

## Kernel Methods

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## 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
- Logistic regression, Perceptron, Max. margin, Fisher's discriminant, Linear regression, Ridge Regression, LASSO, ...:

$$
f(x)=
$$

- Logistic regression, Perceptron, Max. margin, Fisher's discriminant, Linear regression, Ridge Regression, LASSO, ...:

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

Logistic regression, Perceptron, Max. margin, Fisher's discriminant, Linear regression, Ridge Regression, LASSO, ...:

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

- PCA, LDA, ICA, ...:

$$
f(x)=
$$

Logistic regression, Perceptron, Max. margin, Fisher's discriminant, Linear regression, Ridge Regression, LASSO, ...:

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

- PCA, LDA, ICA, ...:

$$
f(x)=A x
$$

Logistic regression, Perceptron, Max. margin, Fisher's discriminant, Linear regression, Ridge Regression, LASSO, ...:

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

- PCA, LDA, ICA, ...:

$$
f(x)=A x
$$

(K-means:

$$
\boldsymbol{c}_{i}=\frac{1}{m} \boldsymbol{X}_{i} \mathbf{1}
$$

- CCA, GLM, ...


## Too much linear

Logistic regression, Perceptron, Max. margin,

Fish
Reg

- PCA
, K-m

- CCA, GLM, ...
dge


## Linear is not enough

- Limited generalization ability



## Linear is not enough

- Limited generalization ability


## $0>$

## Linear is not enough

- Limited applicability


## Text?

## Ordinal/Nominal data?

## Graphs/Trees/Networks?

Shapes?

## Graph nodes?

## Solutions

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## Solutions

- Feature space
- Kernels


## Solutions

- Feature space
- Nonlinear feature spaces


## Important idea \#|

- Kernels
- The Kernel Trick
- Dual representation


$$
f(x)=w x
$$



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$$
x \rightarrow x^{\prime}:=\phi(x):=\left(x, x^{2}, x^{3}\right)
$$



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## Nonlinear feature space

$$
\begin{aligned}
& x \rightarrow x^{\prime}:=\phi(x):=\left(x, x^{2}, x^{3}\right) \\
& f\left(x^{\prime}\right)=w_{1} x+w_{2} x^{2}+w_{3} x^{3}
\end{aligned}
$$



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X


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| - 0 |  | - $\bullet \bullet 0 \cdot 0$ |  | - $0 \cdot 0$ |  | $\bullet$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 1 | 1 | 1 | 1 | 1 | , |
| -1.5 | -1.0 | -0.5 | 0.0 | 0.5 | 1.0 | 1.5 |

$$
x \rightarrow \phi(x)=\left(x, x^{3}-x\right)
$$





$$
x \rightarrow \phi(x)=\left(x, x^{3}-x\right)
$$

## Nonlinear feature space

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



## +Support for arbitrary data types

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

## What if the dimensionality is highes

$$
\left(x_{1}, x_{2}, \ldots, x_{m}\right) \rightarrow\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)
$$

## 

$$
\begin{gathered}
\left(x_{1}, x_{2}, \ldots, x_{m}\right) \rightarrow\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right) \\
O\left(m^{2}\right) \text { elements }
\end{gathered}
$$

For all k-wise products: $O\left(\mathrm{~m}^{k}\right)$


## The Kernel Trick

- Let $\phi(\boldsymbol{x})=\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)$
- Consider

$$
\langle\phi(x), \phi(y)\rangle=\sum_{i j} \phi(x)_{i j} \phi(y)_{i j}
$$

## The Kernel Trick

- Let $\phi(\boldsymbol{x})=\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)$
- Consider

$$
\begin{aligned}
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& =\sum_{i j} x_{i} x_{j} y_{i} y_{j}
\end{aligned}
$$

## The Kernel Trick

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& =\sum_{i j} x_{i} x_{j} y_{i} y_{j}=\sum_{i j} x_{i} y_{i} x_{j} y_{j}
\end{aligned}
$$

## The Kernel Trick

- Let $\phi(\boldsymbol{x})=\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)$
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& =\sum_{i j} x_{i} x_{j} y_{i} y_{j}=\sum_{i j} x_{i} y_{i} x_{j} y_{j} \\
& =\sum_{i} x_{i} y_{i} \sum_{j} x_{j} y_{j}
\end{aligned}
$$

