Lecture #4: Support Vector Machines

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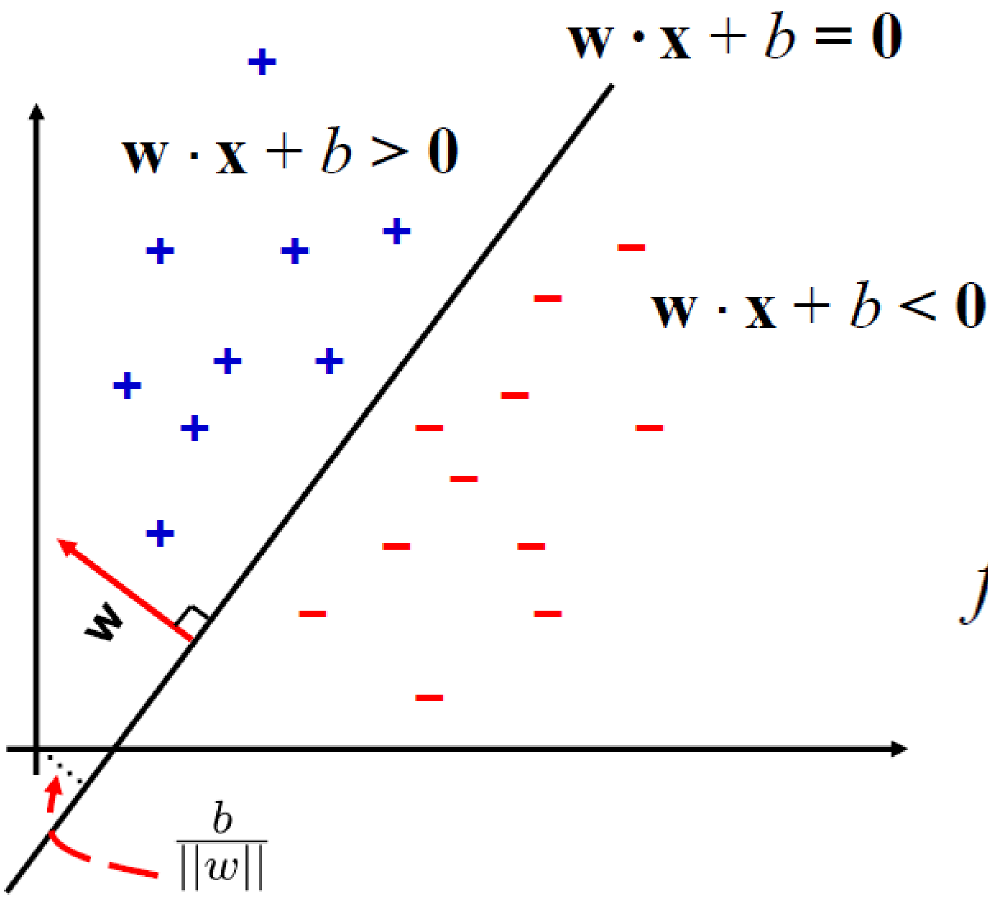
Perceptron Revisited: Linear Separator

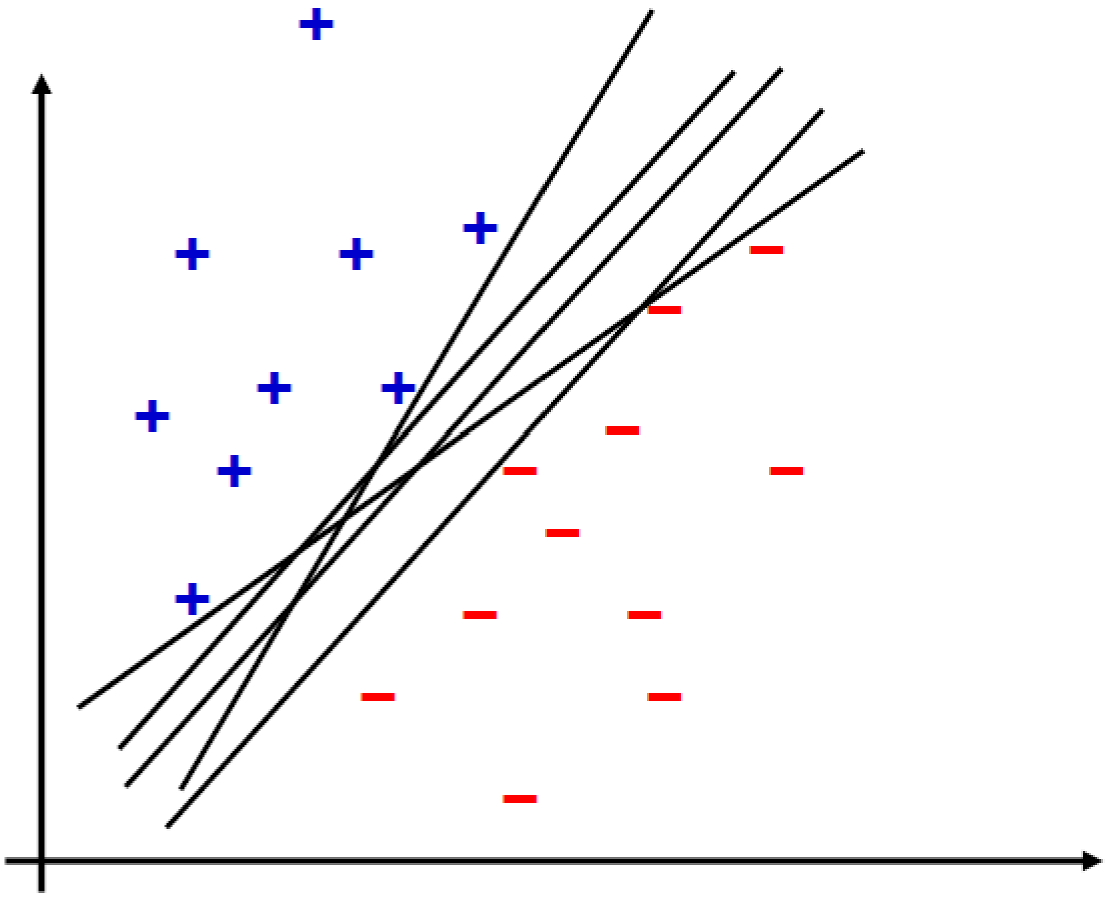
- Binary classification can be viewed as the task of separating classes in a given feature space



$$f(\mathbf{x}) = \text{sign}(\mathbf{w} \cdot \mathbf{x} + b)$$

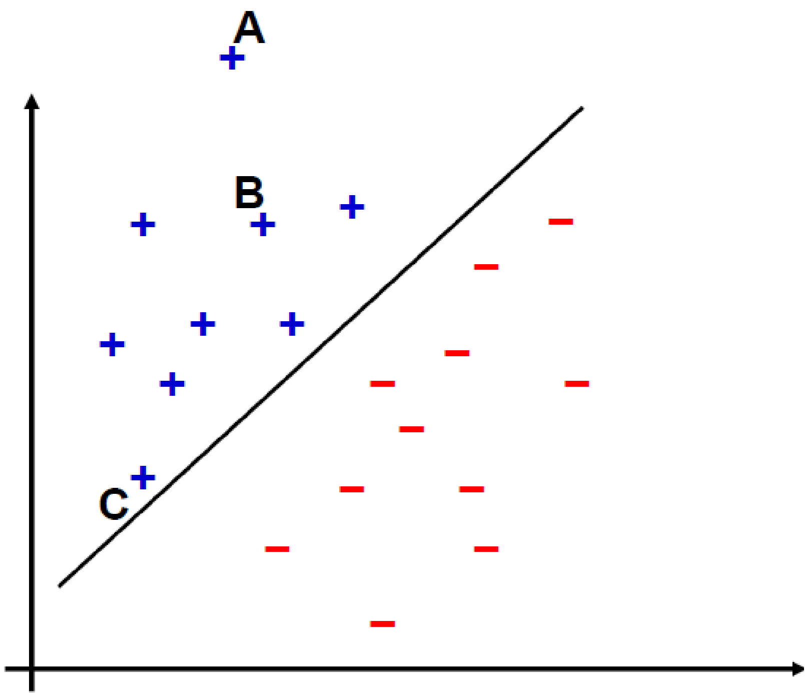
Linear Separators

- Which of the linear separators is optimal?



