Machine Learning Course
basic track

Lecture 04:
SVM, PCA

MIPT, Moscow
Spring 2021

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Outline

1. Support Vector Machine (SVM)
   - Linearly separable and inseparable cases
2. Dimensionality reduction and PCA
   - Connections with SVD

Recap: linear classification

$$X^l = (x_i, y_i)_{i=1}^l, x_i \in R^n, y_i \in \{-1, 1\}$$

- Linear classification model

$$a(x; w, w_0) = \mathrm{sign}\big(\langle x, w\rangle - w_0\big) \qquad w \in R^n, w_0 \in R$$

- Loss function – empirical risk

$$\sum_{i=1}^{\ell}\big[a(x_i; w, w_0) \neq y_i\big] = \sum_{i=1}^{\ell}\big[M_i(w, w_0) < 0\big] \to \min_{w, w_0}.$$

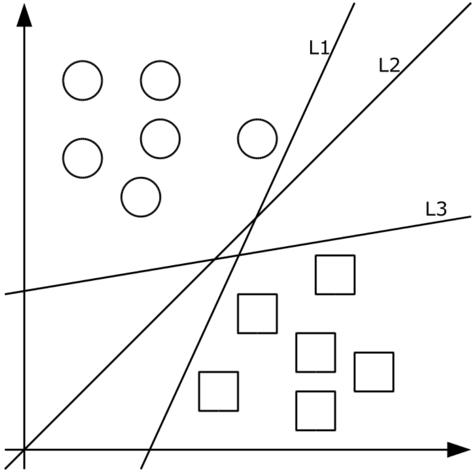
- Margin $\quad M_i(w, w_0) = \big(\langle x_i, w\rangle - w_0\big)y_i$

Optimal classification hyperplane

- In linearly separable case:

$$\exists w, w_0 : \quad M_i(w, w_0) = y_i\big(\langle w, x_i \rangle - w_0\big) > 0, \quad i = 1, \dots, \ell$$

- Trivia: which classification hyperplane is optimal?



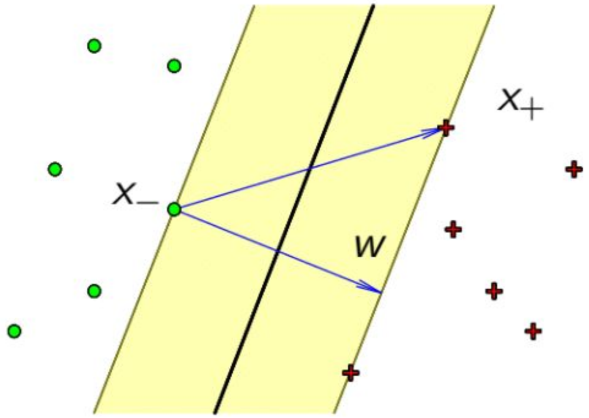
Optimal classification hyperplane

- In linearly separable case:

$$\exists w, w_0 : \quad M_i(w, w_0) = y_i\big(\langle w, x_i \rangle - w_0\big) > 0, \quad i = 1, \ldots, \ell$$

Weight normalization: $\min\limits_{i=1,\ldots,\ell} M_i(w, w_0) = 1$

Maximum margin hyperplane:



$$\forall x_+ : \langle w, x_+ \rangle \quad -w_0 \geq 1$$

$$\forall x_- : \langle w, x_- \rangle \quad -w_0 \leq -1$$

Optimal classification hyperplane

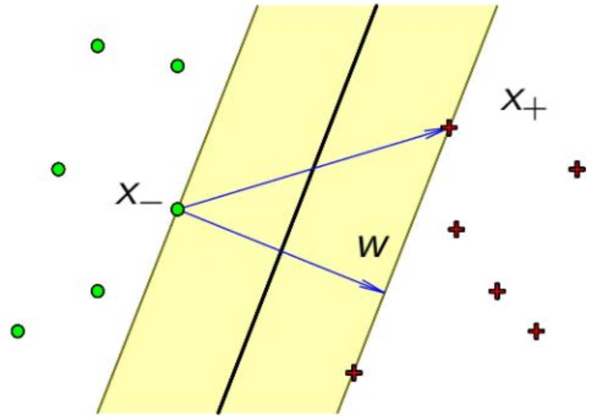
Maximum margin hyperplane:

$$\forall x_+ : \langle w, x_+ \rangle \quad -w_0 \geq 1$$

$$\forall x_- : \langle w, x_- \rangle \quad -w_0 \leq -1$$

Goal: maximize the margin

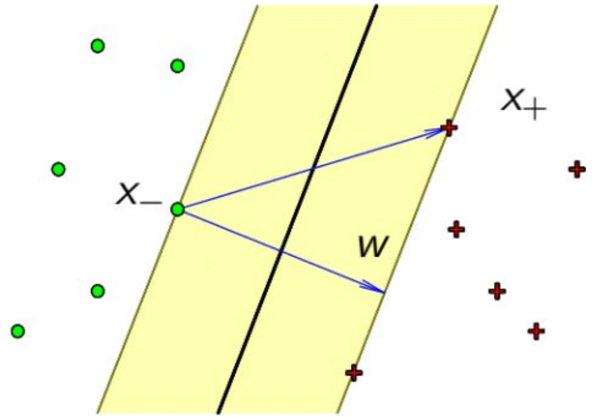
$$\frac{\langle x_+ - x_-, w \rangle}{||w||} \geq \frac{2}{||w||} \to max$$



Optimization problem in SVM

- Separable data optimization problem:

$$\begin{cases} \frac{1}{2}\|w\|^2 \to \min\limits_{w,w_0}; \\ M_i(w, w_0) \geqslant 1, \quad i = 1, \dots, \ell. \end{cases}$$



Inseparable case

- Separable data optimization problem:

$$\begin{cases} \frac{1}{2}\|w\|^2 \to \min\limits_{w,w_0}; \\ M_i(w, w_0) \geqslant 1, \quad i = 1, \dots, \ell. \end{cases}$$

- Heuristic: introduce penalties for violating the margin:

$$M_i(w, w_0) \geqslant 1 - \xi_i, \quad i = 1, \dots, \ell;$$

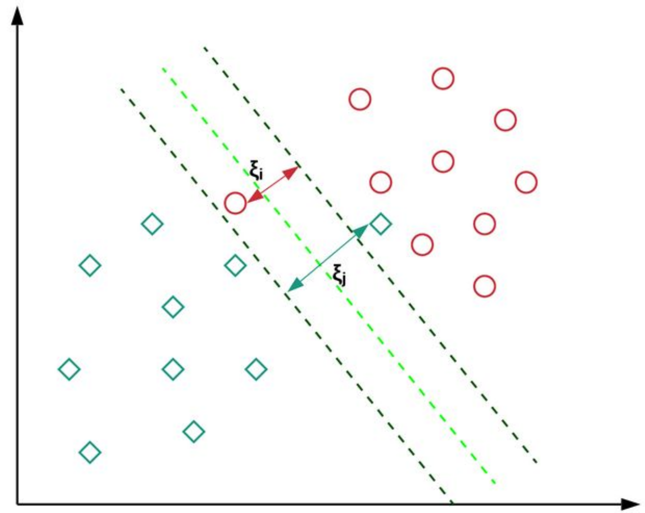
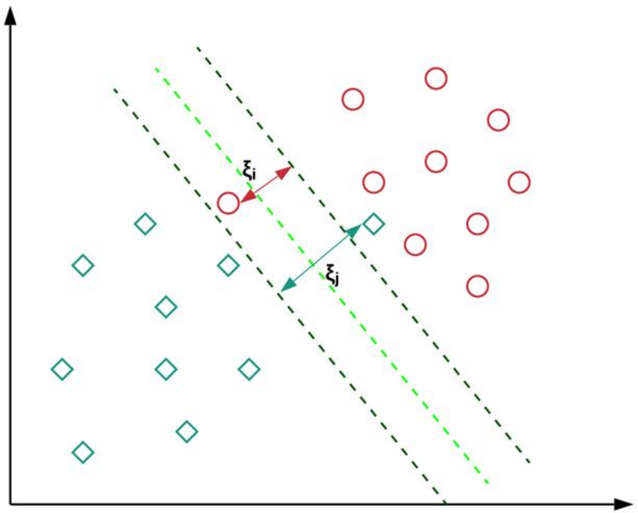


Image source: awesome blog post https://towardsdatascience.com/support-vector-machines-soft-margin-formulation-and-kernel-trick-4c9729dc8efe