## The Kernel Trick

- Let $\phi(\boldsymbol{x})=\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)$
- Consider

$$
\begin{aligned}
& \langle\phi(\boldsymbol{x}), \phi(\boldsymbol{y})\rangle=\sum_{i j} \phi(\boldsymbol{x})_{i j} \phi(\boldsymbol{y})_{i j} \\
& =\sum_{i j} x_{i} x_{j} y_{i} y_{j}=\sum_{i j} x_{i} y_{i} x_{j} y_{j} \\
& =\sum_{i} x_{i} y_{i} \sum_{j} x_{j} y_{j}=\left(\sum_{i} x_{i} y_{i} y_{\text {max } 2}\right)^{2}, 2013
\end{aligned}
$$

## The Kernel Trick

- Let $\phi(\boldsymbol{x})=\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)$
- Consider

$$
\begin{aligned}
& \langle\phi(\boldsymbol{x}), \phi(\boldsymbol{y})\rangle=\sum_{i j} \phi(\boldsymbol{x})_{i j} \phi(\boldsymbol{y})_{i j} \\
& =\left(\sum_{i} x_{i} y_{i}\right)^{2}=\langle\boldsymbol{x}, \boldsymbol{y}\rangle^{2}
\end{aligned}
$$

## The Kernel Trick

- Let $\phi(\boldsymbol{x})=\left(x_{1} x_{1}, x_{1} x_{2}, \ldots, x_{m} x_{m}\right)$
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$$
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& =\left(\sum_{i} x_{i} y_{i}\right)^{2}=\langle\boldsymbol{x}, \boldsymbol{y}\rangle^{2}
\end{aligned}
$$

## The Kernel Trick

- Let
- Coı Polynomial kernel

$$
K(\boldsymbol{x}, \boldsymbol{y})=(\langle\boldsymbol{x}, \boldsymbol{y}\rangle+R)^{d}
$$

$\backslash \digamma_{i} \quad$


## The Kernel Trick

## What about:

$K(x, y)=\langle x, y\rangle+0.5\langle x, y\rangle^{2} ?$

## The Kernel Trick

What about:

$$
\begin{aligned}
& K(\boldsymbol{x}, \boldsymbol{y})=\langle\boldsymbol{x}, \boldsymbol{y}\rangle+0.5\langle\boldsymbol{x}, \boldsymbol{y}\rangle^{2} \\
= & \sum_{i} x_{i} y_{i}+0.5 \sum_{i j} \phi_{i j}(\boldsymbol{x}) \phi_{i j}(\boldsymbol{y})
\end{aligned}
$$

## The Kernel Trick

What about:
$K(\boldsymbol{x}, \boldsymbol{y})=\langle\boldsymbol{x}, \boldsymbol{y}\rangle+0.5\langle\boldsymbol{x}, \boldsymbol{y}\rangle^{2}$
$=\sum_{i} x_{i} y_{i}+0.5 \sum_{i j} \phi_{i j}(\boldsymbol{x}) \phi_{i j}(\boldsymbol{y})$
$\begin{aligned}= & \left\langle\left(x_{1}, \ldots, x_{m}, \sqrt{ } 0.5 x_{1} x_{1}, \ldots, \sqrt{ } 0.5 x_{m} x_{m}\right)\right. \\ & \left.\left(y_{1}, \ldots, y_{m}, \sqrt{ } 0.5 y_{1} y_{1}, \ldots, \sqrt{ } 0.5 y_{m} y_{m}\right)\right\rangle\end{aligned}$

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## The Kernel Trick

## What about:



## $K(\boldsymbol{x}, \boldsymbol{y})=\langle\boldsymbol{x}, \boldsymbol{y}\rangle+0.5\langle\boldsymbol{x}, \boldsymbol{y}\rangle^{2}$

$=\sum_{i} x_{i} y_{i}+0.5 \sum_{i j} \phi_{i j}(\boldsymbol{x}) \phi_{i j}(\boldsymbol{y})$
$=\left\langle\left(x_{1}, \ldots, x_{m}, \sqrt{ } 0.5 x_{1} x_{1}, \ldots, \sqrt{ } 0.5 x_{m} x_{m}\right)\right.$,
$\left.\left(y_{1}, \ldots, y_{m}, \sqrt{ } 0.5 y_{1} y_{1}, \ldots, \sqrt{ } 0.5 y_{m} y_{m}\right)\right\rangle$

