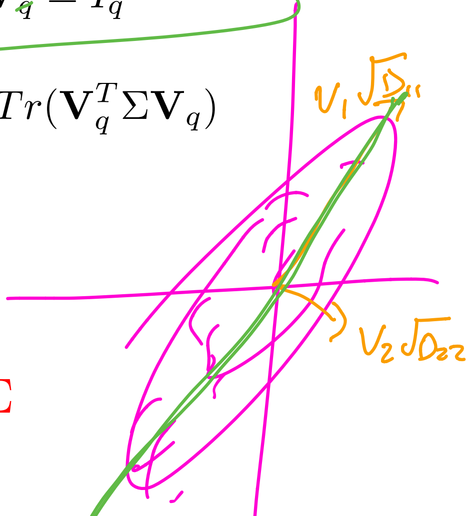
$$\sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2$$

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||_2^2 = \min_{\mathbf{V}_q} Tr(\Sigma) - Tr(\mathbf{V}_q^T \Sigma \mathbf{V}_q)$$

Eigenvalue decomposition of $\sum =$



$\mathbf{V}_q$ are the first q eigenvectors of Σ

Minimize reconstruction error and capture the most variance in your data.

Pictures

$\mathbf{V}_q$ are the first q eigenvectors of Σ

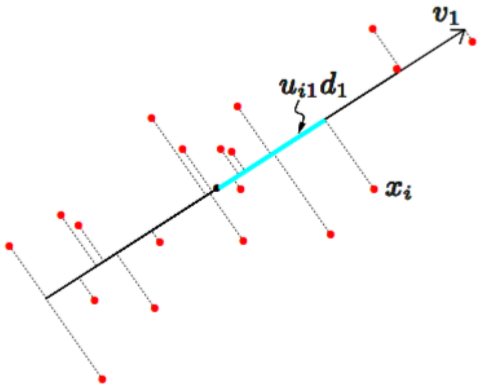
$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Linear projections

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$



where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$

$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \text{diag}(d_1, \ldots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$

Singular Value Decomposition (SVD)

Theorem (SVD): Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with rank $r \leq \min\{m, n\}$. Then $\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^T$ where $\mathbf{S} \in \mathbb{R}^{r \times r}$ is diagonal with positive entries, $\mathbf{U}^T\mathbf{U} = I$, $\mathbf{V}^T\mathbf{V} = I$.

$$\mathbf{A}^T\mathbf{A}v_i =$$

$$\mathbf{A}\mathbf{A}^T u_i =$$

Singular Value Decomposition (SVD)

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$$\mathbf{A}^T\mathbf{A}v_i = \mathbf{S}_{i,i}^2 v_i$$

$$\mathbf{A}\mathbf{A}^T u_i = \mathbf{S}_{i,i}^2 u_i$$

$\mathbf{V}$ are the first r eigenvectors of $\mathbf{A}^T\mathbf{A}$ with eigenvalues $\text{diag}(\mathbf{S})$
$\mathbf{U}$ are the first r eigenvectors of $\mathbf{A}\mathbf{A}^T$ with eigenvalues $\text{diag}(\mathbf{S})$

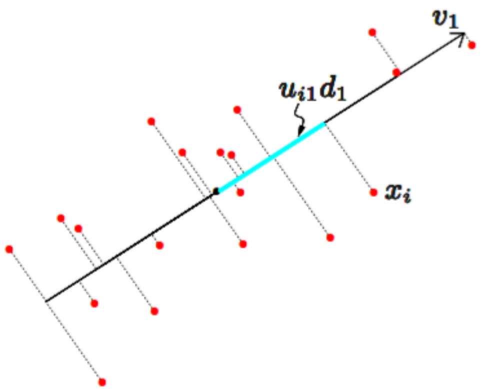
Linear projections

Given $x_i \in \mathbb{R}^d$ and some $q < d$ consider

$$\min_{\mathbf{V}_q} \sum_{i=1}^{N} ||(x_i - \bar{x}) - \mathbf{V}_q \mathbf{V}_q^T (x_i - \bar{x})||^2.$$

where $\mathbf{V}_q = [v_1, v_2, \ldots, v_q]$ is orthonormal:

$$\mathbf{V}_q^T \mathbf{V}_q = I_q$$



$\mathbf{V}_q$ are the first q eigenvectors of Σ

$\mathbf{V}_q$ are the first q *principal components*

$$\Sigma := \sum_{i=1}^{N} (x_i - \bar{x})(x_i - \bar{x})^T$$

Principal Component Analysis (PCA) projects $(\mathbf{X} - \mathbf{1}\bar{x}^T)$ down onto $\mathbf{V}_q$