Intuition of Margin

- Consider points A, B, and C
- We are quite confident in our prediction for A because it is far from the decision boundary
- In contrast, we are not so confident in our prediction for C because a slight change in the decision boundary may flip the decision



Given a training set, we would like to make all predictions correct and confident! This leads to the concept of margin.

Functional Margin

- Given a linear classifier parameterized by $(\mathbf{w}, b)$, we define its functional margin w.r.t training example (x_i, y_i) as:

$$\gamma_i = y_i(w \cdot x_i + b)$$

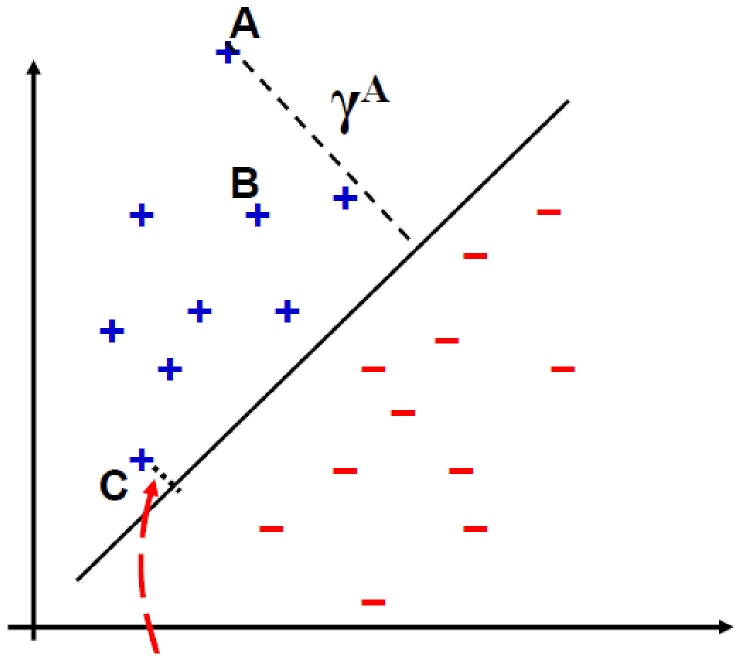
$\gamma_i > 0$ if the example is classified correctly

- If we rescale $(\mathbf{w}, b)$ by a factor α, functional margin gets multiplied by α
  - we can make it arbitrarily large without changing anything meaningful

Geometric Margin

- The geometric margin of $(\boldsymbol{w}, b)$ w.r.t. example (x_i, y_i) is the distance from x_i to the decision surface, which can be computed as:

$$\gamma_i = \frac{y_i(w \cdot x_i + b)}{\|w\|}$$



- Given a training set $S = (x_i, y_i): i = 1,2,..N$ the geometric margin of the classifier w.r.t. S is

$$\gamma = min_{i=1,2,..N} \quad \gamma_i$$

Maximum Margin Classifier

- Given a linearly separable training set $(x_i, y_i): i = 1,2, .. N$, we would like to find a linear classifier with maximum margin
- This can be represented as an optimization problem

$$\boxed{\begin{aligned}&\max_{\mathbf{w},b,\gamma} \gamma \\ &\text{subject to}: \ y^{(i)} \frac{(\mathbf{w}\cdot\mathbf{x}^{(i)}+b)}{\|\mathbf{w}\|} \geq \gamma, \quad i=1,\cdots,N\end{aligned}}$$

Maximum Margin Classifier

- Let $\gamma' = \gamma \|w\|$, we can rewrite the optimization problem as follows:

$$\max_{\mathbf{w},b,\gamma} \gamma$$

$$\text{subject to: } y^{(i)} \frac{(\mathbf{w} \cdot \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|} \geq \gamma, \quad i = 1, \cdots, N$$

$$\Downarrow$$

$$\max_{\mathbf{w},b,\gamma'} \frac{\gamma'}{\|\mathbf{w}\|}$$

$$\text{subject to: } y^{i}(\mathbf{w} \cdot \mathbf{x}^{i} + b) \geq \gamma', \quad i = 1, \cdots, N$$

Maximum Margin Classifier

- Note that rescaling w and b by $1/\gamma'$ will not change the classifier -- we can thus further reformulate the optimization problem

$$\max_{\mathbf{w},b} \frac{\gamma'}{\|\mathbf{w}\|}$$
$$\text{subject to}: \; y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq \gamma', \quad i = 1,\cdots,N$$

$$\Downarrow$$

$$\max_{\mathbf{w},b} \frac{1}{\|\mathbf{w}\|} \quad (\text{or equivalently } \min_{\mathbf{w},b} \|\mathbf{w}\|^2)$$
$$\text{subject to}: \; y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N$$

Maximum Margin Classifier

- Maximizing the geometric margin is equivalent to minimizing the magnitude of w subject to maintaining a functional margin of at least 1

$$\boxed{\begin{array}{l} \max\limits_{\mathbf{w},b} \dfrac{\gamma'}{\|\mathbf{w}\|} \\ \text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq \gamma', \quad i = 1,\cdots,N \end{array}}$$

$$\Downarrow$$

$$\boxed{\begin{array}{l} \max\limits_{\mathbf{w},b} \dfrac{1}{\|\mathbf{w}\|} \ \left(\text{or equivalently } \min\limits_{\mathbf{w},b} \|\mathbf{w}\|^2\right) \\ \text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N \end{array}}$$

Maximum Margin Classifier: Formulation

$$\boxed{\begin{array}{l} \min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 \\ \text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N \end{array}}$$

- This results in a **quadratic optimization (QP) problem** with linear inequality constraints
- This is a well-known class of mathematical programming problems for which several (non-trivial) algorithms exist
  - One could solve for w using any of these methods

Maximum Margin Classifier: Formulation

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N$$

- We will see that it is useful to first formulate an equivalent dual optimization problem and solve it instead
  - This requires a bit of machinery!

Aside: Constrained Optimization

- Suppose we want to: minimize $f(x)$ subject to constraints $g_i(x) \leq 0, i = 1, \ldots, m$
  - $min_x\, f(x) \quad subject\ to \quad g_i(x) \leq 0, i = 1, \ldots, m$
- Consider the following function known as the lagrangian

$$\mathcal{L}(x, \alpha) = f(\mathbf{x}) + \sum_i \alpha_i g_i(\mathbf{x})$$

- Under certain conditions it can be shown that for a solution x' to the above problem we have

$$f(x') = \underbrace{\min_x \max_\alpha \mathcal{L}(x, \alpha)}_{\text{Primal form}} = \underbrace{\max_\alpha \min_x \mathcal{L}(x, \alpha)}_{\text{Dual form}}$$

subject to $\alpha_i \geq 0$

Back to the Original Problem

$$\text{Minimize } \frac{1}{2}||\mathbf{w}||^2$$

$$\text{subject to } 1 - y_i(\mathbf{w}^T\mathbf{x}_i + b) \le 0 \qquad \text{for } i = 1, \ldots, N$$

- The lagrangian is

$$\mathcal{L}(w, b, \alpha) = \frac{1}{2}\mathbf{w}^T\mathbf{w} + \sum_{i=1}^{n} \alpha_i \left(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)\right)$$

- We want to solve

$$\max_{\alpha} \min_{w,b} \mathcal{L}(w, b, \alpha) \quad s.t. \quad \alpha_i \ge 0$$

Back to the Original Problem

- We want to solve

$$\max_{\alpha} \min_{w,b} \mathcal{L}(w, b, \alpha) \quad s.t. \quad \alpha_i \geq 0$$

- Setting the gradient w.r.t w and b to zero, we get

$$\mathbf{w} + \sum_{i=1}^{n} \alpha_i(-y_i)\mathbf{x}_i = \mathbf{0} \quad \Rightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

Back to the Original Problem

- Substitute w in lagrangian

$$
\begin{aligned}
\mathcal{L} &= \frac{1}{2}\sum_{i=1}^{n}\alpha_i y_i \mathbf{x}_i^T \sum_{j=1}^{n}\alpha_j y_j \mathbf{x}_j + \sum_{i=1}^{n}\alpha_i\left(1 - y_i(\sum_{j=1}^{n}\alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i + b)\right) \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n}\alpha_i - \sum_{i=1}^{n}\alpha_i y_i \sum_{j=1}^{n}\alpha_j y_j \mathbf{x}_j^T \mathbf{x}_i - b\sum_{i=1}^{n}\alpha_i y_i \\
&= -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j + \sum_{i=1}^{n}\alpha_i
\end{aligned}
$$

- This is a function of $\alpha's$ only!