## The Kernel Trick

## What about:

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

## The Kernel Trick

What about:

$$
K(x, y)=\sum_{i=0}^{\infty} \frac{\langle x, y\rangle^{i}}{i!}
$$

## The Kernel Trick

## What about:

$$
K(x, y)=\sum_{i=0}^{\infty} \frac{\langle x, y\rangle^{i}}{i!}=\exp \langle x, y\rangle
$$

## The Kernel Trick

## What about:

$$
K(x, y)=\sum_{i=0}^{\infty} \frac{\langle x, y\rangle^{i}}{i!}=\exp \langle x, y\rangle
$$

## Infinite-dimensional feature space!

MOTHER OF GOD...


## The Kernel Trick

## Gaussian kernel

$K$

$$
\begin{aligned}
& K(\boldsymbol{x}, \boldsymbol{y})= \\
& =\exp \left(-\gamma\|\boldsymbol{x}-\boldsymbol{y}\|^{2}\right) \\
& =\exp \left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|^{2}}{2 \sigma^{2}}\right)
\end{aligned}
$$



## The Kernel Trick

## Exponential kernel

$K(\boldsymbol{x}, \boldsymbol{y})=\exp \left(-\frac{\|\boldsymbol{x}-\boldsymbol{y}\|}{2 \sigma^{2}}\right)$

## Kernels

$$
\begin{aligned}
& k(x, y)=x^{T} y+c \quad k(x, y)=\sqrt{\|x-y\|^{2}+c^{2}} \quad k(x, y)=\frac{\theta}{\|x-y\|} \sin \frac{\|x-y\|}{\theta} \\
& k(x, y)=\left(\alpha x^{T} y+c\right)^{d} \\
& k(x, y)=\exp \left(-\frac{\|x-y\|^{2}}{2 \sigma^{2}}\right) \\
& k(x, y)=\frac{1}{\sqrt{\|x-y\|^{2}+c^{2}}} \\
& k(x, y)=\exp \left(-\frac{\|x-y\|}{2 \sigma^{2}}\right) \\
& k(x, y)=\frac{2}{\pi} \arccos \left(-\frac{\|x-y\|}{\sigma}\right)-\frac{2}{\pi} \frac{\|x-y\|}{\sigma} \sqrt{1-\left(\frac{\|x-y\|}{\sigma}\right)^{2}} \\
& k(x, y)=\sum_{k=1}^{n} \exp \left(-\sigma\left(x^{k}-y^{k}\right)^{2}\right)^{d} \\
& k(x, y)=1-\frac{3}{2} \frac{\|x-y\|}{\sigma}+\frac{1}{2}\left(\frac{\|x-y\|}{\sigma}\right)^{3} \quad k(x, y)=-\log \left(\|x-y\|^{d}+1\right) \\
& k(x, y)=\tanh \left(\alpha x^{T} y+c\right) \\
& k(x, y)=-\|x-y\|^{d} \\
& k(x, y)=\frac{1}{1+\frac{\|x-y\|^{2}}{\sigma}} \\
& k(x, y)=1-\frac{\|x-y\|^{2}}{\|x-y\|^{2}+c} \quad k(x, y)=1+x y+x y \min (x, y)-\frac{x+y}{2} \min (x, y)^{2}+\frac{{ }_{1}^{0}}{3} \min (x, y)^{3} \\
& k(x, y)=B_{2 p+1}(x-y) \quad k(x, y)=\sum_{i=1}^{n} \min \left(x_{i}, y_{i}\right) \quad k(x, y)=\prod_{i=1}^{N} h\left(\frac{x_{i}-c}{a}\right) h\left(\frac{y_{i}-c}{a}\right) \\
& k(x, y)=\sum_{i=1}^{m} \min \left(\left|x_{i}\right|^{\alpha},\left|y_{i}\right|^{\beta}\right) \quad k(x, y)=\frac{J_{v+1}(\sigma\|x-y\|)}{\|x-y\|^{-n(v+1)}} \\
& \kappa_{l}(a, b)=\sum_{c \in\{0 ; 1\}} P\left(Y=c \mid X_{l}=a\right) P\left(Y=c \mid X_{l}=b\right) \quad k(x, y)=\frac{1^{i=1}}{1+\|x-y\|^{d}} \\
& \text { May 26, } 2013
\end{aligned}
$$

## 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

- A function $K(\boldsymbol{x}, \boldsymbol{y})$ is a kernel, if

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

for some feature map $\phi$.

