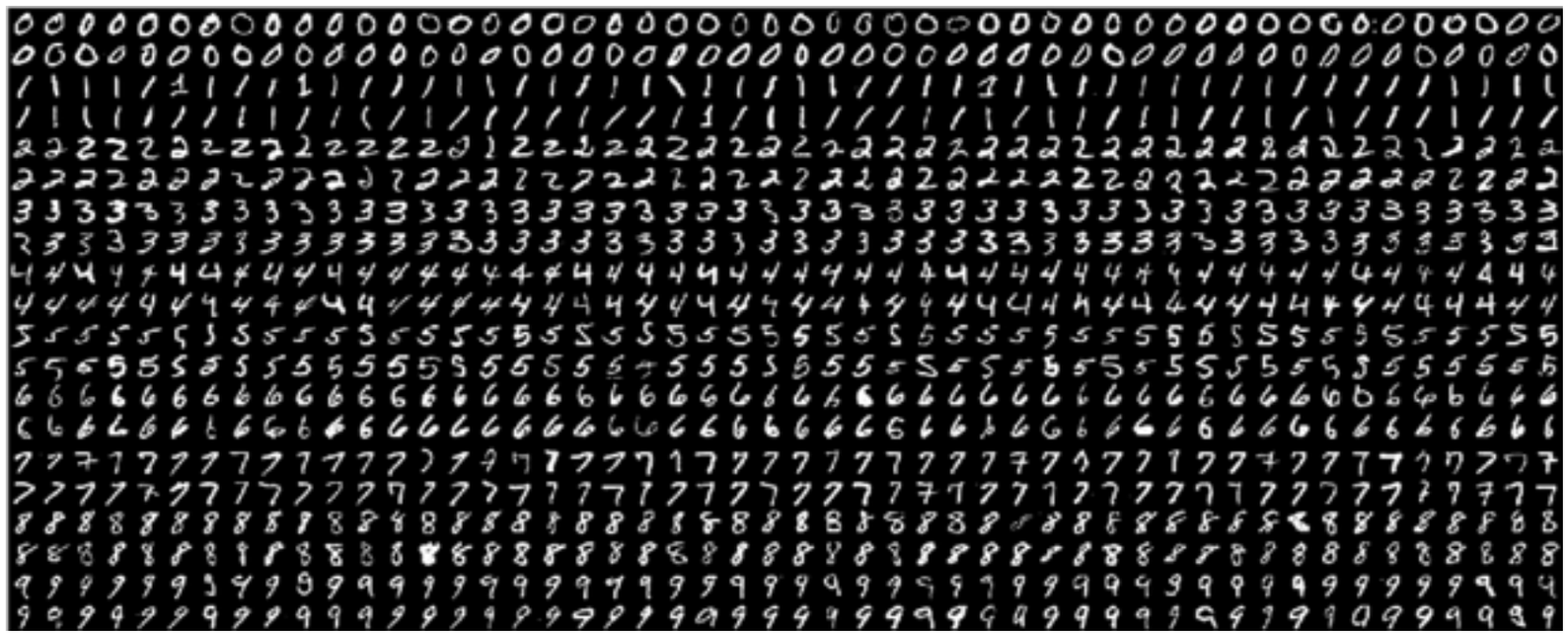
Administrivia

- Mini-project 2 due April 7, in class
  - implement multi-class reductions, naive bayes, kernel perceptron, multi-class logistic regression and two layer neural networks
  - training set:



- Project proposals due April 2, in class
  - one page describing the project topic, goals, etc
  - list your team members (2+)
  - project presentations: April 23 and 27
  - final report: May 3

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Active
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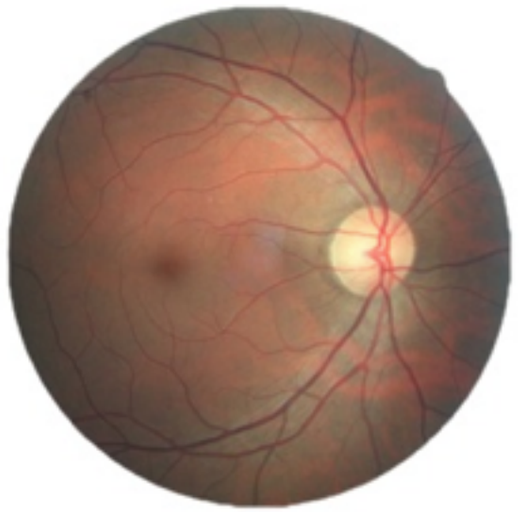
Competition Name			
Diabetic Retinopathy Detection Identify signs of diabetic retinc images			
Restaurant Revenue Predict annual restaurant sale objective measurements			
Microsoft Malware Classification Challen 2015) Classify malware into families based on file content and characteristics			
March Machine Learning Mania 2015 Predict the 2015 NCAA Basketball	$15,000	341	14 days

Competition Details » Get the Data » Make a submission

Identify signs of diabetic retinopathy in eye images

Diabetic retinopathy is the leading cause of blindness in the working-age population of the developed world. It is estimated to affect over 93 million people.