Dual Problem

- The new objective function is a function of $\alpha's$ only
- It is known as the dual problem
  - If we know all the $\alpha's$, we know the weights w
- The original problem is known as the primal problem
- The objective function of the dual problem needs to be maximized!

Dual Problem

- The objective function of the dual problem needs to be maximized!
- Therefore, the dual problem is:

$$\max_{\alpha} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } \alpha_i \geq 0, \qquad \sum_{i=1}^{n} \alpha_i y_i = 0$$

Properties of α_i when we introduce the Lagrange multipliers

The result when we differentiate the original Lagrangian w.r.t. b

Dual Problem

$$\max_{\alpha} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1,j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

$$\text{subject to } \alpha_i \geq 0, \qquad \sum_{i=1}^{n} \alpha_i y_i = 0$$

- This is also a QP problem
  - A global maxima of $\alpha's$ can always be found
- Weights w can be recovered by $$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$
- b can also be recovered (we will skip the details)

Characteristics of Solution

- Many of the $\alpha's$ are zero
  - Weights w is a linear combination of small number of data points
- x_i with non-zero α_i are called support vectors (SVs)
  - The decision boundary is determined only by the SVs
  - Let $t_j (j = 1,2, \ldots, s)$ be the indices of the s support vectors. We can write

$$\mathbf{w} = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} \mathbf{x}_{t_j}$$

Characteristics of Solution

- For classifying a new input example z, compute

$$\mathbf{w}^T\mathbf{z} + b = \sum_{j=1}^{s} \alpha_{t_j} y_{t_j} (\mathbf{x}_{t_j}^T \mathbf{z}) + b$$

  - Classify z as positive if the sum is positive, and negative otherwise
  - Note: w need not be formed explicitly, rather we can classify z by taking inner products with the support vectors (useful when we generalize the notion of inner product later)

The Quadratic Programming Problem

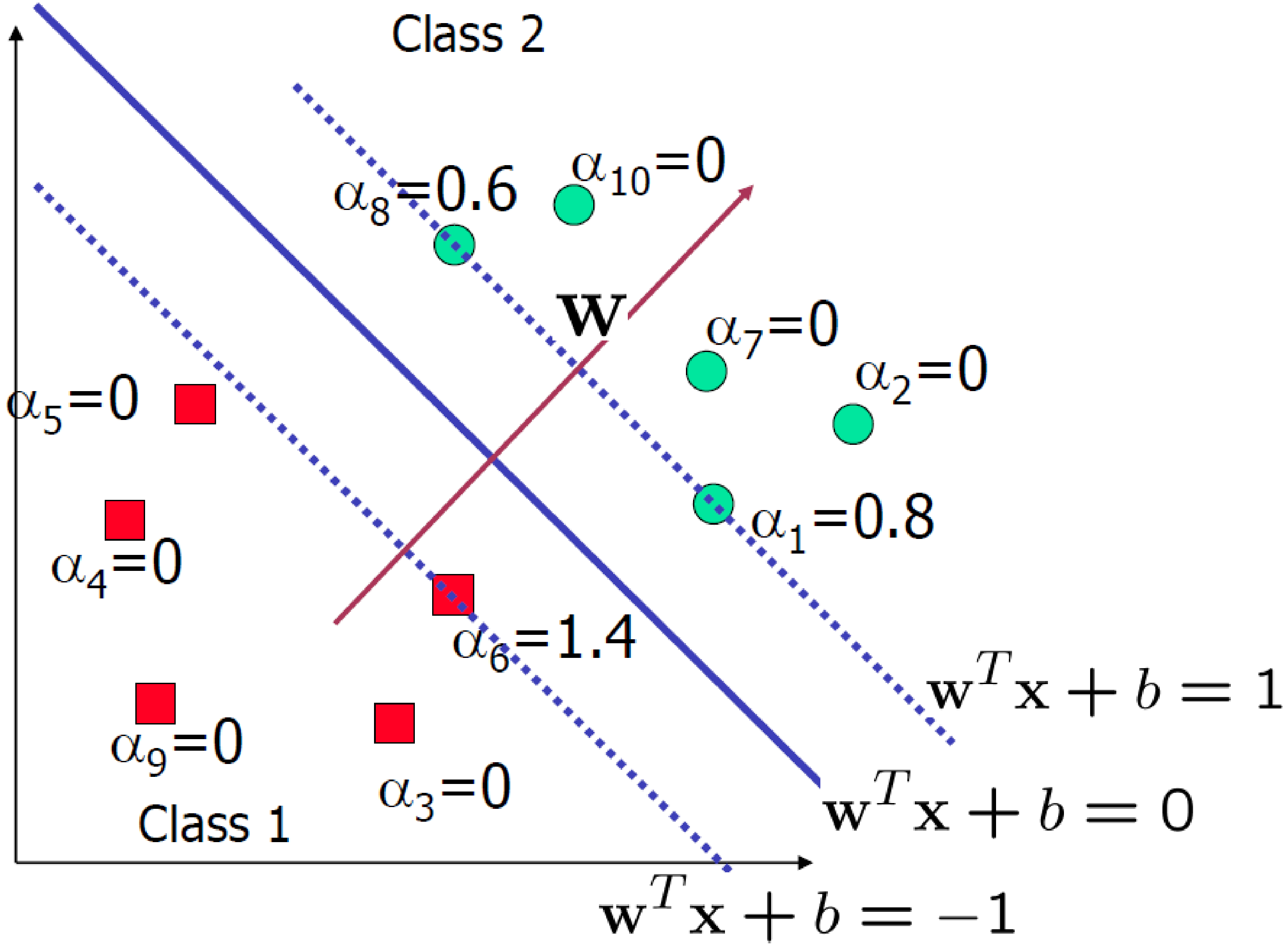
- Many approaches have been proposed
  - Loqo, cplex, etc. (see http://www.numerical.rl.ac.uk/qp/qp.html)
- Most are “interior-point” methods
  - Start with an initial solution that can violate the constraints
  - Improve this solution by optimizing the objective function and/or reducing the amount of constraint violation
- For SVM, sequential minimal optimization (SMO) seems to be the most popular

The Quadratic Programming Problem

- **SMO algorithm**
  - A QP with two variables is trivial to solve
  - Each iteration of SMO picks a pair of (α_i, α_j) and solve the QP with these two variables
  - repeat until convergence

- In practice, we can just regard the QP solver as a "black-box" without bothering how it works

A Geometric Interpretation

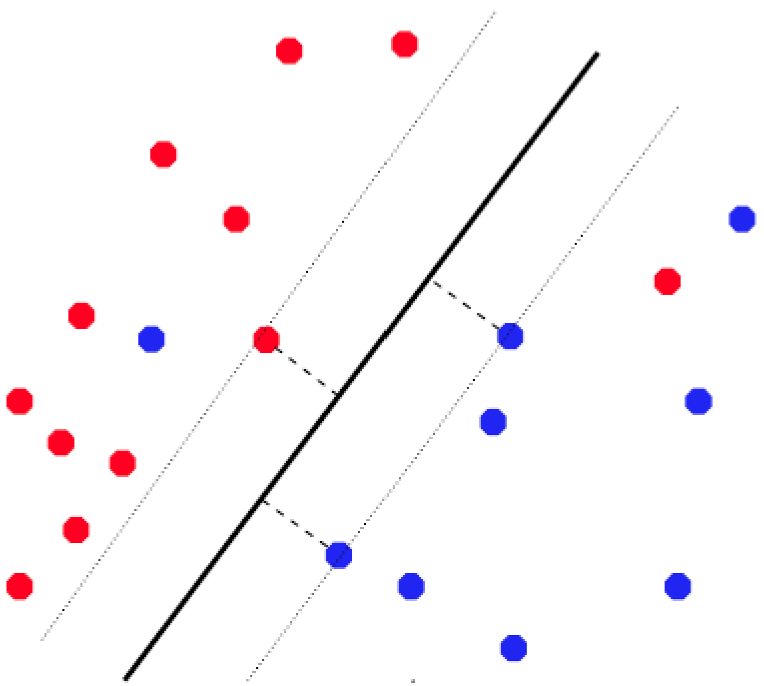


Summary so far

- We demonstrated that we prefer to have linear classifiers with large margin
- We formulated the problem of finding the maximum margin linear classifier as a quadratic optimization problem
- This problem can be solved by solving its dual problem, and efficient QP algorithms are available
- Problem Solved?