## Kernel matrix

- For a given kernel function $K$ and a finite dataset $\left(\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right)$ the $n \times n$ matrix

$$
\boldsymbol{K}_{i j}:=K\left(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}\right)
$$

is called the kernel matrix.

## Kernel matrix

- Let $\boldsymbol{X}$ be the data matrix, then

$$
\boldsymbol{K}=\boldsymbol{X} \boldsymbol{X}^{T}
$$

is the kernel matrix for the linear kernel

$$
K(\boldsymbol{x}, \boldsymbol{y})=\boldsymbol{x}^{T} \boldsymbol{y}
$$

## Kernel matrix

- Let $\boldsymbol{X}$ be the data matrix, then

$$
\boldsymbol{K}=\boldsymbol{X} \boldsymbol{X}^{T}
$$

is the kernel matrix for the linear kernel

$$
K(\boldsymbol{x}, \boldsymbol{y})=\boldsymbol{x}^{T} \boldsymbol{y}
$$

- Let $\phi$ be a feature mapping. Then*

$$
\boldsymbol{K}=\phi(\boldsymbol{X}) \phi(\boldsymbol{X})^{T}
$$

is the kernel matrix for the corresponding kernel $K(\boldsymbol{x}, \boldsymbol{y})=\langle\phi(\boldsymbol{x}), \phi(\boldsymbol{y})\rangle$.

## Kernel theorem

- Not every function K is a kerne!!


## Example?

## Kernel theorem

- Not every function K is a kerne!!

$$
\text { e.g. } K(x, y)=-1 \text { is not }
$$

- 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 $\left\{\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right\}$ the corresponding kernel matrix is positive semidefinite.


## Kernel closure

$\kappa(x, z)=\kappa_{1}(x, z)+\kappa_{2}(x, z)$
$\kappa(x, z)=\alpha \kappa_{1}(x, z)$
$\kappa(x, z)=\kappa_{1}(x, z) \kappa_{2}(x, z)$
$\kappa(x, z)=f(x) f(z)$ where $f$ is a real-valued function
$\kappa(x, z)=\kappa_{3}(\phi(x), \phi(z))$
$\kappa(x, z)=x^{T} B z$ where $B$ is a psd matrix.
P. Agius - L3, Spring 2008

## Kernel closure

Feature space concatenation
$\kappa(x, z)=\kappa_{1}(x, z)+\kappa_{2}(x, z)$
$\kappa(x, z)=\alpha \kappa_{1}(x, z)$
$\kappa(x, z)=\kappa_{1}(x, z) \kappa_{2}(x, z)$
$\kappa(x, z)=f(x) f(z)$ where $f$ is a real-valued function
$\kappa(x, z)=\kappa_{3}(\phi(x), \phi(z))$
$\kappa(x, z)=x^{T} B z$ where $B$ is a psd matrix.
P. Agius - L3, Spring 2008

## Kernel closure

$\kappa(x, z)=\kappa_{1}(x, z)+\kappa_{2}(\infty, \sim) \quad$ Feature space scaling
$\kappa(x, z)=\alpha \kappa_{1}(x, z)$
$\kappa(x, z)=\kappa_{1}(x, z) \kappa_{2}(x, z)$
$\kappa(x, z)=f(x) f(z)$ where $f$ is a real-valued function
$\kappa(x, z)=\kappa_{3}(\phi(x), \phi(z))$
$\kappa(x, z)=x^{T} B z$ where $B$ is a psd matrix.
P. Agius - L3, Spring 2008

## Kernel closure

$$
\begin{aligned}
& \kappa(x, z)=\kappa_{1}(x, z)+\kappa \\
& \kappa(x, z)=\alpha \kappa_{1}(x, z) \\
& \kappa(x, z)=\kappa_{1}(x, z) \kappa_{2}(x, z) \\
& \kappa(x, z)=f(x) f(z) \text { wheature space tensor product } f \text { is a real-valued function } \\
& \kappa(x, z)=\kappa_{3}(\phi(x), \phi(z)) \\
& \kappa(x, z)=x^{T} B z \text { where } B \text { is a psd matrix. }
\end{aligned}
$$