The US Center for Disease Control and Prevention estimates that 29.1 million people in the US have diabetes and the World Health Organization estimates that 347 million people have the disease worldwide. Diabetic Retinopathy (DR) is an eye disease associated with long-standing diabetes. Around 40% to 45% of Americans with diabetes have some stage of the disease. Progression to vision impairment can be slowed or averted if DR is detected in time, however this can be difficult as the disease often shows few symptoms until it is too late to provide effective treatment.

Currently, detecting DR is a time-consuming and manual process that requires a trained clinician to examine and evaluate digital color fundus photographs of the retina. By the time human readers submit their reviews, often a day or two later, the delayed results lead to lost follow up, miscommunication, and delayed treatment.

Kernel Methods

Subhransu Maji

CMPSCI 689: Machine Learning

24 March 2015

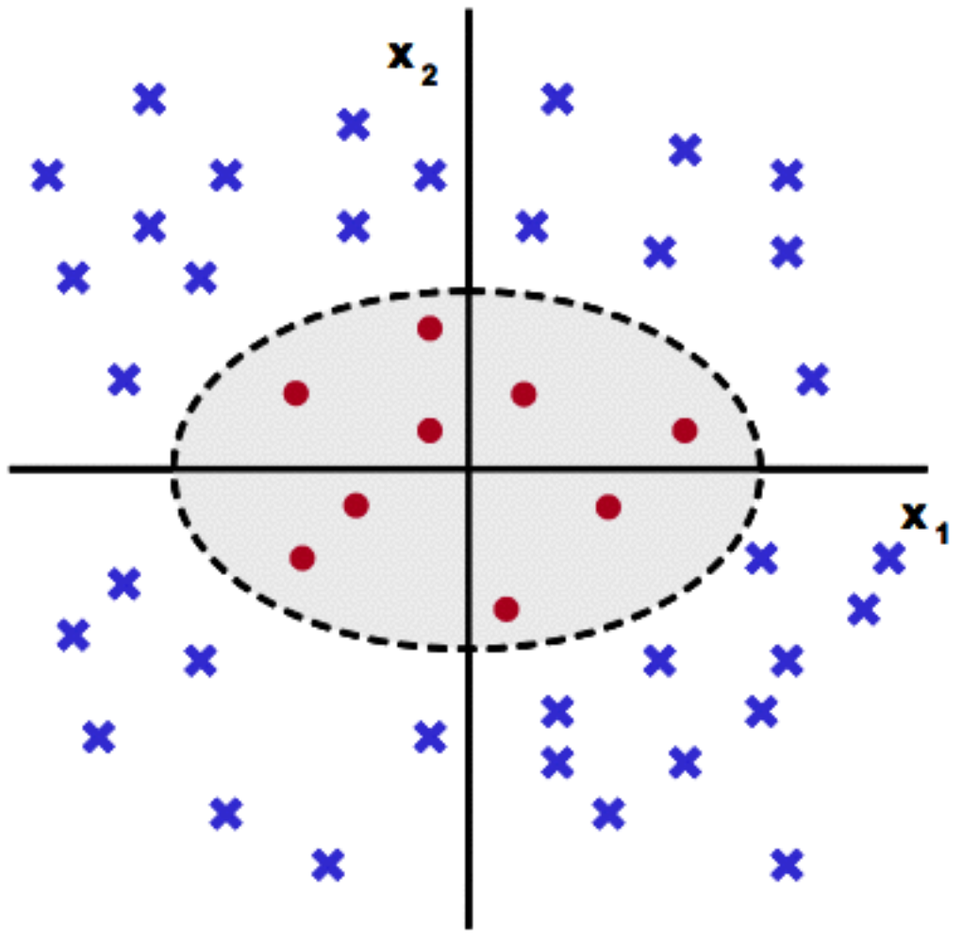
26 March 2015

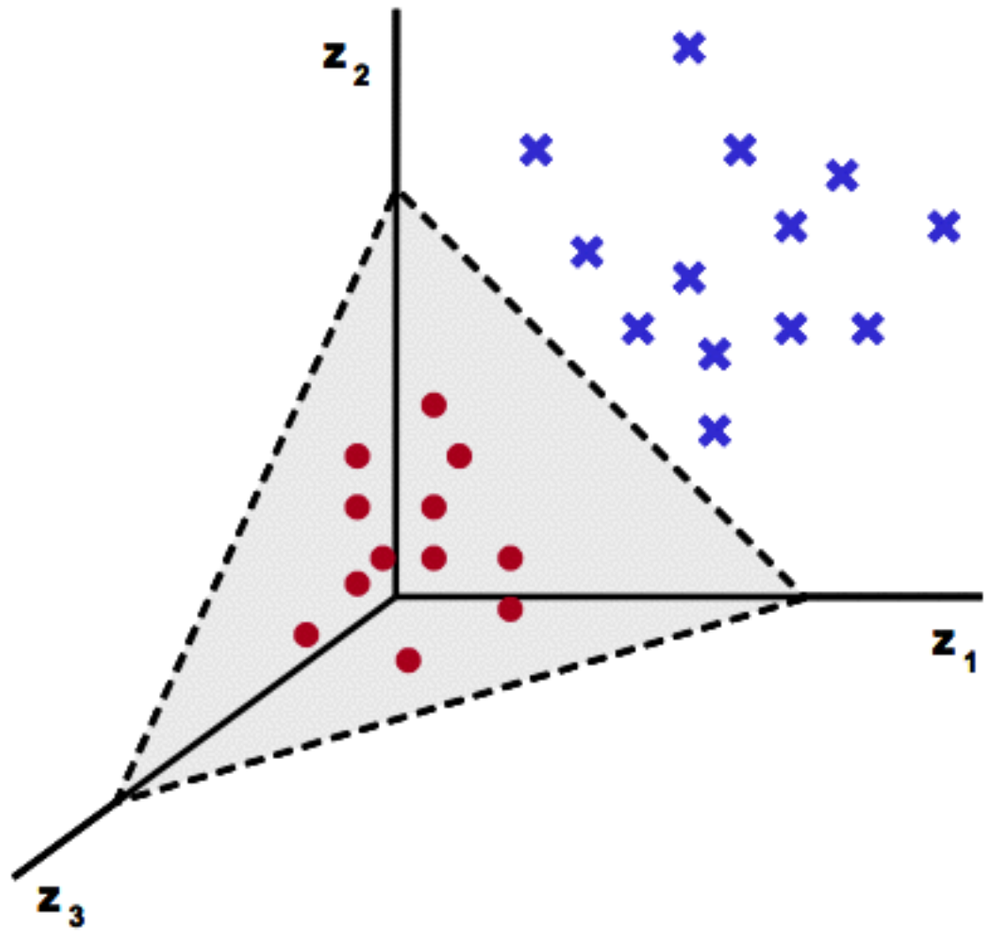
Feature mapping

- Learn non-linear classifiers by mapping features

$$\varphi : \mathbf{R}^2 \rightarrow \mathbf{R}^3$$

$$(x_1, x_2) \mapsto (z_1, z_2, z_3) = \left(x_1^2, \sqrt{2}x_1x_2, x_2^2\right)$$





Can we learn the XOR function with this mapping?

Quadratic feature map

- Let, $\mathbf{x} = [x_1, x_2, \ldots, x_D]$
- Then the quadratic feature map is defined as:

$$\begin{aligned}\phi(\mathbf{x}) = &[1, \sqrt{2}x_1, \sqrt{2}x_2, \ldots, \sqrt{2}x_D, \\ &x_1^2, x_1x_2, x_1x_3 \ldots, x_1x_D, \\ &x_2x_1, x_2^2, x_2x_3 \ldots, x_2x_D, \\ &\ldots, \\ &x_Dx_1, x_Dx_2, x_Dx_3 \ldots, x_D^2]\end{aligned}$$

- Contains all single and pairwise terms