Inseparable case

- Optimization task (with constraints)

$$\begin{cases} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{\ell}\xi_i \to \min_{w, w_0, \xi}; \\ M_i(w, w_0) \geqslant 1 - \xi_i, \quad i = 1, \dots, \ell; \\ \xi_i \geqslant 0, \quad i = 1, \dots, \ell. \end{cases}$$



- Equivalent unconstrained target

$$C\sum_{i=1}^{\ell}\left(1 - M_i(w, w_0)\right)_+ + \frac{1}{2}\|w\|^2 \to \min_{w, w_0}.$$

Image source: awesome blog post https://towardsdatascience.com/support-vector-machines-soft-margin-formulation-and-kernel-trick-4c9729dc8efe

Karush-Kuhn-Tucker conditions

- Consider nonlinear optimization problem

$$\begin{cases} f(x) \to \min\limits_{x}; \\ g_i(x) \leqslant 0, \quad i = 1, \dots, m; \\ h_j(x) = 0, \quad j = 1, \dots, k. \end{cases}$$

- The following conditions are necessary for any local minimum

$$\begin{cases} \frac{\partial \mathscr{L}}{\partial x} = 0, \mathscr{L} = f(x) + \sum_{i=1}^{m} \mu_i g_i(x) + \sum_{j=1}^{k} \lambda_j h_j(x); \\ g_i(x) \leq 0; h_j(x) = 0; \\ \mu_i(x) \geq 0; \\ \mu_i g_i(x) = 0; \end{cases}$$

Karush-Kuhn-Tucker conditions for SVM

- Lagrangian function

$$\mathscr{L}(w, w_0, \xi, \lambda, \eta) = \frac{1}{2}||w|| - \sum_{i=1}^{l} \lambda_i (M_i(w, w_0) - 1) - \sum_{i=1}^{l} \xi_i(\lambda_i + \eta_i - C)$$

- Necessary conditions for an optimum

$$\begin{cases} \frac{\partial \mathscr{L}}{\partial w} = 0, \frac{\partial \mathscr{L}}{\partial w_0} = 0, \frac{\partial \mathscr{L}}{\partial \xi} = 0; \\ \xi_i \geq 0, \lambda_i \geq 0, \eta_i \geq 0; \\ \lambda_i = 0 \vee M_i(w, w_0) = 1 - \xi_i; \\ \eta_i = 0 \vee \xi_i = 0; \end{cases}$$

Karush-Kuhn-Tucker conditions for SVM

- Lagrangian function

$$\mathscr{L}(w, w_0, \xi, \lambda, \eta) = \frac{1}{2}||w|| - \sum_{i=1}^{l} \lambda_i (M_i(w, w_0) - 1) - \sum_{i=1}^{l} \xi_i (\lambda_i + \eta_i - C)$$

- Necessary conditions for an optimum

$$\frac{\partial \mathscr{L}}{\partial w} = w - \sum_{i=1}^{\ell} \lambda_i y_i x_i = 0 \quad \Longrightarrow \quad w = \sum_{i=1}^{\ell} \lambda_i y_i x_i;$$

$$\frac{\partial \mathscr{L}}{\partial w_0} = -\sum_{i=1}^{\ell} \lambda_i y_i = 0 \quad \Longrightarrow \quad \sum_{i=1}^{\ell} \lambda_i y_i = 0;$$

$$\frac{\partial \mathscr{L}}{\partial \xi_i} = -\lambda_i - \eta_i + C = 0 \quad \Longrightarrow \quad \eta_i + \lambda_i = C, \quad i = 1, \dots, \ell.$$

SVM: object classification

1. $\lambda_i = 0; \eta_i = C; \xi_i = 0; M_i \geq 1.$
Non-informative objects (they don't contribute to a solution vector!)