## Kernel closure

$\kappa(x, z)=\kappa_{1}(x, z)+\kappa_{2}(x, z)$
$\kappa(x, z)=\alpha \kappa_{1}(x, z)$
$\kappa(x, z)=\kappa_{1}(x, z) \kappa_{2}(a \quad$ Feature map composition
$\kappa(x, z)=f(x) f(z)$ where $J$ is a real-valued function
$\kappa(x, z)=\kappa_{\kappa_{3}}(\phi(x), \phi(z))$
$\kappa(x, z)=x^{T} B z$ where $B$ is a psd matrix.
P. Agius - L3, Spring 2008

## Kernel normalization

Let $\phi^{\prime}(x)=\frac{\phi(x)}{\|\phi(x)\|}$

- Then

$$
\begin{aligned}
& K^{\prime}(x, y)=\left\langle\phi^{\prime}(x), \phi^{\prime}(y)\right\rangle= \\
& \left\langle\frac{\phi(x)}{\|\phi(x)\|}, \frac{\phi(y)}{\|\phi(y)\|}\right\rangle=\frac{\langle\phi(x), \phi(y)\rangle}{\sqrt{\|\phi(x)\|^{2}\|\phi(y)\|^{2}}}= \\
& =\frac{K(x, y)}{\sqrt{K(x, x) K(y, y)}}
\end{aligned}
$$

## Kernel matrix normalization

Then

$$
\begin{aligned}
& K^{\prime}(x, y)=\left\langle\phi^{\prime}(x), \phi^{\prime}(y)\right\rangle= \\
& \left\langle\frac{\phi(x)}{\|\phi(x)\|}, \frac{\phi(y)}{\|\phi(y)\|}\right\rangle=\frac{\langle\phi(x), \phi(y)\rangle}{\sqrt{\|\phi(x)\|^{2}\|\phi(y)\|^{2}}}= \\
& =\frac{K(x, y)}{\sqrt{K(x, x) K(y, y)}}
\end{aligned}
$$

$$
K_{i j}^{\prime}:=\frac{K_{i j}}{\sqrt{K_{i i} K_{j j}}}
$$

## Kernel matrix centering

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

## Kernel matrix centering

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

## CHALLENGE ACCEPTED



## Kernel matrix centering

$$
\begin{aligned}
& \boldsymbol{x}_{i} \rightarrow \boldsymbol{x}_{i}-\frac{1}{n} \sum_{k} \boldsymbol{x}_{k} \\
& \boldsymbol{X} \rightarrow \boldsymbol{X}-\frac{1}{n} \mathbf{1}_{n} \mathbf{1}_{n}^{T} \boldsymbol{X}
\end{aligned}
$$

## Kernel matrix centering

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

## Kernel matrix centering

$$
\begin{aligned}
& \boldsymbol{x}_{i} \rightarrow \boldsymbol{x}_{i}-\frac{1}{n} \sum_{k} \boldsymbol{x}_{k} \\
& \boldsymbol{X} \rightarrow \boldsymbol{X}-\frac{1}{n} \mathbf{1}_{n} \mathbf{1}_{n}^{T} \boldsymbol{X} \\
& \boldsymbol{X} \boldsymbol{X}^{T} \rightarrow\left(\boldsymbol{X}-\frac{1}{n} \mathbf{1 1}^{T} \boldsymbol{X}\right)\left(\boldsymbol{X}-\frac{1}{n} \mathbf{1 1}^{T} \boldsymbol{X}\right)^{T} \\
& \boldsymbol{X} \boldsymbol{X}^{T} \\
& \rightarrow \boldsymbol{X} \boldsymbol{X}^{T}-\frac{1}{n} \mathbf{1 1}^{T} \boldsymbol{X} \boldsymbol{X}^{T}-\frac{1}{n} \boldsymbol{X} \boldsymbol{X}^{T} \mathbf{1 1}^{T} \\
& +\frac{1}{n^{2}} \mathbf{1 1}^{T} \boldsymbol{X} \boldsymbol{X}^{T} \mathbf{1 1}^{T}
\end{aligned}
$$