- There are repetitions, e.g., x_1x_2 and x_2x_1, but hopefully the learning algorithm can handle redundant features

Drawbacks of feature mapping

- Computational
  - Suppose training time is linear in feature dimension, quadratic feature map squares the training time
- Memory
  - Quadratic feature map squares the memory required to store the training data
- Statistical
  - Quadratic feature mapping squares the number of parameters
  - For now lets assume that regularization will deal with overfitting

Quadratic kernel

- The dot product between feature maps of **x** and **z** is:

$$\begin{aligned}
\phi(\mathbf{x})^T\phi(\mathbf{z}) &= 1 + 2x_1z_1 + 2x_2z_2, \ldots, 2x_Dz_D + x_1^2z_1^2 + x_1x_2z_1z_2 + \ldots + x_1x_Dz_1z_D + \ldots \\
&\quad \ldots + x_Dx_1z_Dz_1 + x_Dx_2z_Dz_2 + \ldots + x_D^2z_D^2 \\
&= 1 + 2\left(\sum_i x_iz_i\right) + \sum_{i,j} x_ix_jz_iz_j \\
&= 1 + 2\left(\mathbf{x}^T\mathbf{z}\right) + \left(\mathbf{x}^T\mathbf{z}\right)^2 \\
&= \left(1 + \mathbf{x}^T\mathbf{z}\right)^2 \\
&= K(\mathbf{x}, \mathbf{z}) \longleftarrow \text{quadratic kernel}
\end{aligned}$$

- Thus, we can compute $\phi(\mathbf{x})^T\phi(\mathbf{z})$ in almost the same time as needed to compute $\mathbf{x}^T\mathbf{z}$ (one extra addition and multiplication)
- We will rewrite various algorithms using only dot products (or kernel evaluations), and not explicit features

Perceptron revisited

Input: training data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

feature map ϕ

Perceptron training algorithm

- Initialize $\mathbf{w} \leftarrow [0, \ldots, 0]$
- for iter = 1,…,T
  - for i = 1,..,n
    - predict according to the current model

$$\hat{y}_i = \begin{cases} +1 & \text{if } \mathbf{w}^T \phi(\mathbf{x}_i) > 0 \\ -1 & \text{otherwise} \end{cases}$$

