SUPPORT VECTOR MACHINE

Mainly based on
https://nlp.stanford.edu/IR-book/pdf/15svm.pdf

Overview

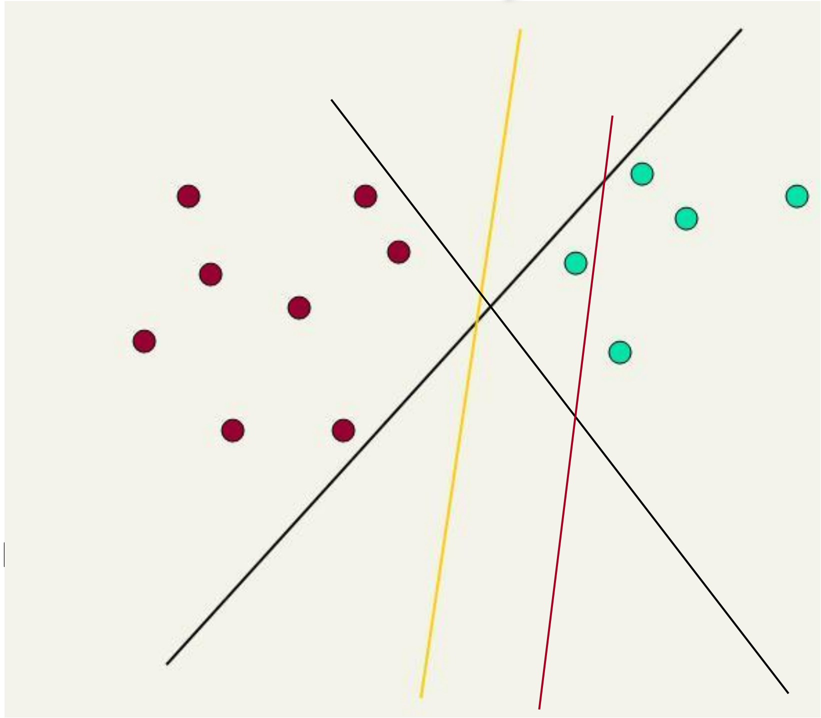
- SVM is a huge topic
  - Integration of MMDS, IIR, and Andrew Moore's slides here
- Our foci:
  - Geometric intuition → Primal form
    - Alternative interpretation from Empirical Risk Minimization point of view.
  - Understand the final solution (in the dual form)
    - Generalizes well to Kernel functions
  - SVM + Kernels

$\mathbf{w}^T\mathbf{x}_i + b = 0$

Linear classifiers: Which Hyperplane?

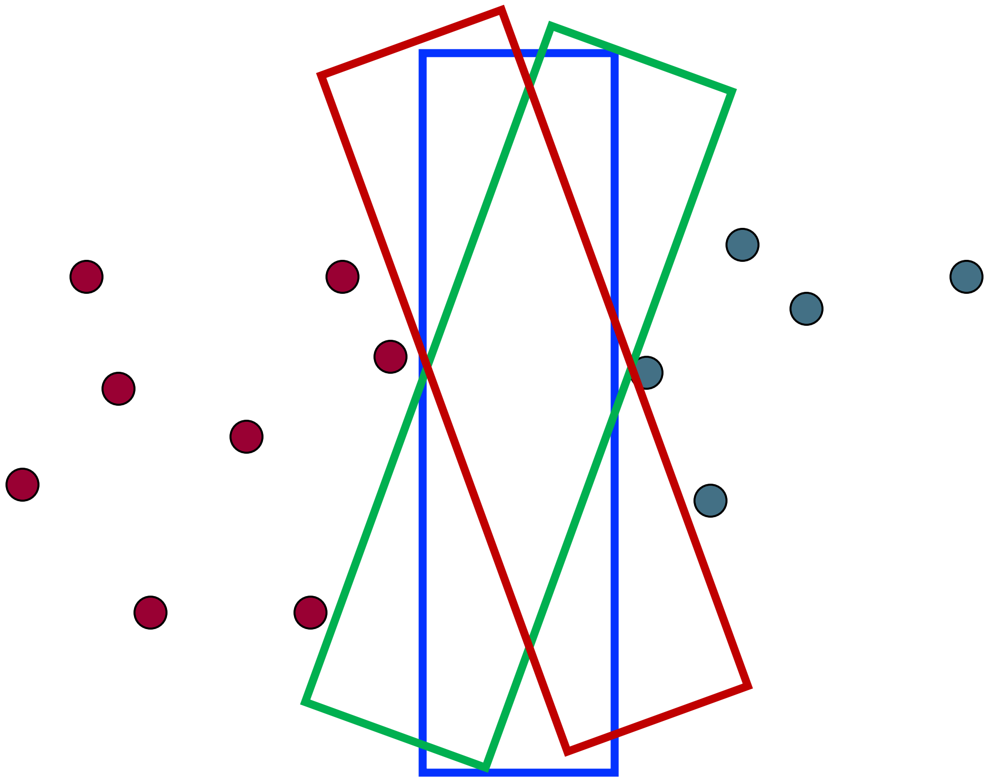
This line represents the decision boundary:
$ax + by - c = 0$

- Lots of possible solutions for *a, b, c.*
- Some methods find a separating hyperplane, but not the optimal one [according to some criterion of expected goodness]
  - E.g., perceptron
- Support Vector Machine (SVM) finds an optimal* solution.
  - Maximizes the distance between the hyperplane and the "difficult points" close to decision boundary
  - One intuition: if there are no points near the decision surface, then there are no very uncertain classification decisions



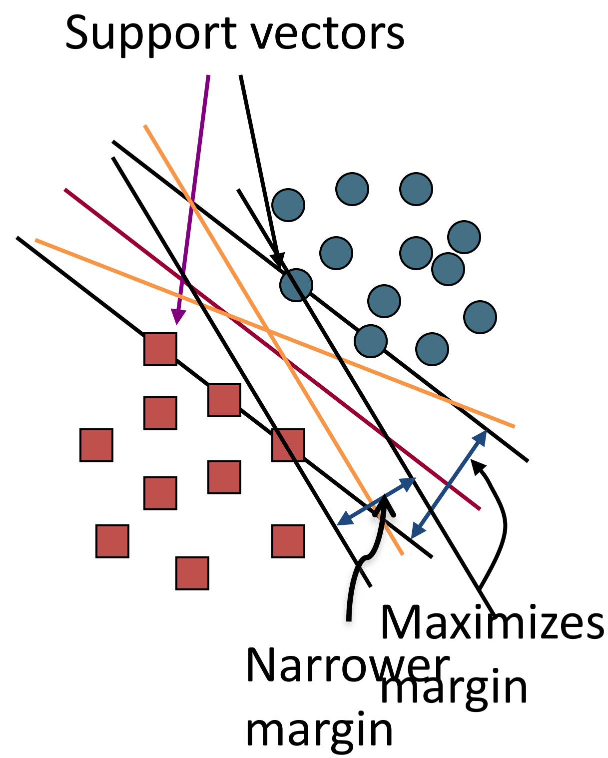
Another intuition

- If you have to place a fat separator between classes, you have less choices, and so the capacity of the model has been decreased