2. $0 < \lambda_i < C; 0 < \eta_i < C; \xi_i = 0; M_i = 1.$
support objects (borderline)

3. $\lambda_i = C; \eta_i = 0; \xi_i > 0; M_i < 1.$
support objects (violators)

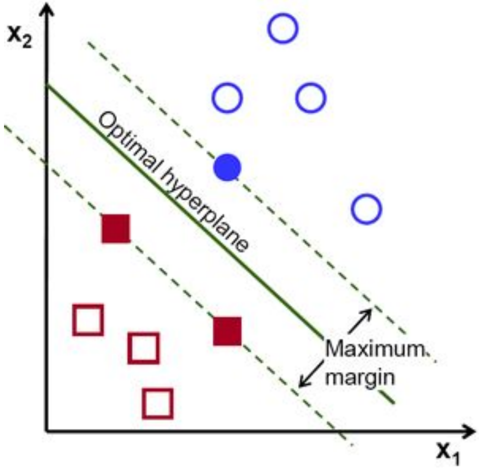


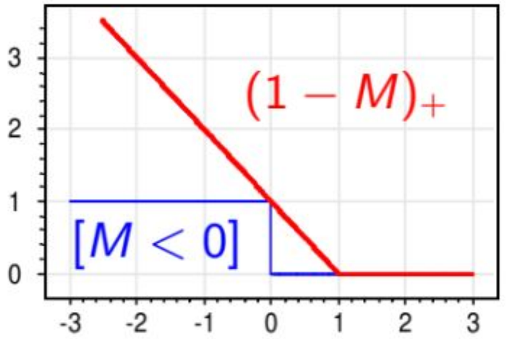
Image source: OpenCV docs: https://docs.opencv.org/3.4/d1/d73/tutorial_introduction_to_svm.html

Hinge loss

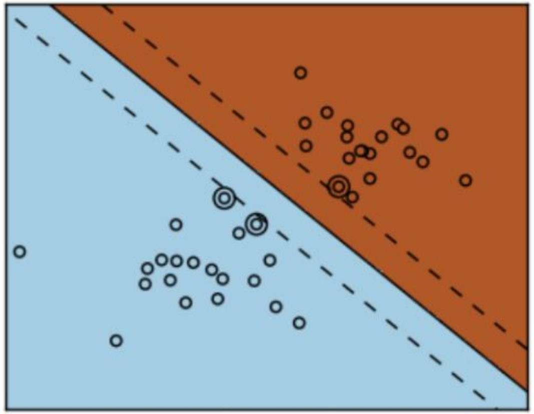
- Can be treated as upper-bound of the empirical risk

$$Q(w, w_0) = \sum_{i=1}^{l} [M_i(w, w_0) < 0] \le$$

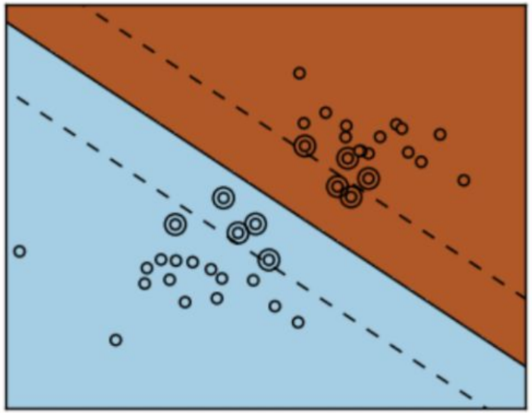
$$\le \underbrace{\sum_{i=1}^{l} (1 - M_i(w, w_0))_+}_{\textit{Approximation}} + \underbrace{\frac{1}{2C}||w||^2}_{\textit{Regularization}} \to min$$



C is large: weak regularization



C is small: strong regularization



Nonlinear SVM

- Can we use other similarity functions apart from dot product?
- Yes, if it can be presented as dot product in another Hilbert space!