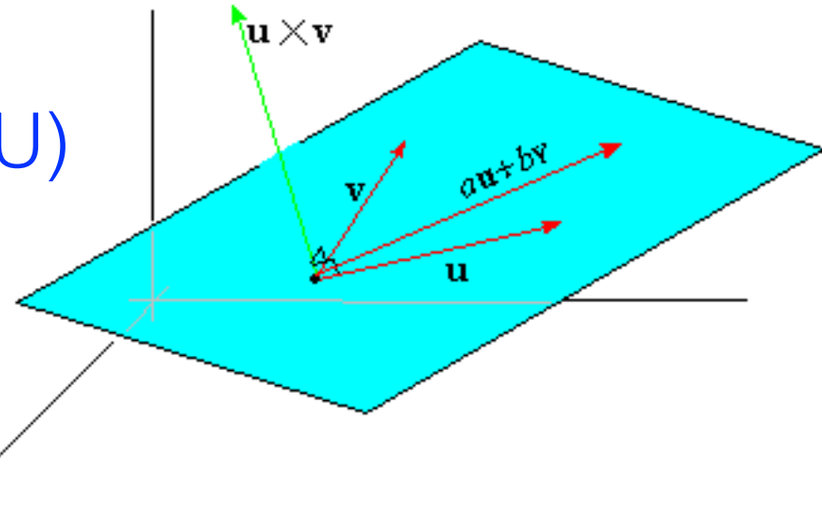
    - if $y_i = \hat{y}_i$, no change
    - else, $\mathbf{w} \leftarrow \mathbf{w} + y_i \phi(\mathbf{x}_i)$

dependence on ϕ

Obtained by replacing **x** by ϕ(**x**)

Properties of the weight vector

- Linear algebra recap:
  - Let U be set of vectors in R^D, i.e., $U = \{\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_D\}$ and $\mathbf{u}_i \in R^D$
  - Span(U) is the set of all vectors that can be represented as $\sum_i a_i \mathbf{u}_i$, such that $a_i \in R$
  - Null(U) is everything that is left i.e., $R^D \setminus$ Span(U)



Perceptron representer theorem: During the run of the perceptron training algorithm, the weight vector **w** is always in the span of $\phi(\mathbf{x}_1)$, $\phi(\mathbf{x}_1)$, …, $\phi(\mathbf{x}_D)$

$$\mathbf{w} = \sum_i \alpha_i \phi(\mathbf{x}_i) \qquad \text{updates} \quad \alpha_i \leftarrow \alpha_i + y_i$$

$$\mathbf{w}^T \phi(\mathbf{z}) = \left(\sum_i \alpha_i \phi(\mathbf{x}_i)\right)^T \phi(\mathbf{z}) = \sum_i \alpha_i \phi(\mathbf{x}_i)^T \phi(\mathbf{z})$$

Kernelized perceptron

Input: training data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

feature map ϕ

Kernelized perceptron training algorithm

- Initialize $\alpha \leftarrow [0, 0, \ldots, 0]$
- for iter = 1,…,T
  - for i = 1,..,n
    - predict according to the current model

$$\hat{y}_i = \begin{cases} +1 & \text{if } \sum_n \alpha_n \phi(\mathbf{x}_n)^T \phi(\mathbf{x}_i) > 0 \\ -1 & \text{otherwise} \end{cases}$$

    - if $y_i = \hat{y}_i$, no change
    - else, $\alpha_i = \alpha_i + y_i$

$$\phi(\mathbf{x})^T \phi(\mathbf{z}) = (1 + \mathbf{x}^T \mathbf{z})^p$$ polynomial kernel of degree p

Support vector machines

- Kernels existed long before SVMs, but were popularized by them
- Does the representer theorem hold for SVMs?
- Recall that the objective function of an SVM is:

$$\min_{\mathbf{w}} \frac{1}{2}||\mathbf{w}||^2 + C\sum_n \max(0, 1 - y_n \mathbf{w}^T \mathbf{x}_n)$$

- Let, $\mathbf{w} = \mathbf{w}_{||} + \mathbf{w}_{\perp}$

only $\mathbf{w}_{||}$ affects classification

$$\begin{aligned}\mathbf{w}^T\mathbf{x}_i &= (\mathbf{w}_{||} + \mathbf{w}_{\perp})^T\mathbf{x}_i \\ &= \mathbf{w}_{||}^T\mathbf{x}_i + \mathbf{w}_{\perp}^T\mathbf{x}_i \\ &= \mathbf{w}_{||}^T\mathbf{x}_i\end{aligned}$$

norm decomposes

$$\begin{aligned}\mathbf{w}^T\mathbf{w} &= (\mathbf{w}_{||} + \mathbf{w}_{\perp})^T(\mathbf{w}_{||} + \mathbf{w}_{\perp}) \\ &= \mathbf{w}_{||}^T\mathbf{w}_{||} + \mathbf{w}_{\perp}^T\mathbf{w}_{\perp} \\ &\geq \mathbf{w}_{||}^T\mathbf{w}_{||}\end{aligned}$$

Hence, $\mathbf{w} \in \text{Span}(\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\})$

Kernel k-means

- Initialize k centers by picking k points randomly
- Repeat till convergence (or max iterations)
  - Assign each point to the nearest center (assignment step)

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} ||\phi(\mathbf{x}) - \mu_i||^2$$

  - Estimate the mean of each group (update step)

$$\arg\min_{\mathbf{S}} \sum_{i=1}^{k} \sum_{\mathbf{x} \in S_i} ||\phi(\mathbf{x}) - \mu_i||^2$$

- Representer theorem is easy here — $\mu_i \leftarrow \frac{1}{|S_i|} \sum_{\mathbf{x} \in S_i} \phi(\mathbf{x})$

- Exercise: show how to compute $||\phi(\mathbf{x}) - \mu_i||^2$ using dot products

What makes a kernel?