Support Vector Machine (SVM)

- SVMs maximize the *margin* around the separating hyperplane.
  - A.k.a. large margin classifiers
- The decision function is fully specified by a subset of training samples, *the support vectors*.
- Solving SVMs is a *quadratic programming* problem
- Seen by many as the most successful current text classification method*



*but other discriminative methods often perform very similarly

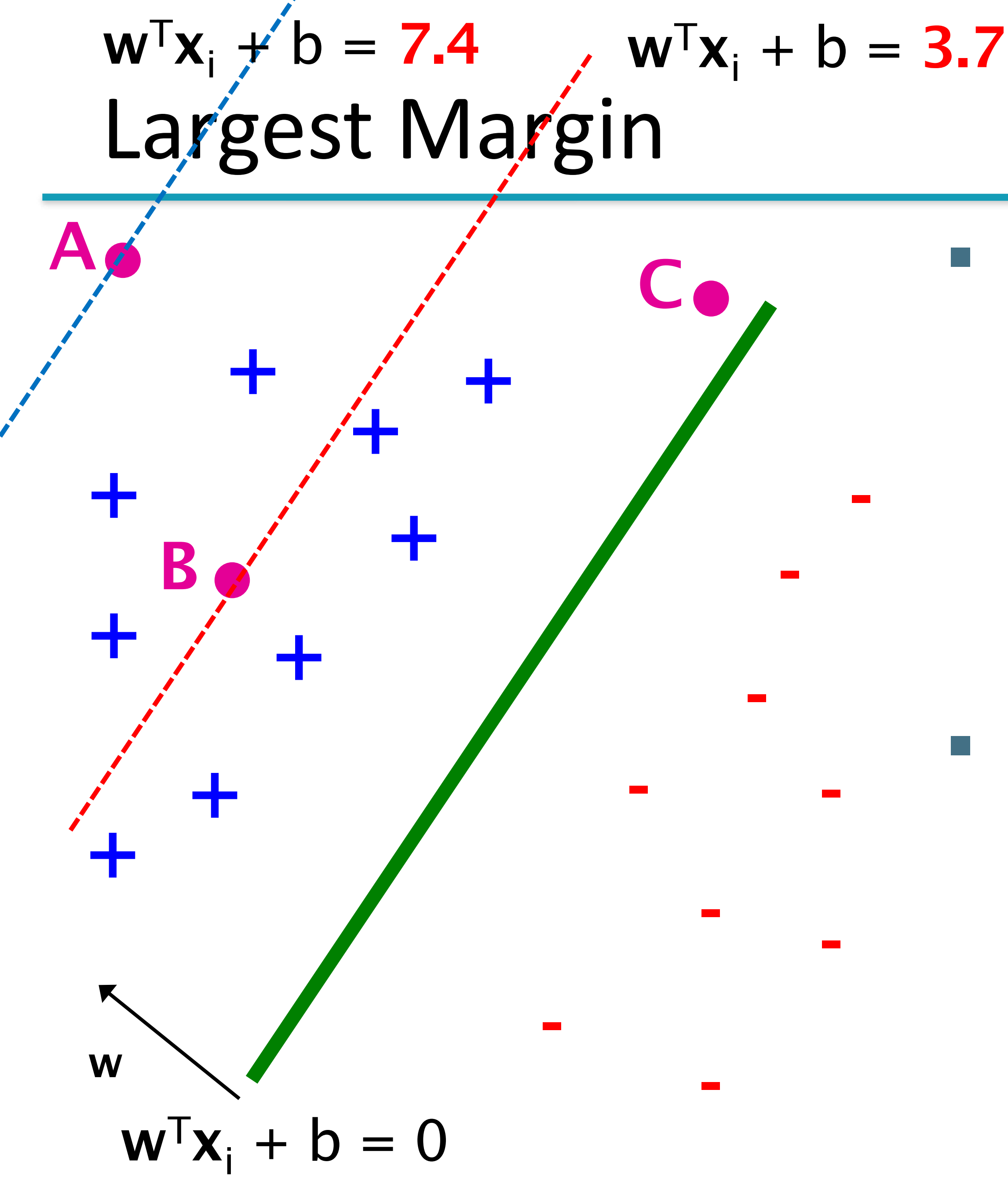
Maximum Margin: Formalization

- **w**: decision hyperplane normal vector
- $\mathbf{x}_i$: data point *i*
- y_i: class of data point *i* (+1 or -1)
- Classifier is: $f(\mathbf{x}_i) = \text{sign}(\mathbf{w}^T\mathbf{x}_i + b)$
- Functional margin of $\mathbf{x}_i$ is: $y_i\,(\mathbf{w}^T\mathbf{x}_i + b)$
  - But note that we can increase this margin simply by scaling **w**, **b**….
- Functional margin of dataset is twice the minimum functional margin for any point
  - The factor of 2 comes from measuring the whole width of the margin