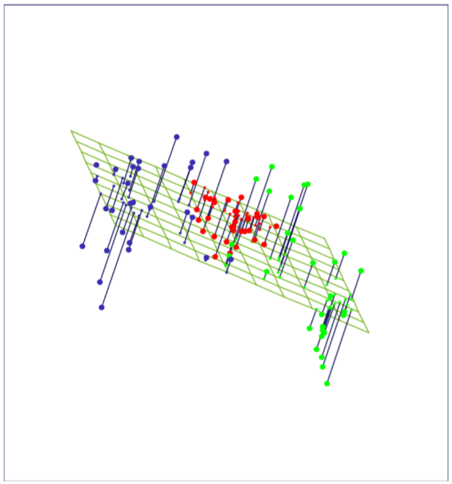
$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U}_q \text{diag}(d_1, \ldots, d_q) \qquad \mathbf{U}_q^T \mathbf{U}_q = I_q$$

Singular Value Decomposition defined as

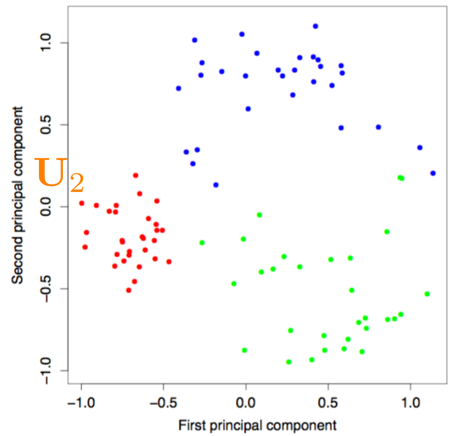
$$\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$$

Dimensionality reduction

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$



$\mathbf{X} - \mathbf{1}\bar{x}^T$



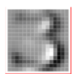
$\mathbf{U}_1$

Dimensionality reduction

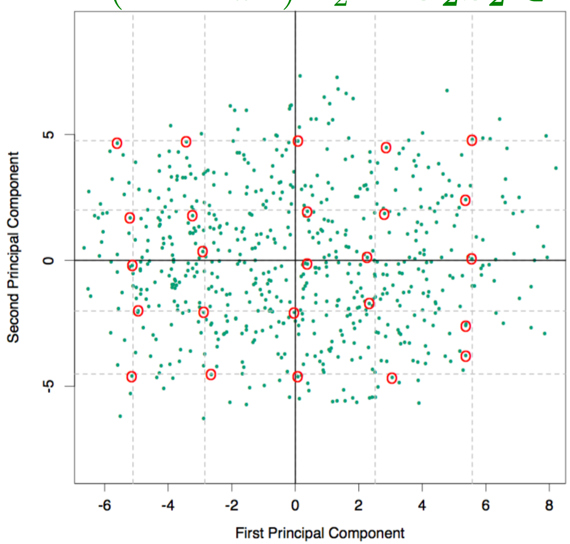
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{USV}^T$

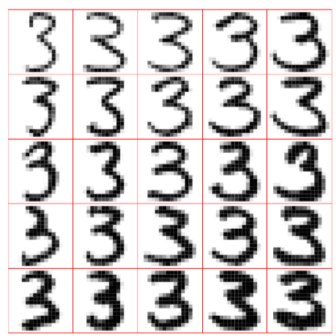
Handwritten 3's, 16x16 pixel image so that $x_i \in \mathbb{R}^{256}$

$$\hat{f}(\lambda) = \bar{x} + \lambda_1 v_1 + \lambda_2 v_2$$

$$=$$  $+ \lambda_1 \cdot$  $+ \lambda_2 \cdot$  .

