

Kernel Methods

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MTAT.03.227 Machine Learning



So far...

- Supervised machine learning
 - Linear models
 - Non-linear models

- Unsupervised machine learning
- Generic scaffolding



So far...

- Supervised machine learning
 - Linear models
 - Least squares regression, SVR
 - Fisher's discriminant, Perceptron, Logistic model, SVM
 - Non-linear models
 - Neural networks, Decision trees, Association rules

Unsupervised machine learning

- Clustering/EM, PCA
- Generic scaffolding
 - Probabilistic modeling, ML/MAP estimation
 - Performance evaluation, Statistical learning theory
 - Linear algebra, Optimization methods



Coming up next...

- Supervised machine learning
 - Linear models
 - Least squares regression, SVR
 - Fisher's discriminant, Perceptron, Logistic model, SVM
 - Non-linear models
 - Neural networks, Decision trees, Association rules
 - Kernel-XXX
- Unsupervised machine learning
 - Clustering/EM, PCA, Kernel-XXX
- Generic scaffolding
 - Probabilistic modeling, ML/MAP estimation
 - Performance evaluation, Statistical learning theory
 - Linear algebra, Optimization methods

Kernels



 $f(\mathbf{x}) =$



$$f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b$$



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▶ PCA, LDA, ICA, ...:



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- ▶ PCA, LDA, ICA, ...:
 - $f(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$



$$f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b$$

▶ PCA, LDA, ICA, ...:

$$f(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}$$

K-means:

CCA, GLM, …

$$\boldsymbol{c}_i = \frac{1}{m} \boldsymbol{X}_i \boldsymbol{1}$$



Too much linear





Linear is not enough

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Limited generalization ability





Linear is not enough

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Limited generalization ability





Linear is not enough

Limited applicability

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Text? Ordinal/Nominal data? Graphs/Trees/Networks? Shapes?

Graph nodes?

Solutions





Solutions

Feature space



Feature space

Solutions

Nonlinear feature spaces

Kernels

- The Kernel Trick
- Dual representation











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 $x \to x' \coloneqq \phi(x) \coloneqq (x, x^2, x^3)$



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Nonlinear feature space









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$$x \rightarrow \phi(x) = (x, x^3 - x)$$



 $x \rightarrow \phi(x) = (x, x^3 - x)$





 $x \rightarrow \phi(x) = (x, x^3 - x)$

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Nonlinear feature space

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 $f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x})$





$\phi(\text{text}) = \text{word counts}$ $\phi(\text{graph}) = \text{node degrees}$ $\phi(\text{tree}) = \text{path lengths}$

. . .



 $(x_1, x_2, \dots, x_m) \rightarrow (x_1 x_1, x_1 x_2, \dots, x_m x_m)$



 $(x_1, x_2, \dots, x_m) \rightarrow (x_1 x_1, x_1 x_2, \dots, x_m x_m)$ $O(m^2)$ elements

For all k-wise products: $O(m^k)$





• Let $\phi(\mathbf{x}) = (x_1 x_1, x_1 x_2, \dots, x_m x_m)$

Consider

$$\langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle = \sum_{ij} \phi(\mathbf{x})_{ij} \phi(\mathbf{y})_{ij}$$



• Let $\phi(\mathbf{x}) = (x_1 x_1, x_1 x_2, \dots, x_m x_m)$

Consider

$$\langle \phi(\boldsymbol{x}), \phi(\boldsymbol{y}) \rangle = \sum_{ij} \phi(\boldsymbol{x})_{ij} \phi(\boldsymbol{y})_{ij}$$
$$= \sum_{ij} x_i x_j y_i y_j$$



• Let $\phi(\mathbf{x}) = (x_1 x_1, x_1 x_2, \dots, x_m x_m)$

Consider

$$\langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle = \sum_{ij} \phi(\mathbf{x})_{ij} \phi(\mathbf{y})_{ij}$$
$$= \sum_{ij} x_i x_j y_i y_j = \sum_{ij} x_i y_i x_j y_j$$