NB: Not 1/0

NB: a common trick

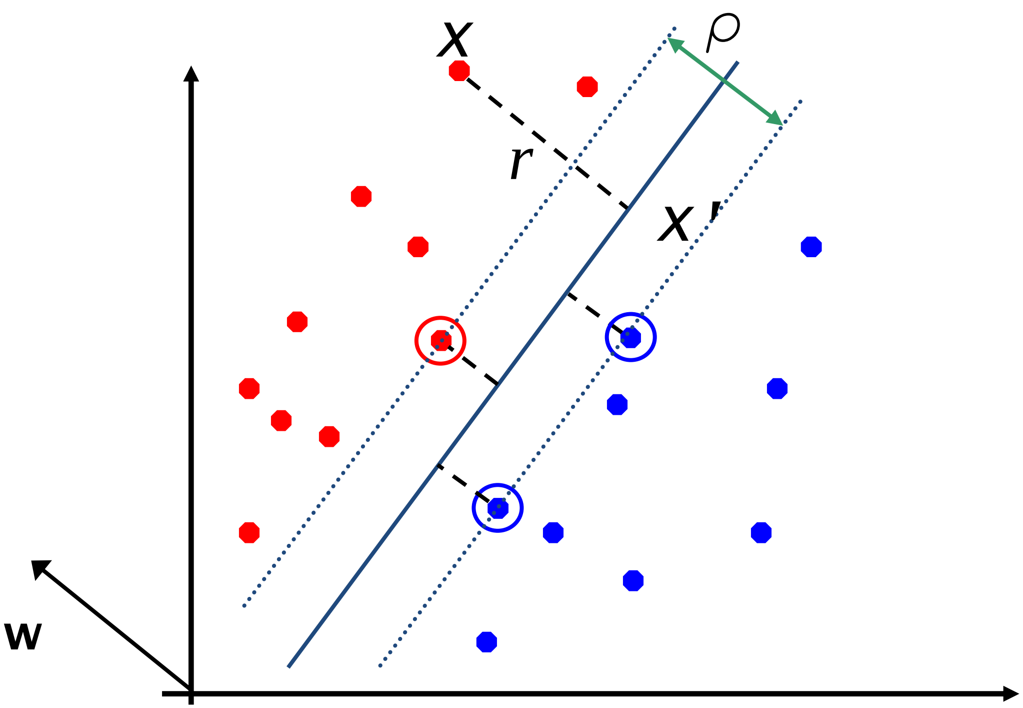
Largest Margin



- Distance from the separating hyperplane corresponds to the “confidence” of prediction
- **Example:**
  - We are more sure about the class of **A** and **B** than of **C**

Geometric Margin

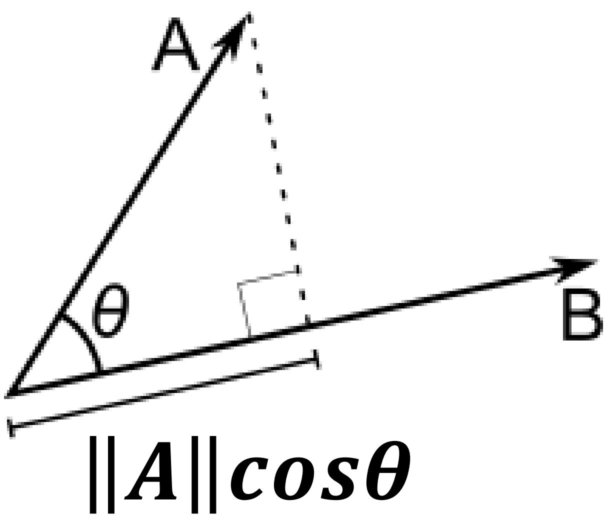
- Distance from example to the separator is $r = y\dfrac{\mathbf{w}^T\mathbf{x}+b}{\|\mathbf{w}\|}$
- Examples closest to the hyperplane are ***support vectors***.
- ***Margin*** ρ of the separator is the width of separation between support vectors of classes.



Algebraic derivation of finding *r*:
Dotted line **x'** −**x** is perpendicular to decision boundary so parallel to **w**.
Unit vector is **w**/||**w**||, so line is rw/||**w**||, for some r.
x' = **x** – yr**w**/||**w**||.
x' satisfies $\mathbf{w}^T\mathbf{x}' + b = 0$.
So $\mathbf{w}^T(\mathbf{x} - yr\mathbf{w}/\|\mathbf{w}\|) + b = 0$
Recall that $\|\mathbf{w}\| = \mathrm{sqrt}(\mathbf{w}^T\mathbf{w})$.
So $\mathbf{w}^T\mathbf{x} - yr\|\mathbf{w}\| + b = 0$
So, solving for r gives:
$r = y(\mathbf{w}^T\mathbf{x} + b)/\|\mathbf{w}\|$

Help from Inner Product

- **Remember: Dot product / inner product**



$$\langle A, B\rangle = \|A\|\|B\|\cos\theta$$

$$\boxed{\|A\|\cos\theta} = \|A\| \cdot \frac{\langle A, B\rangle}{\|A\|\|B\|} = \frac{\langle A, B\rangle}{\|B\|}$$

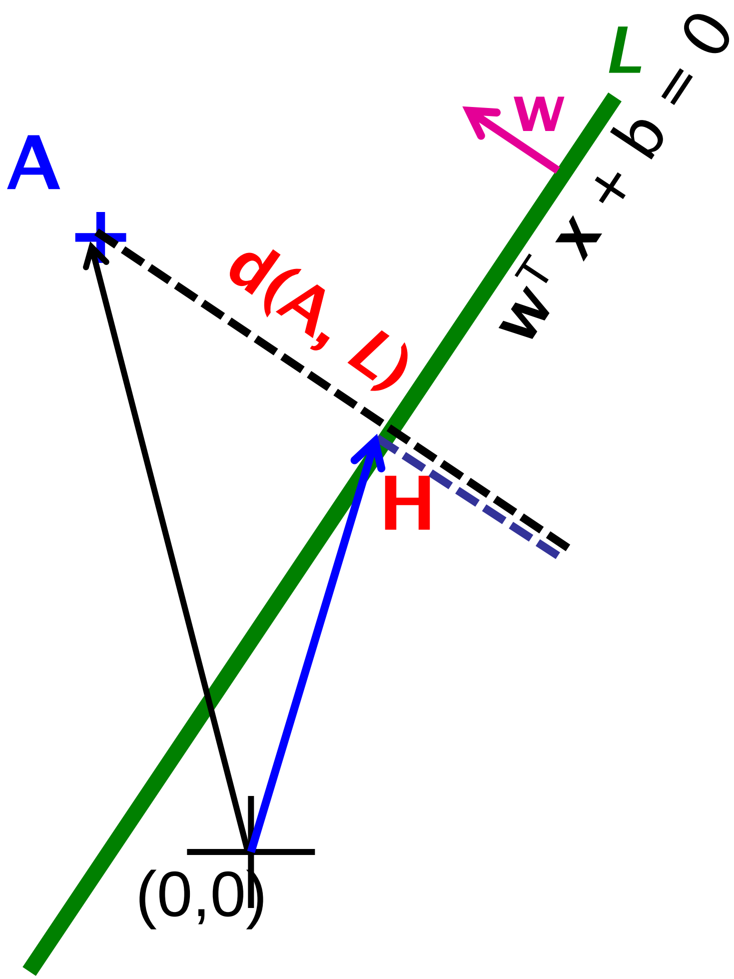
scalar

$$\boxed{(\|A\|\cos\theta)\frac{B}{\|B\|}} = \frac{\langle A, B\rangle}{\|B\|^2}B$$

vector

- **A's projection onto B = (<A, B> / <B, B>) * B**

Derivation of the Geometric Margin



- d(A, L) = <A, w>/<w, w>

  - <H, w>/<w, w>
  - Note that H is on the line L, so <w, H> + b = 0
  - Therefore = (<A, w> + b)/<w, w>