Nonlinear SVM

- **Kernel function**

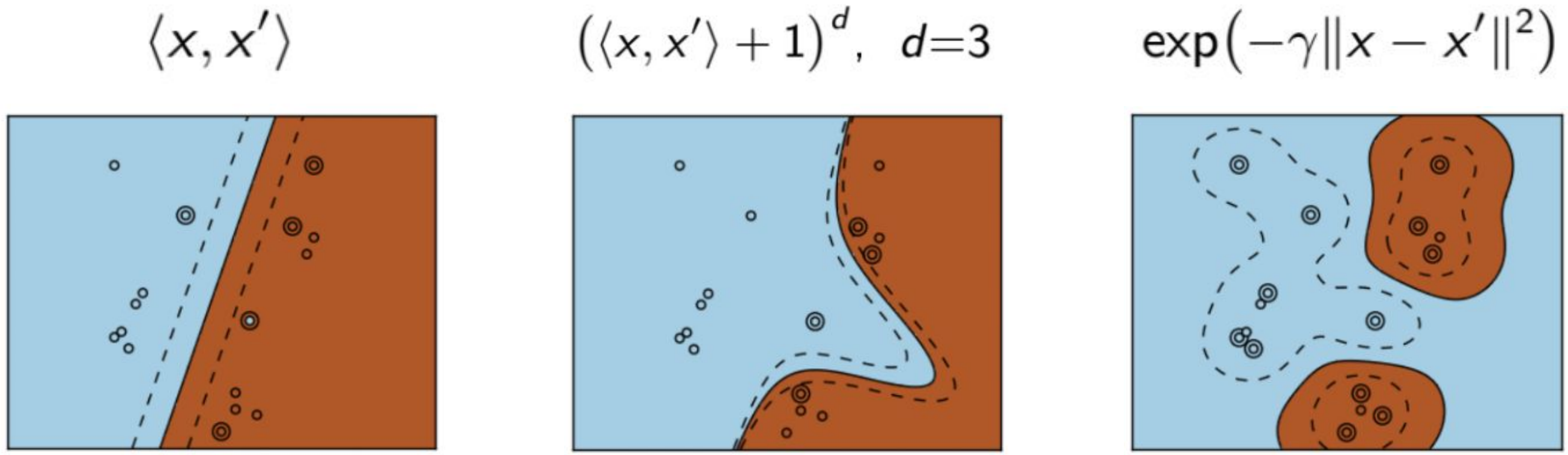
$$K(x, x') : X \times X \to R$$
$$\exists \psi : X \to H : K(x, x') =< \psi(x), \psi(x') >, \text{ H - Hilbert space}$$

- Kernel examples

$$K(x, x') =< x, x' >^2 \text{ - quadratic}$$
$$K(x, x') =< x, x' >^d \text{ - polynomial with degree } d$$
$$K(x, x') = (< x, x' > +1)^d \text{ - polynomial with degree } \leq d$$
$$K(x, x') = exp(-\gamma||x - x'||^2) \text{ - Radial Basis Functions (RBF) kernel}$$

SVM: kernel examples

- SVM finds a linear boundary in linearized feature space
- But for initial features it may be nonlinear!



Principal Component Analysis

Dimensionality reduction

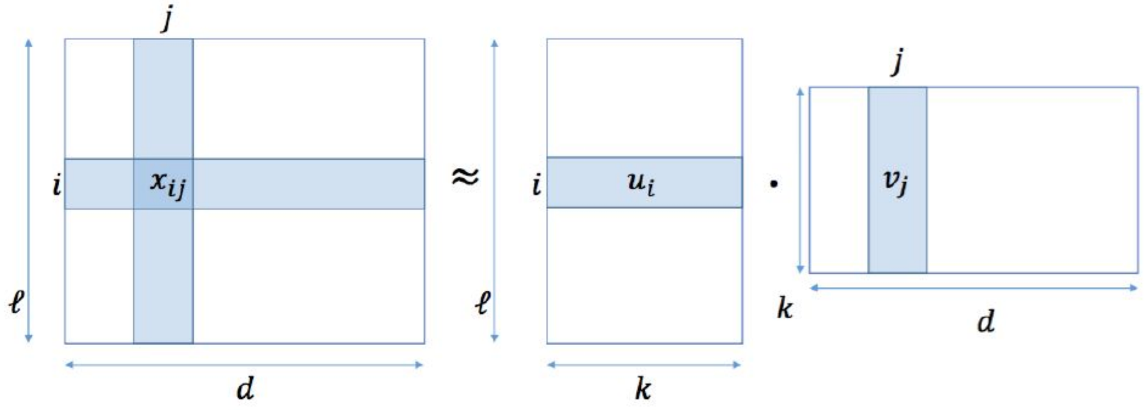
- In ML we often work with high-dimensional data
  - Hundreds or thousands of features

- Hard to visualize
- Slow training
- Some models perform worse on high-dimensional sparse input