• Let $\phi(\mathbf{x}) = (x_1 x_1, x_1 x_2, \dots, x_m x_m)$

Consider





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• Let $\phi(\mathbf{x}) = (x_1 x_1, x_1 x_2, \dots, x_m x_m)$

Consider

$$\langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle = \sum_{ij} \phi(\mathbf{x})_{ij} \phi(\mathbf{y})_{ij}$$
$$= \left(\sum_{i} x_i y_i \right)^2 = \langle \mathbf{x}, \mathbf{y} \rangle^2$$



• Let $\phi(\mathbf{x}) = (x_1 x_1, x_1 x_2, \dots, x_m x_m)$

Consider

 $\langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle = \sum \phi(\mathbf{x})_{ij} \phi(\mathbf{y})_{ij}$ $= \left(\sum_{i} x_i y_i\right)^2 = \langle \boldsymbol{x}, \boldsymbol{y} \rangle^2$







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What about: $K(x, y) = \langle x, y \rangle + 0.5 \langle x, y \rangle^2$?


What about: $K(\mathbf{x}, \mathbf{y}) = \langle \mathbf{x}, \mathbf{y} \rangle + 0.5 \langle \mathbf{x}, \mathbf{y} \rangle^2$ $= \sum x_i y_i + 0.5 \sum \phi_{ij}(\mathbf{x}) \phi_{ij}(\mathbf{y})$









What about: $K(x, y) = \langle x, y \rangle + 0.5 \langle x, y \rangle^2$ $= \sum_{i=1}^{n} x_i y_i + 0.5 \sum_{i=1}^{n} \phi_{ij}(\mathbf{x}) \phi_{ij}(\mathbf{y})$ $= \langle (x_1, \dots, x_m, \sqrt{0.5}x_1x_1, \dots, \sqrt{0.5}x_mx_m), \\ (y_1, \dots, y_m, \sqrt{0.5}y_1y_1, \dots, \sqrt{0.5}y_my_m) \rangle$



What about:

$$K(x,y) = 1 + \langle x, y \rangle + \frac{1}{2} \langle x, y \rangle^{2} + \frac{1}{6} \langle x, y \rangle^{3} + \frac{1}{24} \langle x, y \rangle^{4}?$$



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Infinite-dimensional feature space!



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http://crsouza.blogspot.com/2010/03/kernel-functions-for-machine-learning.html

Kernels



Structured data kernels

String kernels

- P-spectrum kernels
- All-subsequences kernels
- Gap-weighted subsequences kernels

Graph & tree kernels

- Co-rooted subtrees
- All subtrees

. . .

Random walks

Kernel

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• A function K(x, y) is a kernel, if

$$K(\boldsymbol{x},\boldsymbol{y}) = \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{y}) \rangle$$

for some feature map ϕ .

For a given kernel function K and a finite dataset $(x_1, x_2, ..., x_n)$ the $n \times n$ matrix $K_{ij} \coloneqq K(x_i, x_j)$

is called the kernel matrix.

Kernel matrix

• Let X be the data matrix, then $K = XX^T$

is the kernel matrix for the linear kernel $K(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y}$

Kernel matrix

• Let X be the data matrix, then $K = XX^T$

is the kernel matrix for the linear kernel $K(\mathbf{x}, \mathbf{y}) = \mathbf{x}^T \mathbf{y}$

• Let ϕ be a feature mapping. Then* $K = \phi(X)\phi(X)^T$ is the kernel matrix for the corresponding kernel $K(x, y) = \langle \phi(x), \phi(y) \rangle$.

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Not every function K is a kernel!

Kernel theorem

Not every function K is a kernel! e.g. K(x, y) = -1 is not

Not every $n \times n$ matrix is a Kernel matrix!