Linear SVM Mathematically

The linearly separable case

- Assume that all data is at least distance 1 from the hyperplane, then the following two constraints follow for a training set $\{(\mathbf{x_i}, y_i)\}$

$$\mathbf{w^T x_i} + b \geq 1 \quad \text{if } y_i = 1$$

$$\mathbf{w^T x_i} + b \leq -1 \quad \text{if } y_i = -1$$

- For support vectors, the inequality becomes an equality
- Then, since each example's distance from the hyperplane is

$$r = y\frac{\mathbf{w}^T\mathbf{x} + b}{\|\mathbf{w}\|}$$

- The margin is:

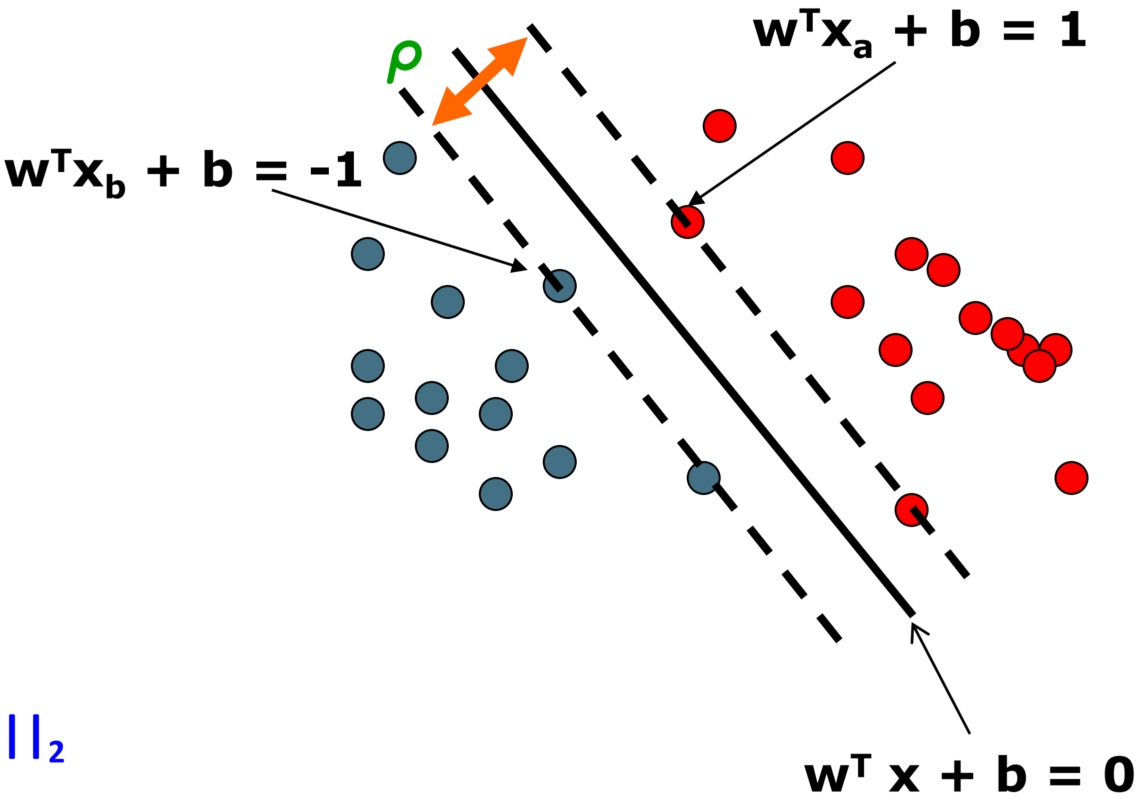
$$r = \frac{2}{\|\mathbf{w}\|}$$

Derivation of ρ

- **Hyperplane**
  $\mathbf{w}^T \mathbf{x} + b = 0$

- **Extra scale constraint**:
  $\min_{i=1,\ldots,n} |\mathbf{w}^T\mathbf{x}_i + b| = 1$

- This implies:
  $w^T(x_a - x_b) = 2$
  $\rho = ||x_a - x_b||_2 = 2/||\mathbf{w}||_2$



Solving the Optimization Problem

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = \frac{1}{2}\,\mathbf{w}^T\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w^T x_i} + b) \geq 1$

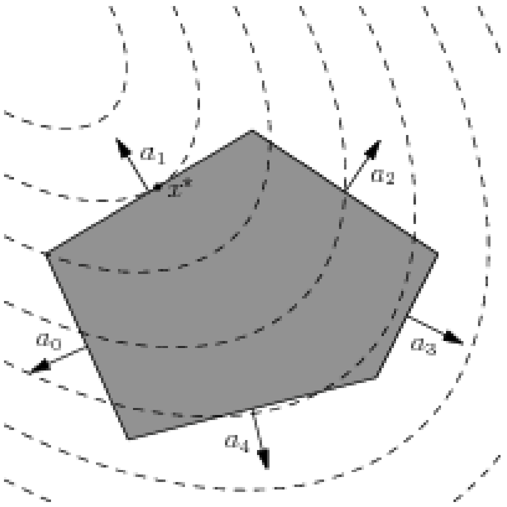
- This is now optimizing a *quadratic* function subject to *linear* constraints
- Quadratic optimization problems are a well-known class of mathematical programming problem, and many (intricate) algorithms exist for solving them (with many special ones built for SVMs)
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every constraint in the primary problem:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $\alpha_i \geq 0$ for all α_i

Geometric Interpretation

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^{\mathrm{T}}\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w}^{\mathbf{T}}\mathbf{x_i} + b) \geq 1$

- What are fixed and what are variables**?**
- **Linear** constraint(s): Where can the variables be?
- **Quadratic** objective function:



The Optimization Problem Solution

- The solution has the form:

$$\mathbf{w} = \Sigma \alpha_i y_i \mathbf{x_i} \qquad b = y_k - \mathbf{w^T x_k} \text{ for any } \mathbf{x_k} \text{ such that } \alpha_k \neq 0$$

- **Each non-zero α_i indicates that corresponding $\mathbf{x_i}$ is a support vector.**
- Then the scoring function will have the form:

$$f(\mathbf{x}) = \Sigma \alpha_i y_i \mathbf{x_i^T x} + b$$

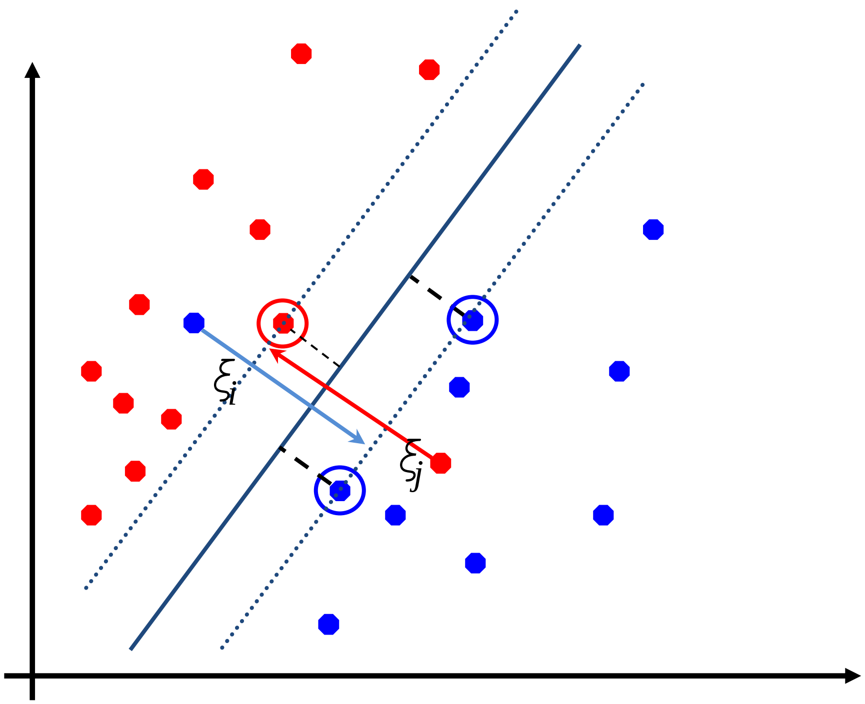
$$f(\mathbf{x}) = \sum_{sv \in SV} y_{sv} \cdot \alpha_{sv} \cdot \langle \mathbf{x}_{sv}, \mathbf{x} \rangle + b$$

Q: What are the model parameters? What does f(x) mean intuitively?

  - Classification is based on the sign of f(**x**)
- Notice that it relies on an ***inner product*** between the test point **x** and the support vectors $\mathbf{x}_i$
  - We will return to this later.
- Also *keep in mind* that solving the optimization problem involved computing the inner products $<\mathbf{x}_i, \mathbf{x}_j>$ between all pairs of training points.

Soft Margin Classification

- If the training data is not linearly separable, *slack variables* ξ_i can be added to allow misclassification of difficult or noisy examples.
- Allow some errors
  - Let some points be moved to where they belong, at a cost
- Still, try to minimize training set errors, and to place hyperplane "far" from each class (large margin)



Soft Margin Classification Mathematically

[Optional]

- The old formulation:

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^{T}\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
$y_i (\mathbf{w}^{\mathbf{T}}\mathbf{x_i} + \mathrm{b}) \geq 1$

- The new formulation incorporating slack variables:

Find $\mathbf{w}$ and b such that
$\mathbf{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^{T}\mathbf{w} + C\Sigma\, \xi_i$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$
$y_i (\mathbf{w}^{\mathbf{T}}\mathbf{x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

- Parameter *C* can be viewed as a way to control overfitting
  - A regularization term

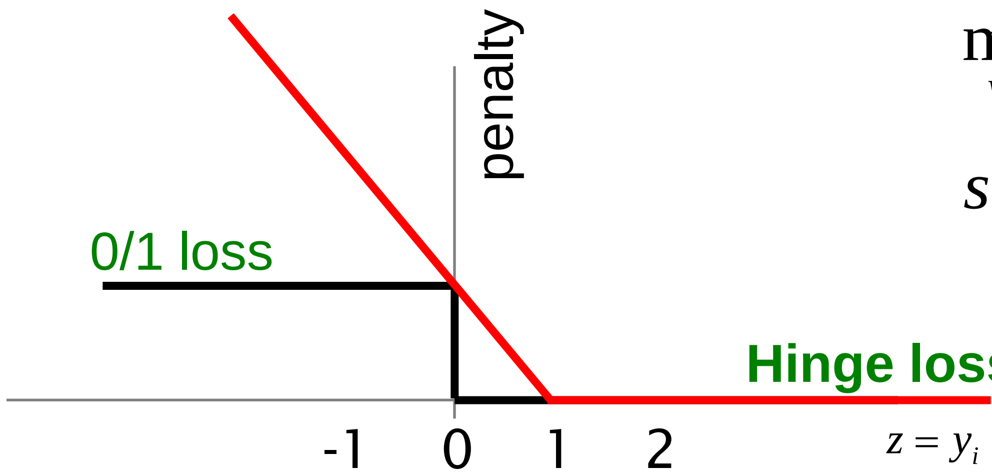
Alternative View

- **SVM in the "natural" form**

$$\underset{w,b}{\arg\min}\ \underbrace{\tfrac{1}{2}\, w \cdot w}_{\text{Margin}} + C \cdot \underbrace{\sum_{i=1}^{n} \max\{0, 1 - y_i (w \cdot x_i + b)\}}_{\text{Empirical loss L (how well we fit training data)}}$$

Hyper-parameter related to regularization

- **SVM uses "Hinge Loss":**



Hinge loss: max{0, 1-z}

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

$$\min_{w,b}\ \tfrac{1}{2}\|w\|^2 + C\sum_{i=1}^{n} \xi_i$$

$$s.t. \forall i,\ y_i \cdot (w \cdot x_i + b) \geq 1 - \xi_i$$

[Optional]

Soft Margin Classification – Solution

- The dual problem for soft margin classification:

Find $\alpha_1 \dots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

- Neither slack variables ξ_i nor their Lagrange multipliers appear in the dual problem!
- Again, $\mathbf{x_i}$ with non-zero α_i will be support vectors.
- Solution to the dual problem is:

$$\mathbf{w} = \Sigma\alpha_i y_i \mathbf{x_i}$$
$$b = y_k(1 - \xi_k) - \mathbf{w}^T\mathbf{x}_k \text{ where } k = \underset{k'}{\operatorname{argmax}}\ \alpha_{k'}$$

w is not needed explicitly for classification!

$$f(\mathbf{x}) = \Sigma\alpha_i y_i \mathbf{x_i}^T\mathbf{x} + b$$

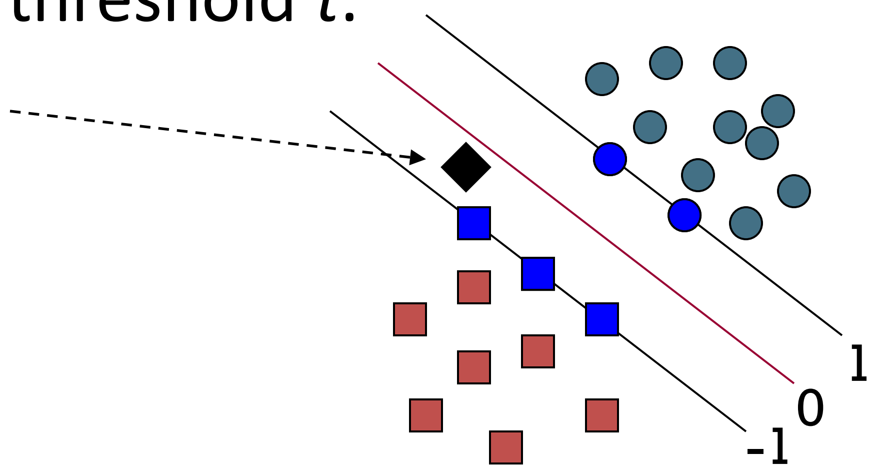
Classification with SVMs

- Given a new point **x**, we can score its projection onto the hyperplane normal:
  - I.e., compute score: $\mathbf{w}^T\mathbf{x} + b = \Sigma\alpha_i y_i \mathbf{x}_\mathbf{i}^T\mathbf{x} + b$
    - Decide class based on whether < or > 0
  - Can set confidence threshold *t*.

Score > *t*: yes

Score < -*t*: no

Else: don't know



Linear SVMs: Summary

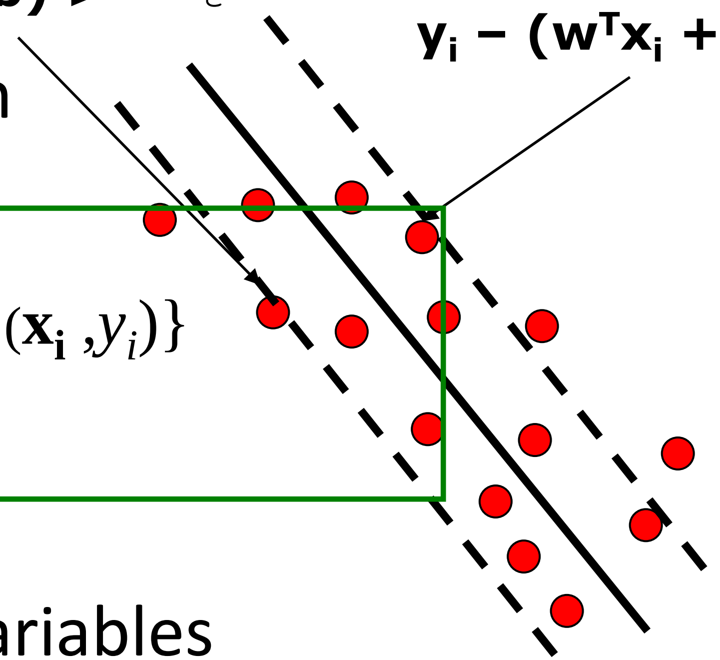
- The classifier is a *separating hyperplane.*
- The most "important" training points are the support vectors; they define the hyperplane.
- Quadratic optimization algorithms can identify which training points $\mathbf{x}_i$ are **support vectors** with non-zero Lagrangian multipliers α_i.
- Both in the dual formulation of the problem and in the solution, training points appear only inside inner products:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - \frac{1}{2}\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and
(1) $\Sigma\alpha_i y_i = 0$
(2) $0 \leq \alpha_i \leq C$ for all α_i

$$f(\mathbf{x}) = \sum_{sv \in SV} y_{sv} \cdot \alpha_{sv} \cdot \langle \mathbf{x}_{sv}, \mathbf{x} \rangle + b$$

Support Vector Regression

- Find a function f(x) with at most ε-deviation frm the target y
- The optimization problem



Find **w** and *b* such that

$\mathbf{\Phi}$ $(\mathbf{w}) = \frac{1}{2}\, \mathbf{w}^T\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}, y_i)\}$

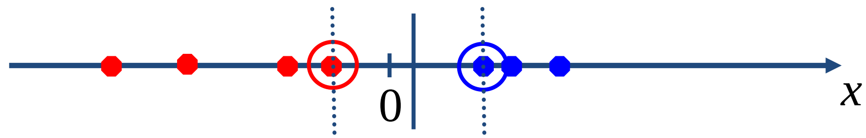
$y_i - (\mathbf{w}^T\mathbf{x_i} + \mathrm{b}) \geq -\ \varepsilon$

$y_i - (\mathbf{w}^T\mathbf{x_i} + \mathrm{b}) \leq \varepsilon$

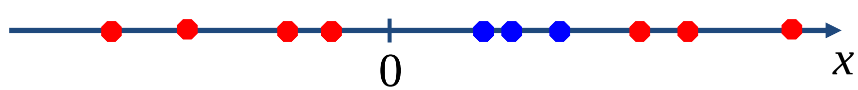
- We can introduce slack variables
  - Similar to soft margin loss function