$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_2 = \mathbf{U_2 S_2} \in \mathbb{R}^{n \times 2}$





$\text{diag}(\mathbf{S})$

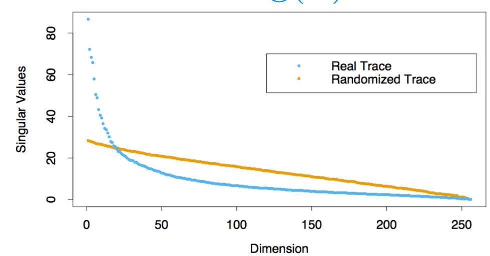


FIGURE 14.24. *The 256 singular values for the digitized threes, compared to those for a randomized version of the data (each column of* $\mathbf{X}$ *was scrambled).*

Kernel PCA

$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q}\mathbf{S_q} \in \mathbb{R}^{n \times q}$$

$$\mathbf{J}\mathbf{X} = \mathbf{X} - 1\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$$

$$(\mathbf{J}\mathbf{X})(\mathbf{J}\mathbf{X})^T =$$

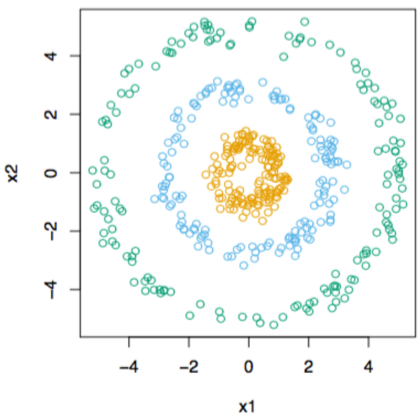
Kernel PCA

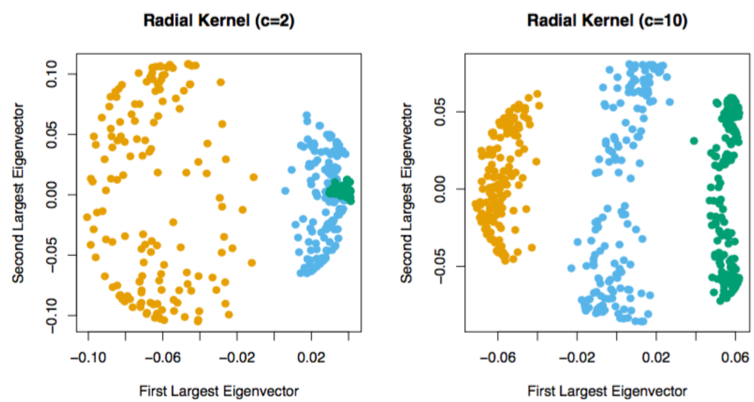
$\mathbf{V}_q$ are the first q eigenvectors of Σ and *SVD* $\mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T$

$$(\mathbf{X} - \mathbf{1}\bar{x}^T)\mathbf{V}_q = \mathbf{U_q}\mathbf{S_q} \in \mathbb{R}^{n \times q}$$

$$\mathbf{J}\mathbf{X} = \mathbf{X} - \mathbf{1}\bar{x}^T = \mathbf{U}\mathbf{S}\mathbf{V}^T \qquad \mathbf{J} = I - \mathbf{1}\mathbf{1}^T/n$$

$$(\mathbf{J}\mathbf{X})(\mathbf{J}\mathbf{X})^T = \mathbf{U}\mathbf{S}^2\mathbf{U}^T$$





PCA Algorithm

PCA

input

A matrix of m examples $X \in \mathbb{R}^{m,d}$

number of components n

if $(m > d)$

$A = X^\top X$

Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be the eigenvectors of A with largest eigenvalues

else

$B = X X^\top$

Let $\mathbf{v}_1, \ldots, \mathbf{v}_n$ be the eigenvectors of B with largest eigenvalues

for $i = 1, \ldots, n$ set $\mathbf{u}_i = \frac{1}{\|X^\top \mathbf{v}_i\|} X^\top \mathbf{v}_i$

output: $\mathbf{u}_1, \ldots, \mathbf{u}_n$