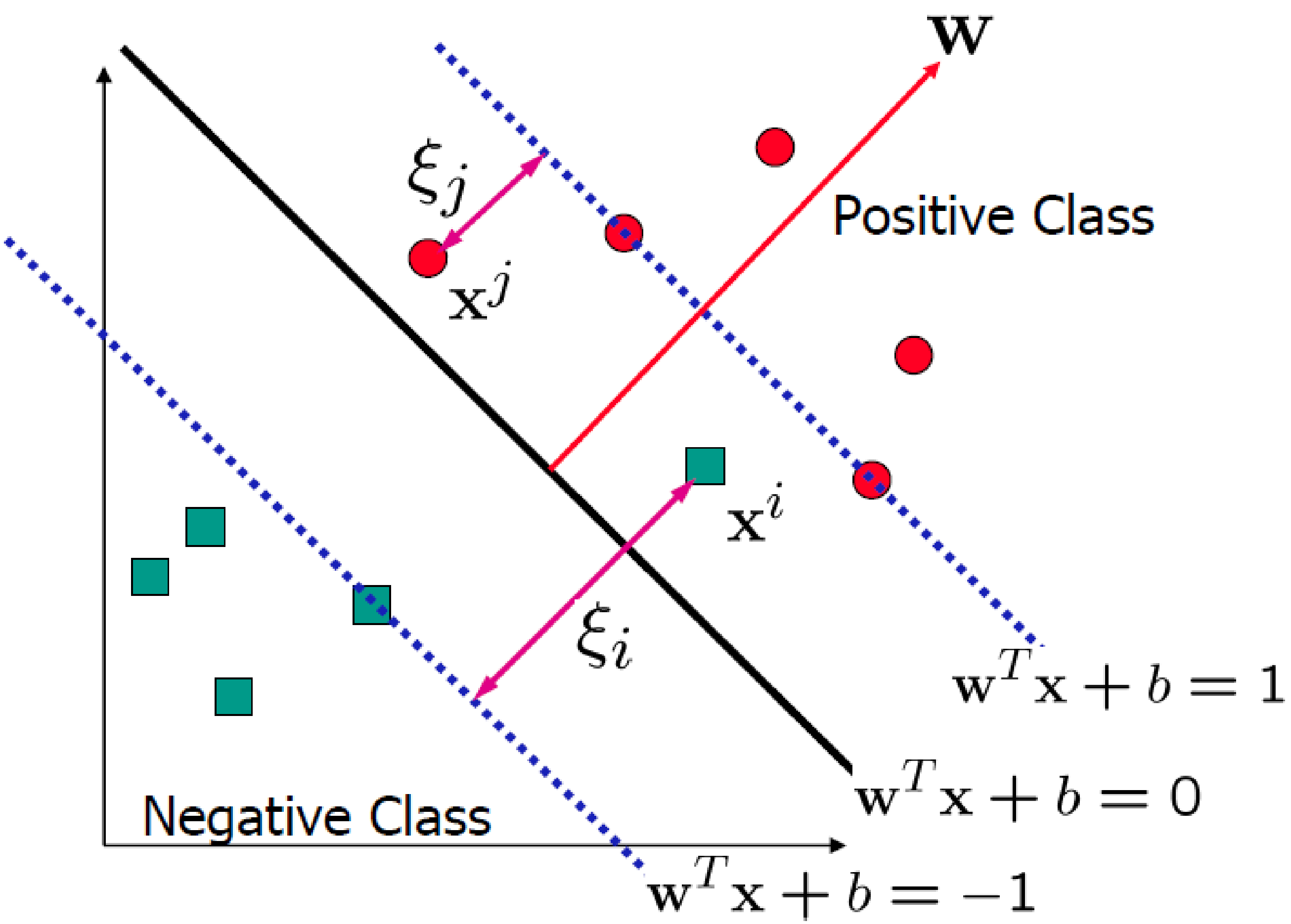
Non-Separable data and Noise

- What if the data is not linearly separable?
- We may have noise in data, and maximum margin classifier is not robust to noise!



Hard Margin → Soft Margin

- Allow functional margins to be less than 1
  - But we will charge a penalty



Soft Margin Maximization

Hard margin

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1, \quad i = 1,\cdots,N$$

$$\Downarrow$$

Soft margin

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 + c\sum_{i=1}^{N}\xi_i$$

$$\text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1 - \xi_i, \quad i = 1,\cdots,N$$

$$\xi_i \geq 0, \quad i = 1,\cdots,N$$

- Introduce slack variables ξ_i to allow functional margins to be smaller than 1

Soft Margin Maximization

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 + c\sum_{i=1}^{N}\xi_i$$

$$\text{subject to: } y^i(\mathbf{w}\cdot\mathbf{x}^i + b) \geq 1 - \xi_i, \quad i = 1, \cdots, N$$

$$\xi_i \geq 0, \quad i = 1, \cdots, N$$

- Parameter C controls the tradeoff between maximizing the margin (generalization error) and fitting the training examples (training error)

Dual Formulation of Soft Margin

$$max \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y^i y^j < \mathbf{x}^i \cdot \mathbf{x}^j >$$

Subject to: $\sum_{i=1}^{N} \alpha_i y^i = 0$

$0 \leq \alpha_i \leq c \qquad i=1, \ldots, N$

- The dual problem is almost identical to the separable case, except for that α_i's are now bounded by C (tradeoff parameter)
- C puts a box constraint on α_i's, the weights of the support vectors
- Limits the influence of outliers

Dual Formulation of Soft Margin

support vectors (α_i>0)

$c > \alpha_i > 0$:	$y^i(w \cdot x^i + b) = 1$, i.e., $\xi_i = 0$
$\alpha_i = c$:	$y^i(w \cdot x^i + b) \leq 1$, i.e., $\xi_i \geq 0$

- We now also have support vectors for data that have functional margin less than one (in addition to those that equal 1), but their α_i's will only equal C
- Optimal weights can be computed as:

$$\mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

Linear SVMs: Overview

- So far our classifier is a *separating hyperplane*
- Most “important” training points are support vectors; they define the hyperplane
- Quadratic optimization algorithms can identify which training points x_i are support vectors with non-zero Lagrange multipliers α_i

Summary of Last Lecture

- Hard-Margin SVMs for linearly separable data
  - Characteristics of the dual solution
  - Weight vector is determined by a small no. of training examples called Support Vectors
- Soft-Margin SVMs
  - To deal with non-separable and noisy data
  - Relax the margin requirement by introducing slack variables
  - C parameter trades-off the training error (sum of slacks) and the generalization error (margin)

Linear SVMs: Overview

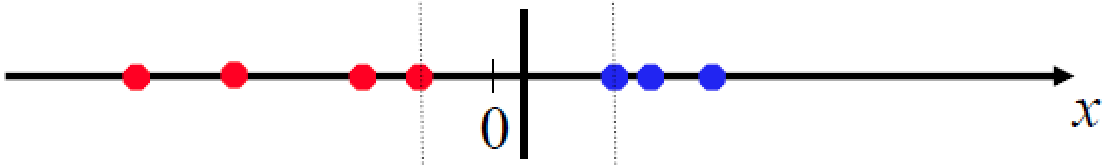
- For both training and classification, we see training data appear only inside inner products

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y^i y^j \boxed{<\mathbf{x}^i \cdot \mathbf{x}^j>}$ is maximized
and
(1) $\Sigma\alpha_i y^i = 0$
(2) $0 \leq \alpha_i \leq c$ for all α_i

$$f(\mathbf{x}) = \Sigma\alpha_i y^i \boxed{<\mathbf{x}^i \cdot \mathbf{x}>} + b$$