- A kernel is a mapping $K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$
- Functions that can be written as dot products are valid kernels

$$K(\mathbf{x}, \mathbf{z}) = \phi(\mathbf{x})^T \phi(\mathbf{z})$$

- Examples: polynomial kernel $K^d_{(\text{poly})}(\mathbf{x}, \mathbf{z}) = (1 + \mathbf{x}^T \mathbf{z})^d$

Alternate characterization of a kernel

- A function $K: \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a kernel if K is positive semi-definite (psd)
- This property is also called as Mercer's condition
- This means that for all functions f that are squared integrable except the zero function, the following property holds:

$$\int \int f(\mathbf{x}) K(\mathbf{x}, \mathbf{z}) f(\mathbf{z}) d\mathbf{z} d\mathbf{x} > 0 \qquad \int f(\mathbf{x})^2 d\mathbf{x} < \infty$$

Why is this characterization useful?

- We can prove some properties about kernels that are otherwise hard to prove
- Theorem: If K_1 and K_2 are kernels, then $K_1 + K_2$ is also a kernel
- Proof:

$$\begin{aligned}\int\int f(\mathbf{x})K(\mathbf{x},\mathbf{z})f(\mathbf{z})d\mathbf{z}d\mathbf{x} &= \int\int f(\mathbf{x})\left(K_1(\mathbf{x},\mathbf{z}) + K_2(\mathbf{x},\mathbf{z})\right)f(\mathbf{z})d\mathbf{z}d\mathbf{x} \\ &= \int\int f(\mathbf{x})K_1(\mathbf{x},\mathbf{z})f(\mathbf{z})d\mathbf{z}d\mathbf{x} + \int\int f(\mathbf{x})K_2(\mathbf{x},\mathbf{z})f(\mathbf{z})d\mathbf{z}d\mathbf{x} \\ &\geq 0 + 0\end{aligned}$$

- More generally if K_1, K_2,…, K_n are kernels then $\sum_i \alpha_i K_i$ with $\alpha_i \geq 0$, is a also a kernel
- Can build new kernels by linearly combining existing kernels

Why is this characterization useful?

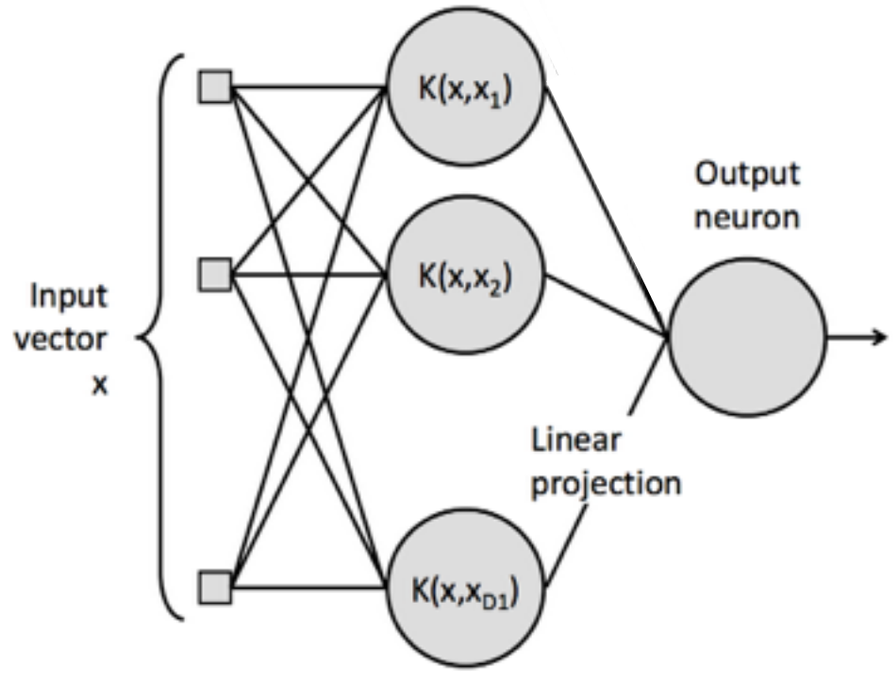
- We can show that the Gaussian function is a kernel
  - Also called as radial basis function (RBF) kernel

$$K_{(\mathrm{rbf})}(\mathbf{x}, \mathbf{z}) = \exp\left(-\gamma||\mathbf{x} - \mathbf{z}||^2\right)$$

- Lets look at the classification function using a SVM with RBF kernel:

$$f(\mathbf{z}) = \sum_i \alpha_i K_{(\mathrm{rbf})}(\mathbf{x}_i, \mathbf{z})$$

$$= \sum_i \alpha_i \exp\left(-\gamma||\mathbf{x}_i - \mathbf{z}||^2\right)$$



- This is similar to a two layer network with the RBF as the link function
- Gaussian kernels are examples of universal kernels — they can approximate any function in the limit as training data goes to infinity