Kernel theorem

• Theorem:

K is a kernel function $\Leftrightarrow K$ is symmetric positive semidefinite

A function is positive semidefinite iff for any finite dataset {x₁, x₂, ..., x_n} the corresponding kernel matrix is positive semidefinite.

P. Agius - L3, Spring 2008

Feature space concatenation

$$\begin{aligned} \star & \kappa(x,z) = \kappa_1(x,z) + \kappa_2(x,z) \\ \star & \kappa(x,z) = \alpha \kappa_1(x,z) \\ \star & \kappa(x,z) = \kappa_1(x,z) \kappa_2(x,z) \\ \star & \kappa(x,z) = f(x) f(z) \text{ where } f \text{ is a real-valued function} \\ \star & \kappa(x,z) = \kappa_3(\phi(x),\phi(z)) \\ \star & \kappa(x,z) = x^T Bz \text{ where } B \text{ is a psd matrix.} \end{aligned}$$

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$$\begin{aligned} &\star \kappa(x,z) = \kappa_1(x,z) + \kappa_{2}^{\text{Feature space scaling}} \\ &\star \kappa(x,z) = \alpha \kappa_1(x,z) \\ &\star \kappa(x,z) = \kappa_1(x,z) \kappa_2(x,z) \\ &\star \kappa(x,z) = f(x)f(z) \text{ where } f \text{ is a real-valued function} \\ &\star \kappa(x,z) = \kappa_3(\phi(x),\phi(z)) \\ &\star \kappa(x,z) = x^T Bz \text{ where } B \text{ is a psd matrix.} \end{aligned}$$

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P. Agius – L3, Spring 2008

P. Agius – L3, Spring 2008

Kernel normalization

• Let
$$\phi'(x) = \frac{\phi(x)}{\|\phi(x)\|}$$

• Then
 $K'(x,y) = \langle \phi'(x), \phi'(y) \rangle =$
 $\langle \frac{\phi(x)}{\|\phi(x)\|}, \frac{\phi(y)}{\|\phi(y)\|} \rangle = \frac{\langle \phi(x), \phi(y) \rangle}{\sqrt{\|\phi(x)\|^2 \|\phi(y)\|^2}} =$
 $= \frac{K(x,y)}{\sqrt{K(x,x)K(y,y)}}$

Kernel matrix normalization

Then

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$$K'(x,y) = \langle \phi'(x), \phi'(y) \rangle =$$

$$\langle \frac{\phi(x)}{\|\phi(x)\|}, \frac{\phi(y)}{\|\phi(y)\|} \rangle = \frac{\langle \phi(x), \phi(y) \rangle}{\sqrt{\|\phi(x)\|^2 \|\phi(y)\|^2}} =$$

$$= \frac{K(x,y)}{\sqrt{K(x,x)K(y,y)}}$$

$$K'_{ij} \coloneqq \frac{K_{ij}}{\sqrt{K_{ii}K_{jj}}}$$

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 $x_i \rightarrow x_i - \frac{1}{n} \sum_k x_k$

 $x_i \rightarrow x_i - \frac{1}{n} \sum_k x_k$

$$\begin{aligned} \mathbf{x}_{i} \to \mathbf{x}_{i} - \frac{1}{n} \sum_{k} \mathbf{x}_{k} \\ \mathbf{X} \to \mathbf{X} - \frac{1}{n} \mathbf{1}_{n} \mathbf{1}_{n}^{T} \mathbf{X} \\ \mathbf{X} \mathbf{X}^{T} \to \left(\mathbf{X} - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} \mathbf{X} \right) \left(\mathbf{X} - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} \mathbf{X} \right)^{T} \end{aligned}$$

$$x_{i} \rightarrow x_{i} - \frac{1}{n} \sum_{k} x_{k}$$

$$X \rightarrow X - \frac{1}{n} \mathbf{1}_{n} \mathbf{1}_{n}^{T} X$$

$$XX^{T} \rightarrow \left(X - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} X \right) \left(X - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} X \right)^{T}$$