Non-Linear SVMs

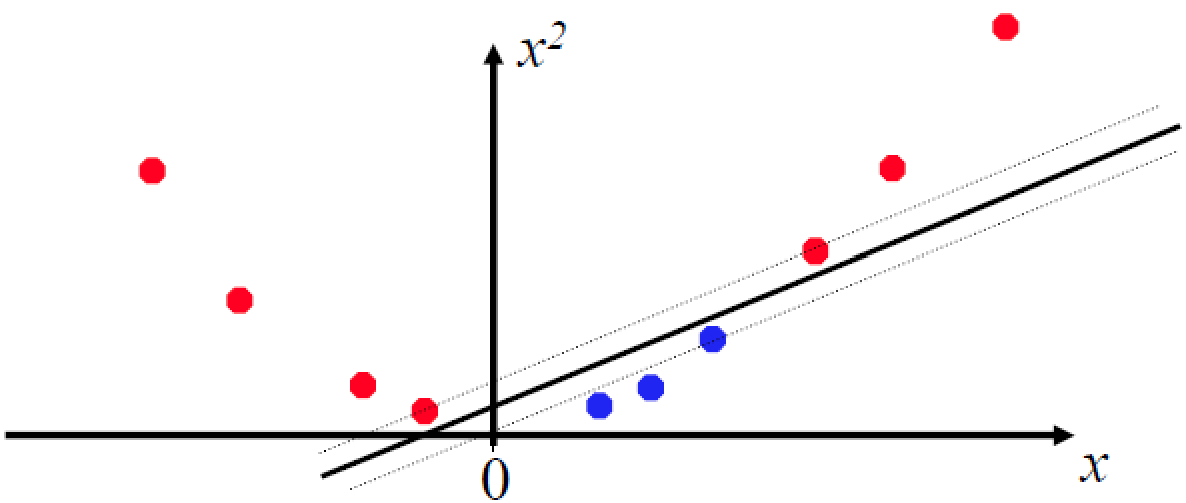
- Datasets that are linearly separable with some noise work out great



- But what are we going to do if the dataset is just too hard?

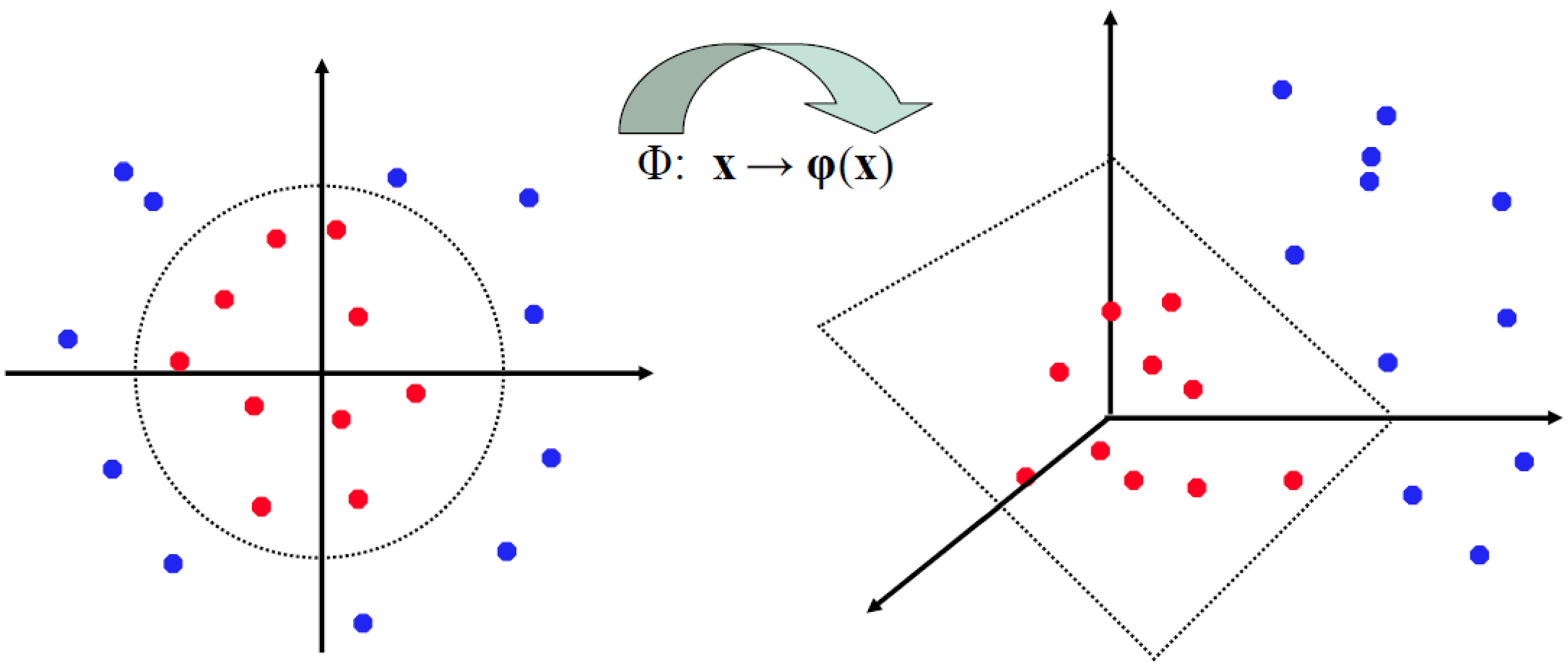
Non-Linear SVMs

- How about mapping the data to a higher dimensional space?



Non-Linear SVMs: Feature Spaces

- **General idea**
  - For <u>any</u> data set, the original feature space can always be mapped to some higher-dimensional feature space such that the data is linearly separable



Example: Quadratic Space

- Assume m input dimensions
  - $x = (x_1, x_2, \ldots, x_m)$
- The number of dimensions increase rapidly
  - Expensive to compute!
- You may be wondering about the $\sqrt{2}'s$
  - You will find out soon!

$$\Phi(\mathbf{x}) = \begin{pmatrix} \left.1\right\} \text{Constant Term} \\ \left.\begin{matrix} \sqrt{2}x_1 \\ \sqrt{2}x_2 \\ \vdots \\ \sqrt{2}x_m \end{matrix}\right\} \text{Linear Terms} \\ \left.\begin{matrix} x_1^2 \\ x_2^2 \\ \vdots \\ x_m^2 \end{matrix}\right\} \text{Pure Quadratic Terms} \\ \left.\begin{matrix} \sqrt{2}x_1x_2 \\ \sqrt{2}x_1x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \sqrt{2}x_2x_3 \\ \vdots \\ \sqrt{2}x_1x_m \\ \vdots \\ \sqrt{2}x_{m-1}x_m \end{matrix}\right\} \text{Quadratic Cross-Terms} \end{pmatrix}$$

Kernel Functions

- The linear classifier relies on inner product between vectors: $K(x_i, x_j) = \langle x_i . x_j \rangle$
- If every data point is mapped into high-dimensional space via some transformation $\Phi: x \rightarrow \phi(x)$, the inner product becomes $K(x_i, x_j) = \langle \phi(x_i) . \phi(x_j) \rangle$
- A ***kernel function*** is a function that is equivalent to an inner product in some feature space
  - Example: $K(x_i, x_j) = (x_i . x_j + 1)^2$
  - This is equivalent to mapping to the quadratic space!

Quadratic Kernel

- Consider a 2-d input space (generalizes to n-d)

$$
\begin{aligned}
K(\mathbf{x}^i, \mathbf{x}^j) &= (\mathbf{x}^i \cdot \mathbf{x}^j + 1)^2 \\
&= (x_1^i x_1^j + x_2^i x_2^j + 1)^2 \\
&= {x_1^i}^2 {x_1^j}^2 + 2 x_1^i x_2^i x_1^j x_2^j + {x_2^i}^2 {x_2^j}^2 + 2 x_1^i x_1^j + 2 x_2^i x_2^j + 1 \\
&= ({x_1^i}^2, \sqrt{2}\, x_1^i x_2^i,\ {x_2^i}^2, \sqrt{2}\, x_1^i, \sqrt{2}\, x_2^i, 1) \cdot \\
&\quad\ ({x_1^j}^2, \sqrt{2}\, x_1^j x_2^j,\ {x_2^j}^2, \sqrt{2}\, x_1^j, \sqrt{2}\, x_2^j, 1) \\
&= \Phi(\mathbf{x}^i) \cdot \Phi(\mathbf{x}^j)
\end{aligned}
$$

nonlinear mapping of $\mathbf{x}^i$ and $\mathbf{x}^j$ to quadratic space

- A kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\phi(x)$ explicitly)

Quadratic Kernel

- A kernel function *implicitly* maps data to a high-dimensional space (without the need to compute each $\phi(x)$ explicitly)

- Computing inner product of quadratic features is $O(m^2)$ time vs. $O(m)$ time for kernel