Kernels in practice

- Feature mapping via kernels often improves performance
- MNIST digits test error:
  - **8.4%** SVM linear
  - **1.4%** SVM RBF
  - **1.1%** SVM polynomial (d=4)

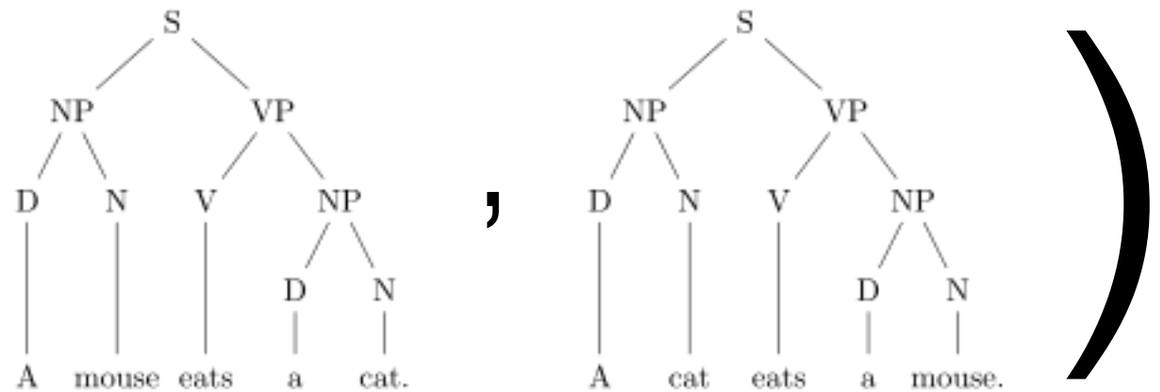
60,000 training examples

http://yann.lecun.com/exdb/mnist/

Kernels over general structures

- Kernels can be defined over any pair of inputs such as strings, trees and graphs!
- Kernel over trees:

$$K\left(\quad , \quad \right) = \text{number of common subtrees}$$



http://en.wikipedia.org/wiki/Tree_kernel

  - This can be computed efficiently using dynamic programming
  - Can be used with SVMs, perceptrons, k-means, etc
- For strings number of common substrings is a kernel
- Graph kernels that measure graph similarity (e.g. number of common subgraphs) have been used to predict toxicity of chemical structures

Kernels for computer vision

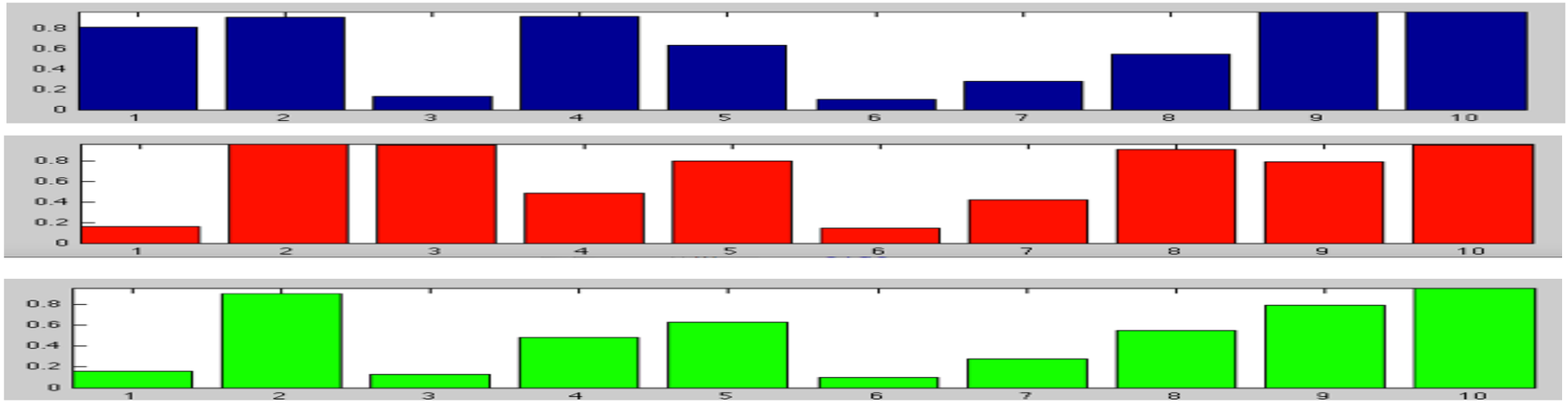
- Histogram intersection kernel between two histograms a and b

$$K_{\min}(a,b) = \sum_{i=1}^{n} \min(a_i, b_i) \quad a_i \geq 0 \quad b_i \geq 0$$