$$XX^{T}$$

$$\rightarrow XX^{T} - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} XX^{T} - \frac{1}{n} XX^{T} \mathbf{1} \mathbf{1}^{T}$$

$$+ \frac{1}{n^{2}} \mathbf{1} \mathbf{1}^{T} XX^{T} \mathbf{1} \mathbf{1}^{T}$$
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Kernel matrix centering

$$XX^{T}$$

$$\rightarrow XX^{T} - \frac{1}{n} \mathbf{1}\mathbf{1}^{T}XX^{T} - \frac{1}{n}XX^{T}\mathbf{1}\mathbf{1}^{T}$$

$$+ \frac{1}{n^{2}} \mathbf{1}\mathbf{1}^{T}XX^{T}\mathbf{1}\mathbf{1}^{T}$$

$$K_{\text{cent}}$$

$$\coloneqq K - \frac{1}{n} \mathbf{1}\mathbf{1}^{T}K - \frac{1}{n}K\mathbf{1}\mathbf{1}^{T} + \frac{1}{n^{2}} \mathbf{1}\mathbf{1}^{T}K\mathbf{1}\mathbf{1}^{T}$$

$$M_{\text{Ma}} 2t$$

The Dual Representation

- Let A be the input space, and let B be the higher-dimensional feature space.
- Let $\phi: A \to B$ be the feature map.
- Fix a dataset $\{x_1, x_2, \dots, x_n\} \subset A$

• Let
$$w = \sum_i \alpha_i \phi(\mathbf{x}_i) \in B$$

• We say that α_i are the dual coordinates for w. May 26, 2013

$$w = \sum_{i} \alpha_{i} \phi(x_{i}) = \phi(X)^{T} \alpha = \Xi^{T} \alpha$$

Note that $\Xi\Xi^{T} = \phi(X)\phi(X)^{T} = K$

Now we can do all of the useful stuff using dual coordinates only.

Dual coordinates

Let

$$w = \Xi^T \alpha$$
$$u = \Xi^T \beta$$

Then

2**w** =

Dual coordinates

Let

$$w = \Xi^T \alpha$$
$$u = \Xi^T \beta$$

Then

 $2\boldsymbol{w} = \boldsymbol{\Xi}^{\mathrm{T}}(2\boldsymbol{\alpha})$

Dual coordinates

Let

$$w = \Xi^T \alpha$$
$$u = \Xi^T \beta$$

Then

$$2w = \Xi^{\mathrm{T}}(2\alpha)$$
$$w + u =$$


Let

$$w = \Xi^T \alpha$$
$$u = \Xi^T \beta$$

Then

$$2\boldsymbol{w} = \boldsymbol{\Xi}^{\mathrm{T}}(2\boldsymbol{\alpha})$$
$$\boldsymbol{w} + \boldsymbol{u} = \boldsymbol{\Xi}^{\mathrm{T}}(\boldsymbol{\alpha} + \boldsymbol{\beta})$$



Let

$$w = \Xi^T \alpha$$

 $u = \Xi^T \beta$

Then

$$2w = \Xi^{T}(2\alpha)$$
$$w + u = \Xi^{T}(\alpha + \beta)$$
$$\langle w, u \rangle =$$