Non-Linear SVMs

- Dual problem formulation

$$\begin{array}{l}\text{Find } \alpha_1 \ldots \alpha_N \text{ such that} \\ \Sigma\alpha_i - \tfrac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y^i y^j \langle \mathbf{x}^i \cdot \mathbf{x}^j \rangle \text{ is maximized and} \\ (1)\ \ \Sigma\alpha_i y^i = 0 \\ (2)\ \ 0 \leq \alpha_i \leq c \text{ for all } \alpha_i \end{array}$$

$K(\mathbf{x}^i,\mathbf{x}^j)$

- To classify a new point, we compute

$$f(\mathbf{x}) = \Sigma\alpha_i y^i \langle \mathbf{x}^i, \mathbf{x}^j \rangle + b$$

$K(\mathbf{x}^i,\mathbf{x}^j)$

- Optimization techniques to find α_i's remain the same
- This shows the utility of the dual formulation

Kernel Functions

- In practice, the user specifies the kernel function *K*, without explicitly stating the transformation $\phi(\cdot)$
- Given a kernel function, finding its corresponding transformation can be very cumbersome
  - This is why people only specify the kernel function without worrying about the exact transformation
- **Another view:** a kernel function computes some kind of measure of similarity between objects
- If you have a reasonable measure of similarity for your application, can we use it as the kernel in an SVM?

What functions are Kernels?

- Consider some finite set of *m* points, let matrix K be defined as follows

K=

$K(\mathbf{x}^1,\mathbf{x}^1)$	$K(\mathbf{x}^1,\mathbf{x}^2)$	$K(\mathbf{x}^1,\mathbf{x}^3)$	…	$K(\mathbf{x}^1,\mathbf{x}^m)$
$K(\mathbf{x}^2,\mathbf{x}^1)$	$K(\mathbf{x}^2,\mathbf{x}^2)$	$K(\mathbf{x}^2,\mathbf{x}^3)$		$K(\mathbf{x}^2,\mathbf{x}^m)$
…	…	…	…	…
$K(\mathbf{x}^m,\mathbf{x}^1)$	$K(\mathbf{x}^m,\mathbf{x}^2)$	$K(\mathbf{x}^m,\mathbf{x}^3)$	…	$K(\mathbf{x}^m,\mathbf{x}^m)$

- This is called **Kernel Matrix**
- Mercer's Theorem:
  - A function K is a kernel function if and only if its corresponding kernel matrix is symmetric and positive semi-definite

Examples of Kernel Functions

- Linear: $K(x_i, x_j) = \langle x_i . x_j \rangle$
  - Mapping: $\Phi: x \rightarrow \phi(x)$, such that $\phi(x) = x$
- Polynomial of power p: $K(x_i, x_j) = (1 + x_i . x_j)^p$
  - Mapping: $\Phi: x \rightarrow \phi(x)$, where $\phi(x)$ has $(d + p)\ Choose\ p$ dimensions
- Gaussian (Radial Basis Function): $K(x_i, x_j) = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}}$
  - Mapping: $\Phi: x \rightarrow \phi(x)$, where $\phi(x)$ has infinite dimensions; every point is mapped to a function (Gaussian)

Examples of Kernel Functions

- Gaussian (Radial Basis Function): $K(x_i, x_j) = e^{-\frac{\|x_i - x_j\|^2}{2\sigma^2}}$
  - Mapping: $\Phi: x \rightarrow \phi(x)$, where $\phi(x)$ has infinite dimensions; every point is mapped to a function (Gaussian)
  - RBF kernel values decreases with distance and ranges between zero (in the limit) and one ($x_i = x_j$)
- String Kernels
  - No. of common substrings of length k
- Graph Kernels
- Time-Series Kernels

Properties of Kernels

- Not all functions $K(x_i, x_j)$ are kernels!
- Conditions for a function to be a kernel
  - **Symmetry**: $\forall\ x_i, x_j$; $K(x_i, x_j) = K(x_j, x_i)$
  - **Positivity:** for a set of m points $x_1, x_2, \ldots, x_m$; define the kernel matrix as $K_{ij} = K(x_i, x_j)$. For all m data points and all $m \times 1$ vectors t, $t^T K t \geq 0$
- These are necessary and sufficient conditions

Properties of Kernels

- How to show that a function $K(x_i, x_j)$ is a kernel?
  - Either find the feature map $\Phi: x \rightarrow \phi(x)$ such that $K(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle$ OR
  - Show that symmetry and positivity conditions hold
- How to show that a function $K(x_i, x_j)$ is not a kernel?
  - Show a counter-example for symmetry or positivity conditions

Multi-Class SVMs

- **One-vs-One Reduction**
  - Learn ${}^{k(k-1)}/_{2}$ binary classifiers
  - Classify a new example via majority vote
- **One-vs-All Reduction**
  - K weight vectors (Rep-I)
  - Single weight vector (Rep-II)

Multi-class Classification

- **Single prototype**

$$\begin{array}{ccccc} & w_1 & w_2 & w_3 & & w_K \\ W = & [\quad\quad] & [\quad\quad] & [\quad\quad] & \dots & [\quad\quad] \end{array}$$

  - $K * D$ parameters

- $\varphi(x,y) = (\llbracket y = 1 \rrbracket x,\ \llbracket y = 2 \rrbracket x, \cdots, \llbracket y = k \rrbracket x)$

  - $\varphi(x,2)$

$$[\quad 0 \quad][\quad x \quad][\quad 0 \quad] \dots [\quad 0 \quad]$$

Multi-Class SVM

- Multi-class SVM [Crammer and Singer 2001]

$$min_w \quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\delta_i$$

$$s.t: \quad w\cdot\varphi(x_i, y_i) - w\cdot\varphi(x_i, y\ ) \geq 1 - \delta_i$$

$$\forall y \in Y\backslash\{y_i\}, \forall i = 1, \cdots, n$$

Critical Steps for using SVM

- Select the kernel function to use (important but often trickiest part of SVM).
- In practice, try the following in the same order
  - linear kernel
  - low degree polynomial kernel
  - RBF kernel with a reasonable width σ
  - Supported by off-the-shelf software (e.g., LibSVM or SVM-Light)
-

Critical Steps for using SVM

- Select the value of tradeoff parameter C and the parameter of the kernel function
  - Try the values suggested by the SVM software
  - $C = \{0.0001, 0.001, 0.01, 0.1, 1, 10, 100, 1000, 10000\}$
  - You can set apart a validation set to determine the values of the parameter

- SVM Software
  - LibSVM -- http://www.csie.ntu.edu.tw/~cjlin/libsvm/
  - SVM-Light -- http://www.cs.cornell.edu/people/tj/svm_light/svm_multiclass.html

SVMs Summary

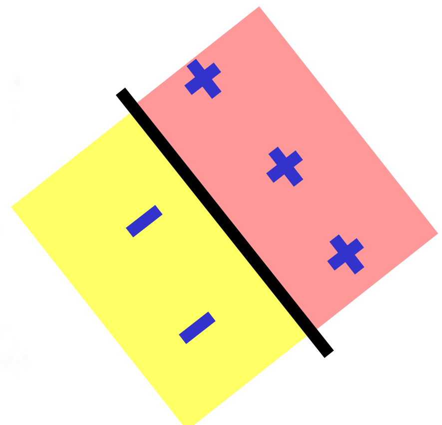
- Advantages of SVMs
  - Polynomial time exact optimization
  - Kernels allow very flexible hypotheses (decision boundaries)
  - Can be applied to very complex data types, e.g., sequences, graphs
- Disadvantages of SVMs
  - Must choose a good kernel and kernel parameters
  - Scalability issues with very-large data sets
    - Recent work has made this much less an issue
    - Stream SVM: http://www.ibis.t.u-tokyo.ac.jp/masin/streamsvm.html
    - SVM-Perf: http://www.cs.cornell.edu/people/tj/svm_light/svm_perf.html

Summary of Last Lecture

- Non-Linear SVMs and Kernels
  - Any data can be transformed into a higher-dimensional space (via mapping $\phi(x)$) to make it linearly separable
  - A Kernel function implicitly maps data to a high-dimensional space (without the need to compute the mapping $\phi(x)$ explicitly)
- Example Kernels: linear, polynomial, and RBF
- Necessary and Sufficient conditions for Kernel functions
- Multi-Class SVM: *one vs. one* and *one vs. all*
- Criticial steps for using SVM