Non-linear SVMs

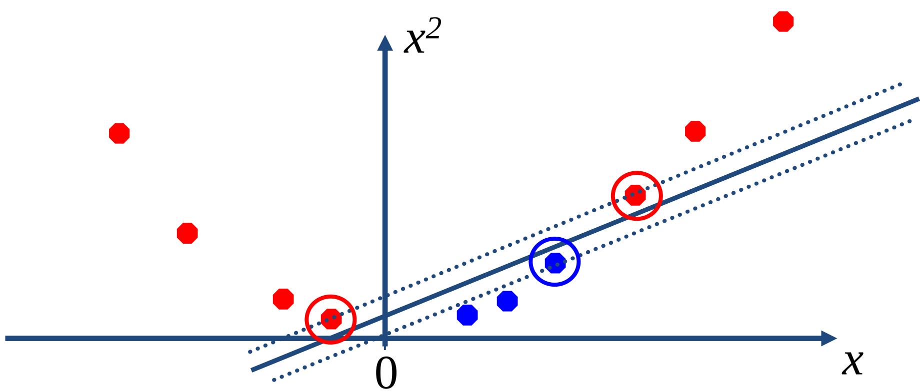
- Datasets that are linearly separable (with some noise) work out great:



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



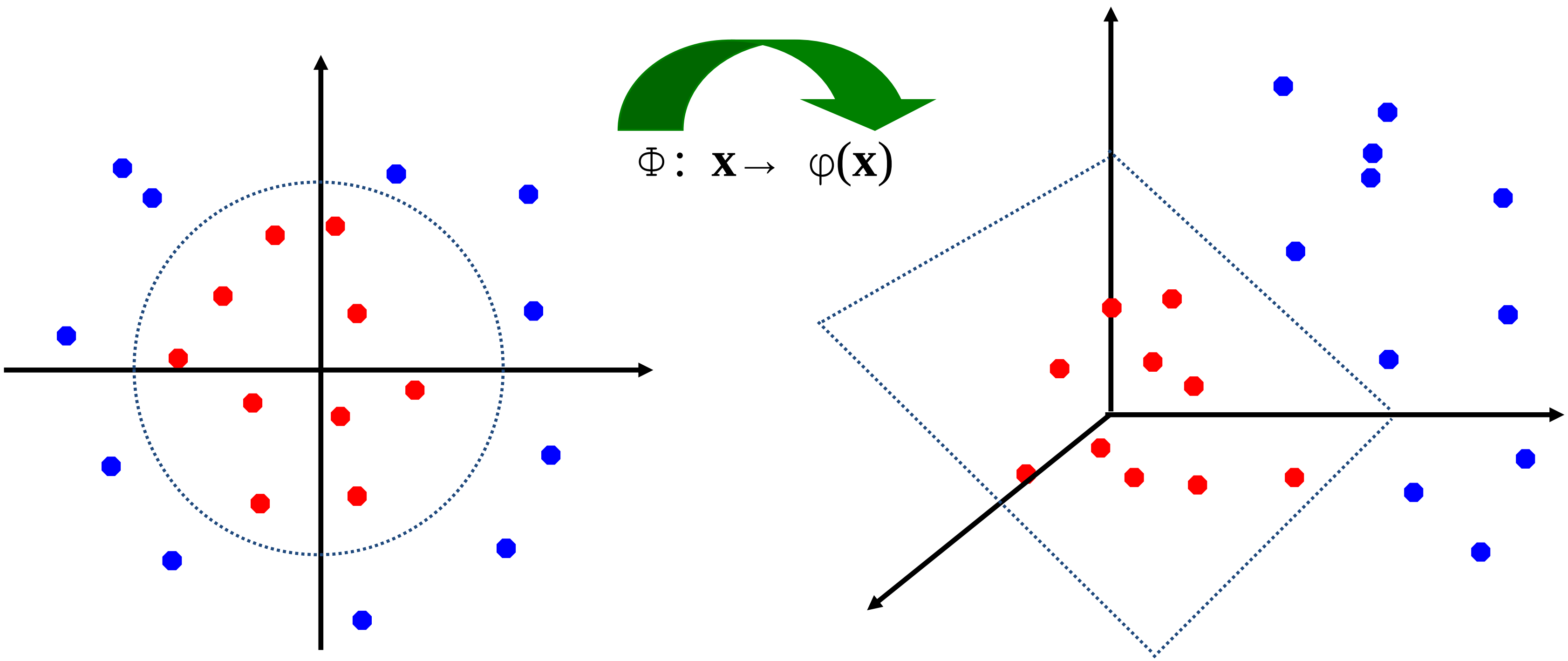
- How about … mapping data to a higher-dimensional space:



c.f., polynomial regression

Non-linear SVMs: Feature spaces

- General idea: the original feature space can always be mapped to some higher-dimensional feature space where the training set is separable:



The "Kernel Trick"

- The linear classifier relies on an inner product between vectors $K(\mathbf{x}_i,\mathbf{x}_j)=\mathbf{x}_i^T\mathbf{x}_j$
- If every datapoint is mapped into high-dimensional space via some transformation $\Phi: \mathbf{x} \rightarrow \varphi(\mathbf{x})$, the inner product becomes:

$$K(\mathbf{x}_i,\mathbf{x}_j)= \varphi(\mathbf{x}_i)^{T}\varphi(\mathbf{x}_j)$$

- A *kernel function* is some function that corresponds to an inner product in **some** expanded feature space.
  - Usually, no need to construct the feature space explicitly.

What about $K(\mathbf{u},\mathbf{v}) = (1+\mathbf{u}^\top\mathbf{v})^3$ **?**

Example

$$\begin{aligned}
K(\mathbf{u},\mathbf{v}) &= (1+\mathbf{u}^\top\mathbf{v})^2 \\
&= 1 + 2\mathbf{u}^\top\mathbf{v} + (\mathbf{u}^\top\mathbf{v})^2 \\
&= 1 + 2\mathbf{u}^\top\mathbf{v} + \left(\sum_i \mathbf{u}_i\mathbf{v}_i\right)^2 \\
&= 1 + 2\mathbf{u}^\top\mathbf{v} + \left(\sum_i \mathbf{u}_i^2\mathbf{v}_i^2 + \sum_{i\neq j} \mathbf{u}_i\mathbf{u}_j\mathbf{v}_i\mathbf{v}_j\right) \\
&= \phi(\mathbf{u})^\top\phi(\mathbf{v})
\end{aligned}$$

O(d²) new cross-term features

$$\phi(\mathbf{u}) = [1 \;\; \sqrt{2}\mathbf{u}_1 \;\; \ldots \;\; \sqrt{2}\mathbf{u}_d \;\; \mathbf{u}_1^2 \;\; \ldots \;\; \mathbf{u}_d^2 \;\; \mathbf{u}_1\mathbf{u}_2 \;\; \ldots \;\; \mathbf{u}_{d-1}\mathbf{u}_d]^\top$$

$$\phi(\mathbf{v}) = [1 \;\; \sqrt{2}\mathbf{v}_1 \;\; \ldots \;\; \sqrt{2}\mathbf{v}_d \;\; \mathbf{v}_1^2 \;\; \ldots \;\; \mathbf{v}_d^2 \;\; \mathbf{v}_1\mathbf{v}_2 \;\; \ldots \;\; \mathbf{v}_{d-1}\mathbf{u}_d]^\top$$

Linear **Non-linear** **Non-linear + feature combination**

Why feature combinations?