Let

$$w = \Xi^T \alpha$$

 $u = \Xi^T \beta$

Then

$$2w = \Xi^{T}(2\alpha)$$

$$w + u = \Xi^{T}(\alpha + \beta)$$

$$\langle w, u \rangle = w^{T}u = \alpha^{T}\Xi\Xi^{T}\beta = \alpha^{T}K\beta$$



Let

$$w = \Xi^T \alpha$$

 $u = \Xi^T \beta$

Then

$$2w = \Xi^{T}(2\alpha)$$

$$w + u = \Xi^{T}(\alpha + \beta)$$

$$\langle w, u \rangle = w^{T}u = \alpha \Xi^{T}\beta = \alpha K\beta$$

$$||w - u||^{2} =$$



Let

$$w = \Xi^T \alpha$$

 $u = \Xi^T \beta$

Then

$$2w = \Xi^{T}(2\alpha)$$

$$w + u = \Xi^{T}(\alpha + \beta)$$

$$\langle w, u \rangle = w^{T}u = \alpha \Xi^{T}\beta = \alpha K\beta$$

$$||w - u||^{2} = w^{T}w + u^{T}u - 2w^{T}u = \cdots$$



Let

 $w = \Xi^T \alpha$ $u = \Xi^T \beta$

Then

$$2w = \Xi^{T}(2\alpha)$$

$$w + u = \Xi^{T}(\alpha + \beta)$$

$$\langle w, u \rangle = w^{T}u = \alpha \Xi^{T}\beta = \alpha K\beta$$

$$||w - u||^{2} = w^{T}w + u^{T}u - 2w^{T}u = \cdots$$





- Initialize $w \coloneqq \mathbf{0}$
- Find a misclassified example (x_i, y_i)
- Update weights:
 - $\mathbf{w} \coloneqq \mathbf{w} + \mu y_i \mathbf{x_i}$
 - $b \coloneqq b + \mu y_i$



- $\blacktriangleright \ \, {\sf Initialize} \ \, w\coloneqq {\bf 0} \Leftrightarrow \alpha\coloneqq {\bf 0}$
- Find a misclassified example (x_i, y_i)
- Update weights:
 - $\mathbf{w} \coloneqq \mathbf{w} + \mu y_i \mathbf{x}_i$
 - $b \coloneqq b + \mu y_i$



- Initialize $w \coloneqq \mathbf{0} \Leftrightarrow \alpha \coloneqq \mathbf{0}$
- Find a misclassified example (x_i, y_i)
- Update weights:

$$\mathbf{w} \coloneqq \mathbf{w} + \mu y_i \mathbf{x}_i \Leftrightarrow \alpha_i \coloneqq \alpha_i + \mu y_i$$

$$b \coloneqq b + \mu y_i$$



- Initialize $\alpha \coloneqq \mathbf{0}$
- Find a misclassified example (x_i, y_i)
- Update weights:
 - $\bullet \ \alpha_i \coloneqq \alpha_i + \mu y_i$
 - $b \coloneqq b + \mu y_i$



- ▶ Initialize $\alpha \coloneqq \mathbf{0}$
- Find a misclassified example (x_i, y_i)

•
$$\mathbf{w}^T \mathbf{x}_i + b \neq y_i \Leftrightarrow \sum_j \alpha_j \mathbf{x}_j^T \mathbf{x}_i + b \neq y_i$$

- Update weights:
 - $\blacktriangleright \alpha_i \coloneqq \alpha_i + \mu y_i$
 - $\flat b \coloneqq b + \mu y_i$



Recall the Perceptron:

- Initialize $\alpha \coloneqq \mathbf{0}$
- Find a misclassified example (x_i, y_i)

$$\mathbf{w}^T \mathbf{x}_i + b \neq y_i \Leftrightarrow \mathbf{K}_i \mathbf{\alpha} + b \neq y_i$$

Update weights:

$$\bullet \ \alpha_i \coloneqq \alpha_i + \mu y_i$$

 $\flat b \coloneqq b + \mu y_i$



- Initialize $\alpha \coloneqq \mathbf{0}$
- Find a misclassified example (x_i, y_i)
 - $K_i \alpha + b \neq y_i$
- Update weights:
 - $\bullet \ \alpha_i \coloneqq \alpha_i + \mu y_i$
 - $b \coloneqq b + \mu y_i$





Quiz

Today we heard three important ideas

- Important idea #I:___
- Important idea #2:
- Important idea #3: ____
- Function/matrix K is a kernel function/matrix iff it is ______

Dual representation: ____ = ____



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Those algoritms have kernelized versions:

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