PEGASOS

Primal Efficient sub-GrAdient SOlver for SVM



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Support Vector Machines

QP form:

$$\operatorname*{argmin}_{\mathbf{w},\xi_i\geq 0} \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{m}\xi_i$$

$$\text{s.t.} \quad \forall i,\ y_i\langle \mathbf{w},\mathbf{x}_i\rangle \geq 1-\xi_i$$

More "natural" form:

$$\operatorname*{argmin}_{\mathbf{w}} f(\mathbf{w}) \qquad \text{where:}$$

$$f(\mathbf{w}) \stackrel{\text{def}}{=} \underbrace{\frac{\lambda}{2}\|\mathbf{w}\|^2}_{\text{Regularization term}} + \underbrace{\frac{1}{m}\sum_{i=1}^{m}\max\{0, 1-y_i\langle \mathbf{w},\mathbf{x}_i\rangle\}}_{\text{Empirical loss}}$$

Previous Work

- Dual-based methods
  - Interior Point methods
    - Memory: m^2, time: $m^3 \log(\log(1/\varepsilon))$
  - Decomposition methods
    - Memory: m, Time: super-linear in m
- Online learning & Stochastic Gradient
  - Memory: O(1), Time: $1/\varepsilon^2$ (linear kernel)
  - Memory: $1/\varepsilon^2$, Time: $1/\varepsilon^4$ (non-linear kernel)

  Typically, online learning algorithms do not converge to the optimal solution of SVM

PEGASOS

A_t = S

Subgradient method

|A_t| = 1

Stochastic gradient

...t S = ...

...ation...

Number of iterations T

INITIALIZE: Choose $\mathbf{w}_1$ s.t. $\|\mathbf{w}_1\| \leq 1/\sqrt{\lambda}$

FOR $t = 1, 2, \ldots, T$

Subgradient

Choose $A_t \subseteq S$

$A_t^+ = \{(\mathbf{x}, y) \in A_t : y\langle \mathbf{w}_t, \mathbf{x}\rangle < 1\}$

$\nabla_t = \lambda \mathbf{w}_t - \frac{\eta_t}{|A_t|} \sum_{(\mathbf{x},y)\in A_t^+} y\,\mathbf{x}$

$\eta_t = \frac{1}{t\,\lambda}$

$\mathbf{w}_t' = \mathbf{w}_t - \eta_t \nabla_t$

Projection $\Leftarrow$ $\mathbf{w}_{t+1} = \min\left\{1, \frac{1/\sqrt{\lambda}}{\|\mathbf{w}_t'\|}\right\} \mathbf{w}_t'$

OUTPUT: $\mathbf{w}_{T+1}$

Run-Time of Pegasos

- Choosing $|A_t|=1$ and a linear kernel over R^n

  ➔ Run-time required for Pegasos to find ε accurate solution w.p. ¸ 1-δ

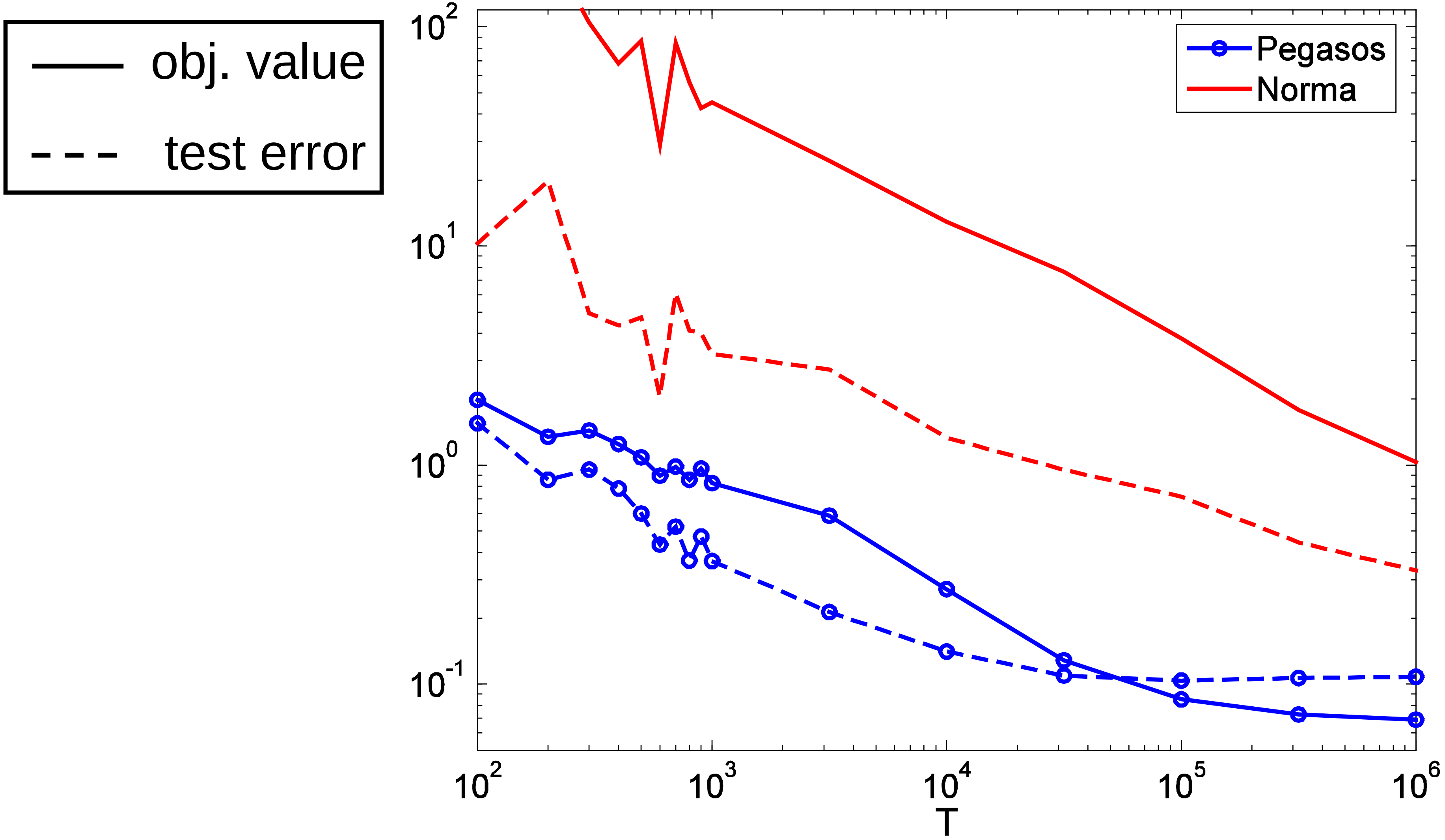
  $$\tilde{O}\left(\frac{d}{\lambda\epsilon\delta}\right)$$, where d is the sparsity bound

- Run-time does not depend on #examples
- Depends on “difficulty” of problem (λ and ε)