a

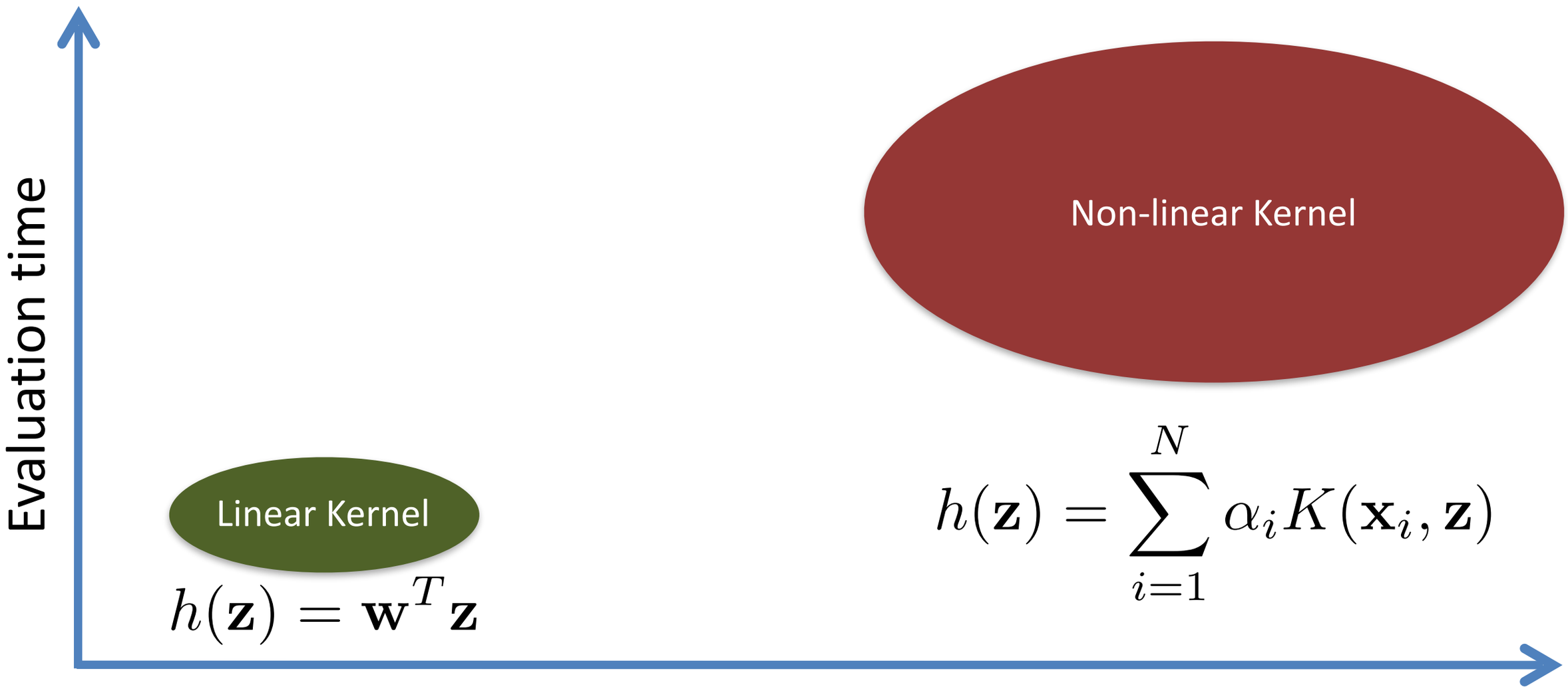
b

min(a,b)



- Introduced by Swain and Ballard 1991 to compare color histograms

Kernel classifiers tradeoffs



Linear: O (feature dimension)

Non Linear: O (**N** X feature dimension)

Kernel classification function

$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}_i, \mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

Kernel classification function

$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}_i, \mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

Key insight: additive property

$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

$$= \sum_{j=1}^{D} \left(\sum_{i=1}^{N} \alpha_i \min(x_{ij}, z_j) \right)$$

$$= \sum_{j=1}^{D} h_j(z_j)$$

$$h_j(z_j) = \sum_{i=1}^{N} \alpha_i \min(x_{ij}, z_j)$$

Kernel classification function

$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}_i, \mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

Algorithm 1

$$h_j(z_j) = \sum_{i=1}^{N} \alpha_i \min(x_{ij}, z_j) \qquad O(N)$$

Kernel classification function

$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}_i, \mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

[Maji et al. PAMI 13]

Algorithm 1

$$h_j(z_j) = \sum_{i=1}^{N} \alpha_i \min(x_{ij}, z_j)$$

~~$O(N)$~~

$$= \sum_{i:x_{ij}<z_j}^{N} \alpha_i x_{ij} + \sum_{i:x_{ij}\geq z_j}^{N} \alpha_i z_j$$

$O(\log N)$

Sort the support vector values in each coordinate, and pre-compute these sums for each rank.

To evaluate, find the position of z_j the sorted list of support vector x_{ij} .This can be done in **O(log N)** time using binary search.