## Kernel matrix centering

$$
\begin{aligned}
& \boldsymbol{X} \boldsymbol{X}^{T} \\
& \rightarrow \boldsymbol{X} \boldsymbol{X}^{T}-\frac{1}{n} \mathbf{1 1}^{T} \boldsymbol{X} \boldsymbol{X}^{T}-\frac{1}{n} \boldsymbol{X} \boldsymbol{X}^{T} \mathbf{1 1}^{T} \\
& +\frac{1}{n^{2}} \mathbf{1 1}^{T} \boldsymbol{X} \boldsymbol{X}^{T} \mathbf{1 1}^{T}
\end{aligned}
$$

$\boldsymbol{K}_{\text {cent }}$

$$
:=\boldsymbol{K}-\frac{1}{n} \mathbf{1 1}^{T} \boldsymbol{K}-\frac{1}{n} \boldsymbol{K} \mathbf{1 1} 1^{T}+\frac{1}{n^{2}} \mathbf{1 1}^{T} \boldsymbol{K} \mathbf{1 1}^{T}
$$



## The Dual Representation

- Let $A$ be the input space, and let $B$ be the higher-dimensional feature space.
- Let $\phi: A \rightarrow B$ be the feature map.
- Fix a dataset $\left\{\boldsymbol{x}_{1}, \boldsymbol{x}_{2}, \ldots, \boldsymbol{x}_{n}\right\} \subset A$

Let $w=\sum_{i} \alpha_{i} \phi\left(\boldsymbol{x}_{i}\right) \in B$

- We say that $\alpha_{i}$ are the dual coordinates for $w$.


## Dual coordinates

$$
\boldsymbol{w}=\sum_{i} \alpha_{i} \phi\left(\boldsymbol{x}_{i}\right)=\phi(\boldsymbol{X})^{T} \boldsymbol{\alpha}=\boldsymbol{\Xi}^{T} \boldsymbol{\alpha}
$$

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

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

## Dual coordinates

## Let

$$
\begin{aligned}
& \boldsymbol{w}=\boldsymbol{\Xi}^{T} \boldsymbol{\alpha} \\
& \boldsymbol{u}=\boldsymbol{\Xi}^{\mathrm{T}} \boldsymbol{\beta}
\end{aligned}
$$

## Then

$2 w=$

## Dual coordinates

Let

$$
\begin{aligned}
& \boldsymbol{w}=\boldsymbol{\Xi}^{T} \boldsymbol{\alpha} \\
& \boldsymbol{u}=\boldsymbol{\Xi}^{\mathrm{T}} \boldsymbol{\beta}
\end{aligned}
$$

Then

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

## Dual coordinates

Let

$$
\begin{aligned}
& \boldsymbol{w}=\boldsymbol{\Xi}^{T} \boldsymbol{\alpha} \\
& \boldsymbol{u}=\boldsymbol{\Xi}^{\mathrm{T}} \boldsymbol{\beta}
\end{aligned}
$$

Then

$$
\begin{aligned}
& 2 \boldsymbol{w}=\Xi^{\mathrm{T}}(2 \boldsymbol{\alpha}) \\
& \boldsymbol{w}+\boldsymbol{u}=
\end{aligned}
$$

## Dual coordinates

Let

$$
\begin{aligned}
& \boldsymbol{w}=\boldsymbol{\Xi}^{T} \boldsymbol{\alpha} \\
& \boldsymbol{u}=\boldsymbol{\Xi}^{\mathrm{T}} \boldsymbol{\beta}
\end{aligned}
$$

Then

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

## Dual coordinates

Let

$$
\begin{aligned}
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& \boldsymbol{u}=\boldsymbol{\Xi}^{\mathrm{T}} \boldsymbol{\beta}
\end{aligned}
$$

Then

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\begin{aligned}
& 2 \boldsymbol{w}=\Xi^{\mathrm{T}}(2 \boldsymbol{\alpha}) \\
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- Recall the Perceptron:


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$$
\boldsymbol{w}^{T} \boldsymbol{x}_{i}+b \neq y_{i} \Leftrightarrow \sum_{j} \alpha_{j} \boldsymbol{x}_{j}^{T} \boldsymbol{x}_{i}+b \neq y_{i}
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Today we heard three important ideas

- Important idea \#I:
- Important idea \#2: $\qquad$
- Important idea \#3:
- Function/matrix $K$ is a kernel function/matrix iff it is
- Dual representation:


Those algoritms have kernelized versions:


May 26, 2013