Dimensionality reduction

- Factorization into smaller-rank matrices

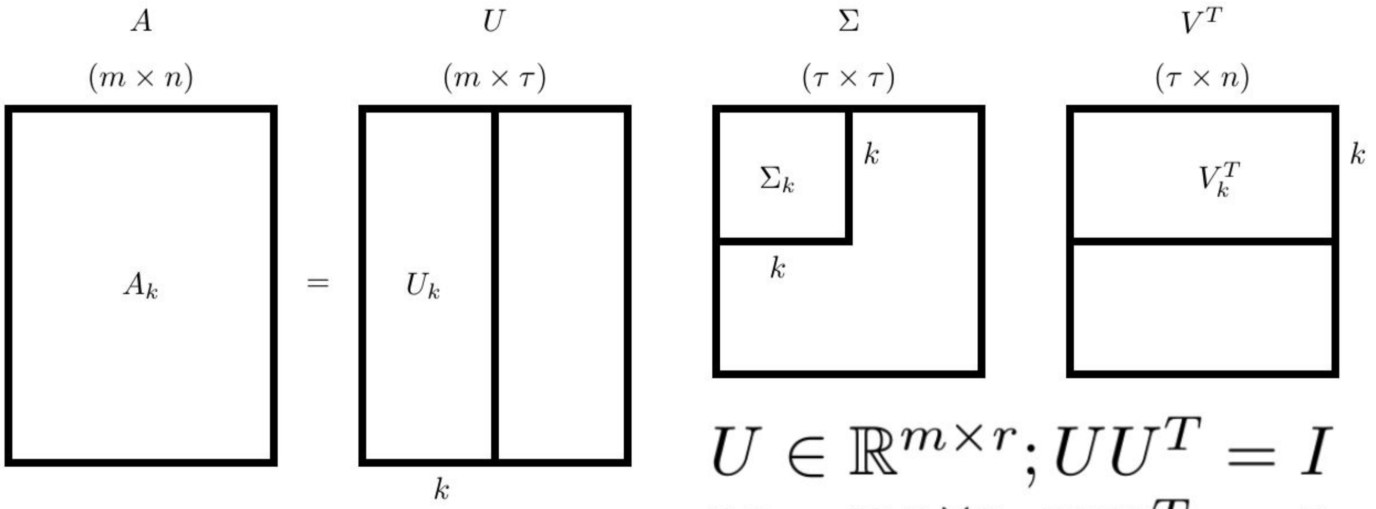
$$X_{l,d} \approx U_{l,k} \cdot V_{k,d}^T \qquad ||X - UV^T|| \to min$$



Dimensionality reduction with SVD

$$A = U\Sigma V^T$$

$$A_k = U_k \Sigma_k V_k^T = (U_k \Sigma_k) V_k^T = U_k(\Sigma_k V_k^T)$$



$$U \in \mathbb{R}^{m \times r}; UU^T = I$$

$$V \in \mathbb{R}^{n \times r}; VV^T = I$$

$$\Sigma = diag(\sigma_1, ..., \sigma_r); r = rank(M)$$

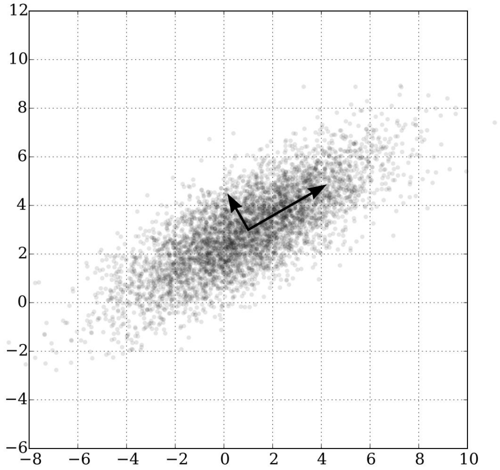
Theorem (Eckart-Young)

- Truncated SVD gives best low-rank approximation for a given matrix A
- More formally,

$$A_k = U_k \Sigma_k V_k^T$$
$$\forall B_k : rank(B_k) = k$$
$$||A - B_k||_F \geq ||A - A_k||_F$$

PCA: projection into a subspace

- Project all data points into a smaller dimension subspace
- Maximize *variance* along new basis vectors