- Examples:
  - Two categorical features (age & married) encoded as one-hot encoding ➔ combination = conjunction rules
    - e.g., 1[age in [30, 40) AND married = TRUE]
  - [..., eagerness-for-travel, income, ...] ➔ combination indicates how much to spend on travel
    - e.g., "travel rarely" AND "high income", among other combinations
  - NLP, feature vector = 1[w ∈ x] ➔ combination indicates two word co-occurrence (where phrase/multi-word expression (MWE) is just a special case)
- $\mathbf{x}$ ➔ $\varphi(\mathbf{x})$, then a linear model in the new feature space is just $\mathbf{w}^{\mathbf{T}}\varphi(\mathbf{x}) + b$
  - each feature combination will be assigned a weight w_i
  - irrelevant features combinations will get 0 weight

Why feature combinations? /2

- Also helpful for linear models
  - Linear regression assumes no interaction between x_i and x_j
  - One can add **manual** interaction terms, typically $x_i * x_j$, to still use linear regression (to learn a non-linear model!)

Inner product in an infinite dimensional space!

[Optional]

RBF kernel:

$$e^{-\gamma\|x_i - x_j\|^2} = e^{-\gamma(x_i - x_j)^2} = e^{-\gamma x_i^2 + 2\gamma x_i x_j - \gamma x_j^2}$$

$$= e^{-\gamma x_i^2 - \gamma x_j^2}\left(1 + \frac{2\gamma x_i x_j}{1!} + \frac{(2\gamma x_i x_j)^2}{2!} + \frac{(2\gamma x_i x_j)^3}{3!} + \cdots\right)$$

$$= e^{-\gamma x_i^2 - \gamma x_j^2}\left(1 \cdot 1 + \sqrt{\frac{2\gamma}{1!}}x_i \cdot \sqrt{\frac{2\gamma}{1!}}x_j + \sqrt{\frac{(2\gamma)^2}{2!}}x_i^2 \cdot \sqrt{\frac{(2\gamma)^2}{2!}}x_j^2 + \ldots\right)$$

$$= \phi(x_i)^T \phi(x_j) \qquad , \text{ where}$$

$$\phi(x) = e^{-\gamma x^2}\left[1, \sqrt{\frac{2\gamma}{1!}}x, \sqrt{\frac{(2\gamma)^2}{2!}}x^2, \sqrt{\frac{(2\gamma)^3}{3!}}x^3, \cdots\right]^T$$

[Optional]

String Kernel

- K(s1, s2) should evaluate the similarity between the two strings
  - Without this, sim("actor", "actress") = 0
- Intuition:
  - consider all substrings as (binary) "features"
  - inner product in that "enhanced" feature space means the number of common substrings the two share.
- Variants:
  - (more complex): consider subsequences (with possibly gap penalty)
  - (simpler): consider all k-grams, and use Jaccard
    - bigrams(actor) = {ac, ct, to, or}
    - bigrams(actress) = {ac, ct, tr, re, es, ss}
    - Jaccard(actor, actress) = 2/8

Kernels

- Why use kernels?
  - Make non-separable problem separable.
  - Map data into better representational space
  - Can be learned to capture some notion of "similarity"
- Common kernels
  - Linear
  - Polynomial **$K(x,z) = (1+x^T z)^d$**
    - Gives feature combinations
  - Radial basis function (infinite dimensional space)

$$K(\mathbf{x}_i, \mathbf{x}_j; \sigma) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

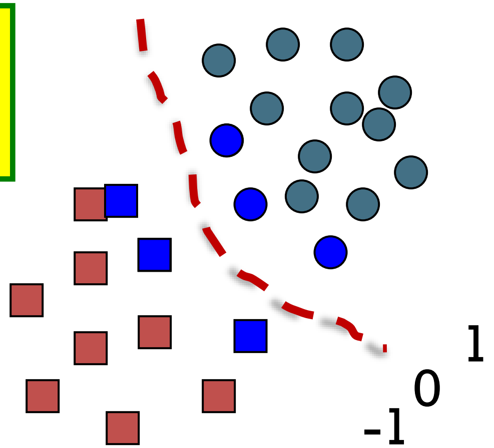
- Text classification:
  - Usually use linear or polynomial kernels

Classification with SVMs **with Kernels**

- Given a new point **x**, we can compute its score i.e.,

$$\boxed{\sum_{sv \in SV} y_{sv} \alpha_{sv} K(\mathbf{x}_{sv}, \mathbf{x}) + b}$$

  - Decide class based on whether < or > 0



- E.g., in scikit-learn

- linear: $\langle x, x' \rangle$.
- polynomial: $(\gamma \langle x, x' \rangle + r)^d$. d is specified by keyword `degree`, r by `coef0`.
- rbf: $\exp(-\gamma \|x - x'\|^2)$. γ is specified by keyword `gamma`, must be greater than 0.
- sigmoid ($\tanh(\gamma \langle x, x' \rangle + r)$), where r is specified by `coef0`.

Pros and Cons of the SVM Classifier

- Pros
  - High accuracy
  - Fast classification speed
  - Works with cases where #features > #samples
  - Can adapt to different objects (due to Kernel)
    - Any K(u, v) can be used if symmetric, continuous, and positive semi-definite.
    - Or explicit engineer the feature space.
- Cons
  - Training does not scale well with number of training samples ($O(d*n^2)$ or $O(d*n^3)$)
  - Hyper-parameters needs tuning

Resources for today's lecture

- Christopher J. C. Burges. 1998. A Tutorial on Support Vector Machines for Pattern Recognition
- S. T. Dumais. 1998. Using SVMs for text categorization, IEEE Intelligent Systems, 13(4)
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- Tie-Yan Liu, Yiming Yang, Hao Wan, et al. 2005. Support Vector Machines Classification with Very Large Scale Taxonomy, SIGKDD Explorations, 7(1): 36-43.
- 'Classic' Reuters-21578 data set: http://www.daviddlewis.com /resources /testcollections/reuters21578/