Kernel classification function

$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}_i, \mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

[Maji et al. PAMI 13]

Algorithm 2

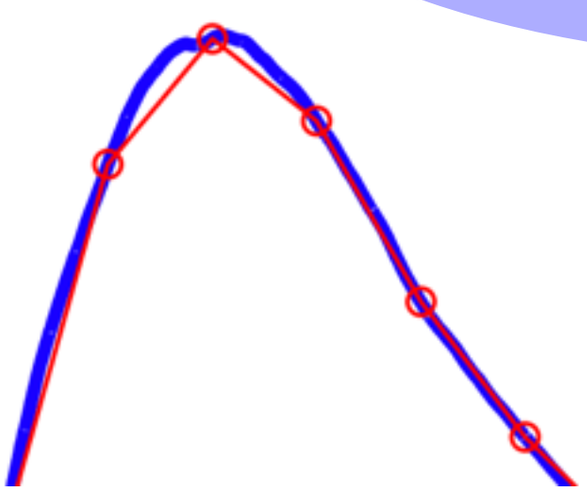
$$h_j(z_j) = \sum_{i=1}^{N} \alpha_i \min(x_{ij}, z_j)$$

$$= \sum_{i:x_{ij}<z_j}^{N} \alpha_i x_{ij} + \sum_{i:x_{ij}\geq z_j}^{N} \alpha_i z_j$$

~~$O(N)$~~

~~$O(\log N)$~~

$O(1)$



For many problems h_j is smooth (blue plot). Hence, we can *approximate* it with fewer uniformly spaced segments (red plot). This saves time and space!

Kernel classification function

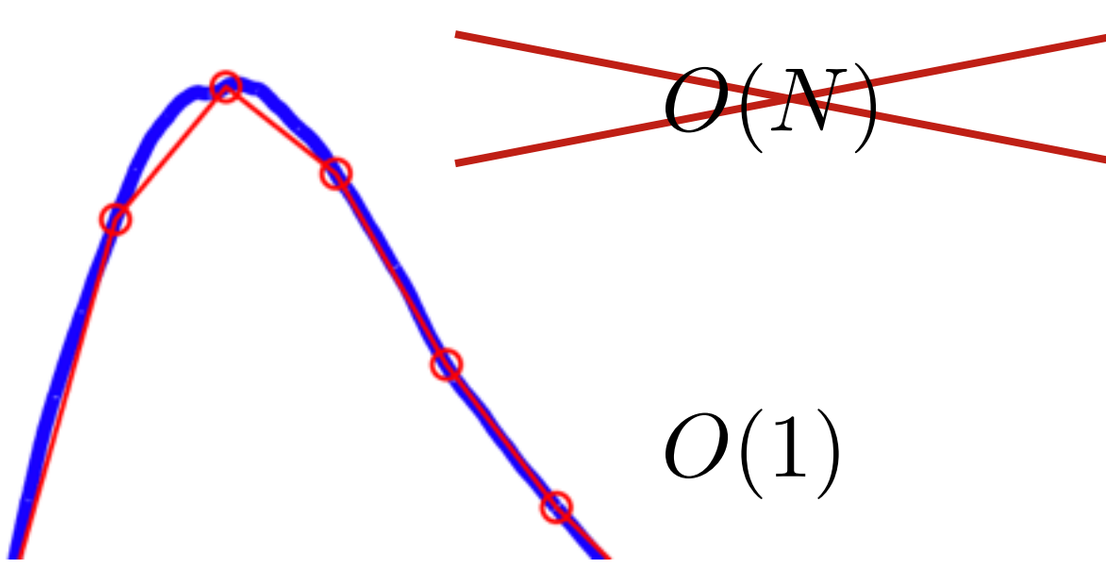
$$h(\mathbf{z}) = \sum_{i=1}^{N} \alpha_i K(\mathbf{x}_i, \mathbf{z}) = \sum_{i=1}^{N} \alpha_i \left(\sum_{j=1}^{D} \min(x_{ij}, z_j) \right)$$

[Maji et al. PAMI 13]

Algorithm 2

$$K(\mathbf{x}, \mathbf{z}) = \sum_{i=1}^{D} k_i(x_i, z_i)$$

additive kernels



Intersection $k(a, b) = \min(a, b)$

Chi-squared $k(a, b) = \dfrac{2ab}{a + b}$

Jensen-Shannon $k(a, b) = a \log \left(\dfrac{a + b}{a} \right) + b \log \left(\dfrac{a + b}{b} \right)$

Linear and intersection kernel SVM

Using histograms of oriented gradients feature:

Dataset	Measure	Linear SVM	IK SVM	Speedup
INRIA pedestrians	Recall@ 2 FPPI	78.9	86.6	2594 X
DC pedestrians	Accuracy	72.2	89.0	2253 X
Caltech101, 15 examples	Accuracy	38.8	50.1	37 X
Caltech101, 30 examples	Accuracy	44.3	56.6	62 X
MNIST digits	Error	1.44	0.77	2500 X
UIUC cars (Single Scale)	Precision@ EER	89.8	98.5	65 X

On average **more accurate** than linear and **100-1000x** faster than standard kernel classifier. Similar idea can be applied to training as well.

Research question: when can we approximate kernels efficiently?

Slides credit

- Some of the slides are based on CIML book by Hal Daume III
- Experiments on various datasets: “Efficient Classification for Additive Kernel SVMs”, S. Maji, A. C. Berg and J. Malik, PAMI, Jan 2013
- Some resources:
  - LIBSVM: kernel SVM classifier training and testing
    - ➡ http://www.csie.ntu.edu.tw/~cjlin/libsvm/
  - LIBLINEAR: fast linear classifier training
    - ➡ http://www.csie.ntu.edu.tw/~cjlin/liblinear/
  - LIBSPLINE: fast additive kernel training and testing
    - ➡ https://github.com/msubhransu/libspline