PCA: projection into a subspace

$$X = U \Sigma V^T$$

orthogonal

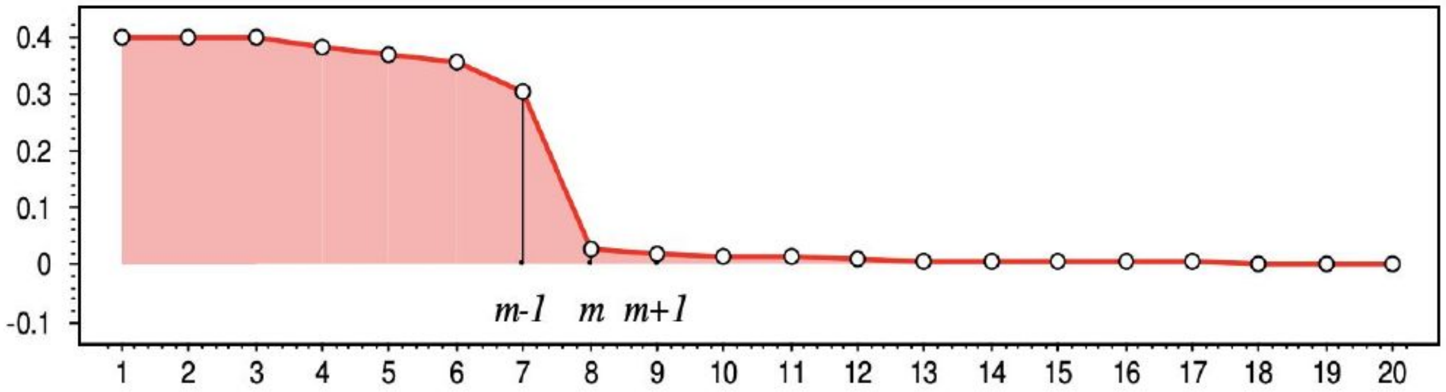
orthogonal

diagonal: sigmas ~ variance

- Consider columns of matrix V new basis vectors: **principal directions**
- Columns of matrix US are called **principal components** of the data
- Singular values are sorted: truncated SVD gives the best projection of dim K

PCA: effective dimensionality

- Often data is noisy and has non-informative features
- Get rid of low-variance components in PCA



$$E_m = \frac{\|GU^\intercal - F\|^2}{\|F\|^2} = \frac{\lambda_{m+1} + \cdots + \lambda_n}{\lambda_1 + \cdots + \lambda_n} \leqslant \varepsilon.$$

PCA in practice

- Above said is correct only if X is centered
  - **Normalize data before PCA!**
- Dimensionality reduction:

$$X_k = U_k \Sigma_k$$

- Reconstruction:

$$\overline{X} = U_k \Sigma_k V_k^T$$

PCA in practice: examples

- Word embeddings visualization

Let's walk through space…

Image source: https://github.com/yandexdataschool/nlp_course/tree/2019/week01_embeddings

PCA in practice: examples

- Eigenfaces: image examples

Image source: awesome blog post https://towardsdatascience.com/eigenfaces-recovering-humans-from-ghosts-17606c328184

PCA in practice: examples

- Eigenfaces: top-16 components

Image source: awesome blog post https://towardsdatascience.com/eigenfaces-recovering-humans-from-ghosts-17606c328184

PCA in practice: examples

- Eigenfaces: reconstruction with n=50

Image source: awesome blog post https://towardsdatascience.com/eigenfaces-recovering-humans-from-ghosts-17606c328184

PCA in practice: examples

- Eigenfaces: reconstruction with n=250

Image source: awesome blog post https://towardsdatascience.com/eigenfaces-recovering-humans-from-ghosts-17606c328184

Outro

Karush-Kuhn-Tucker conditions for SVM

- Dual optimization task for SVM

$$\begin{cases} -\mathscr{L}(\lambda) = -\sum_{i=1}^{\ell} \lambda_i + \frac{1}{2} \sum_{i=1}^{\ell} \sum_{j=1}^{\ell} \lambda_i \lambda_j y_i y_j \langle x_i, x_j \rangle \to \min\limits_{\lambda}; \\ 0 \leqslant \lambda_i \leqslant C, \quad i = 1, \dots, \ell; \\ \sum_{i=1}^{\ell} \lambda_i y_i = 0. \end{cases}$$

SVM: general solution

- Use the dual optimization problem solution

$$\begin{cases} w = \sum_{i=1}^{l} \lambda_i y_i x_i; \\ w_0 =< w, x_i > -y_i, i : \lambda_i > 0; M_i = 1. \end{cases}$$

- SVM classifier general form

$$a(x) = \mathrm{sign}\left(\sum_{i=1}^{\ell} \lambda_i y_i \langle x, x_i \rangle - w_0 \right).$$