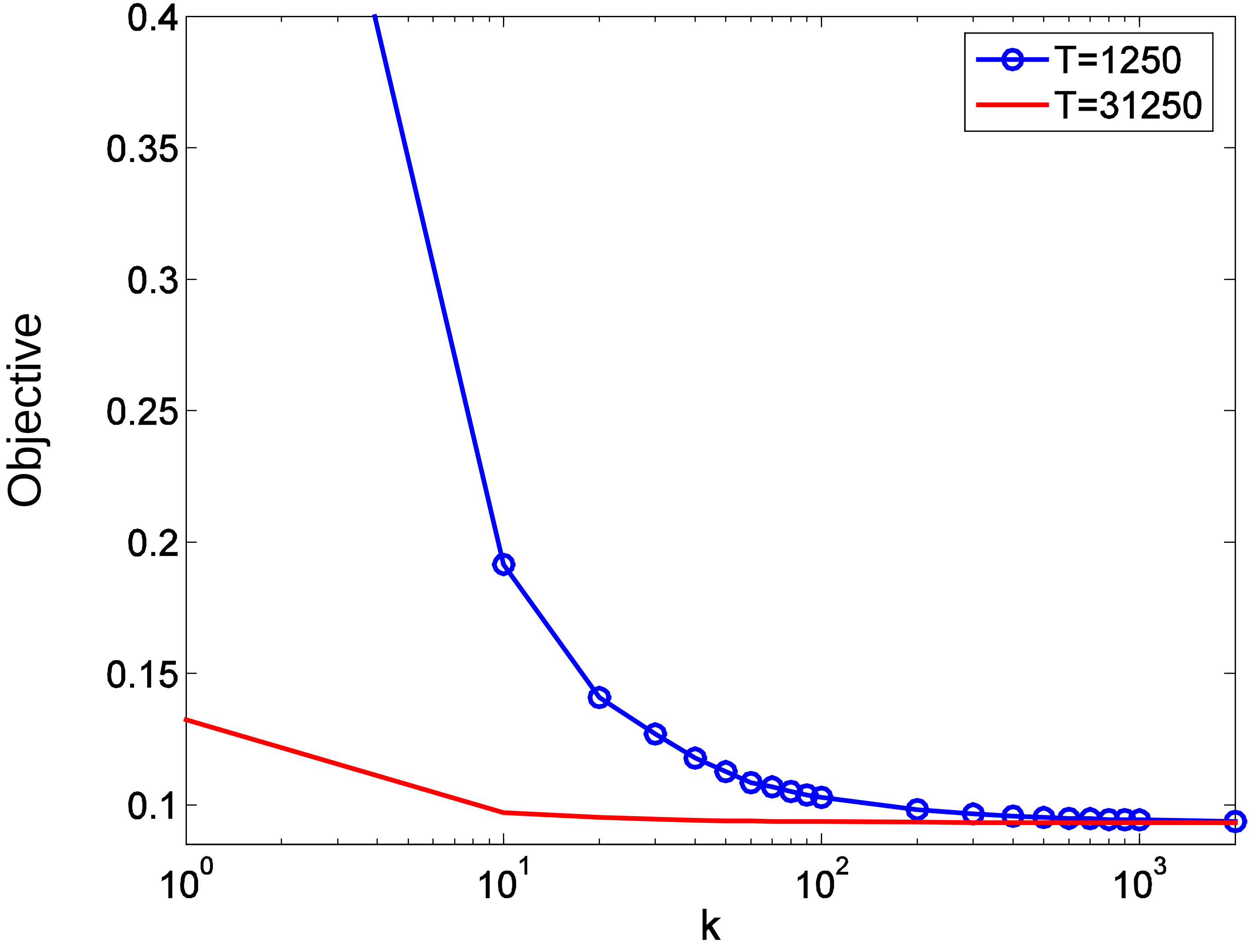
Training Time (in seconds)

	Pegasos	SVM-Perf	SVM-Light
Reuters	**2**	77	20,075
Covertype	**6**	85	25,514
Astro-Physics	**2**	5	80

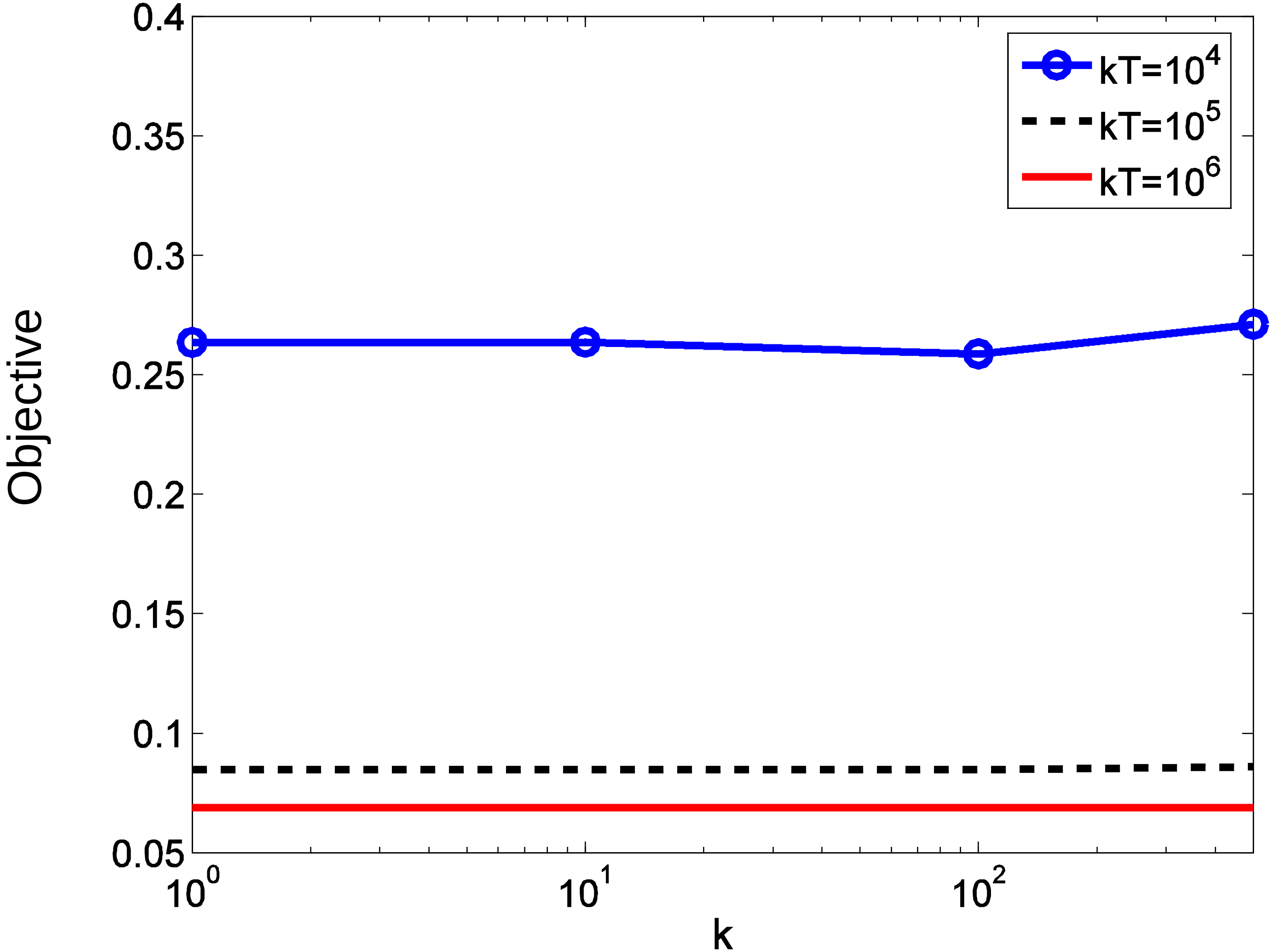
Compare to Norma (on Physics)



Effect of k=$|A_t|$ when T is fixed



Effect of $k=|A_t|$ when kT is fixed



Discussion

- Pegasos: Simple & Efficient solver for SVM
- Sample vs. computational complexity
  - Sample complexity: How many examples do we need as a function of VC-dim (λ), accuracy (ε), and confidence (δ)
  - In Pegasos, we aim at analyzing computational complexity based on λ, ε, and δ (also in Bottou & Bousquet)

Kernelizing Online Learning Algorithms

initialize $f = 0$ **Functional Form**

repeat

Pick (x_i, y_i) from data

if $y_i f(x_i) \leq 0$ then

$f(\cdot) \leftarrow f(\cdot) + y_i k(x_i, \cdot)$

until $y_i f(x_i) > 0$ for all i

- Nothing happens if classified correctly
- Weight vector is a linear combination $w = \sum_{i \in I} \alpha_i \phi(x_i)$
- Classifier is a linear combination of inner products

$$f(x) = \sum_{i \in I} \alpha_i \langle \phi(x_i), \phi(x) \rangle = \sum_{i \in I} \alpha_i k(x_i, x)$$

Kernelized Perceptron

Primal Form

update weights

$$w \leftarrow w + y_i \phi(x_i)$$

classify

$$f(k) = w \cdot \phi(x)$$

Dual Form

update linear coefficients

$$\alpha_i \leftarrow \alpha_i + y_i$$

implicitly equivalent to:

$$w = \sum_{i \in I} \alpha_i \phi(x_i)$$

- Nothing happens if classified correctly
- Weight vector is a linear combination $w = \sum_{i \in I} \alpha_i \phi(x_i)$
- Classifier is a linear combination of inner products

$$f(x) = \sum_{i \in I} \alpha_i \langle \phi(x_i), \phi(x) \rangle = \sum_{i \in I} \alpha_i k(x_i, x)$$

Questions?