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 in

    - Alternative interpretation fro k Minimization point of view.

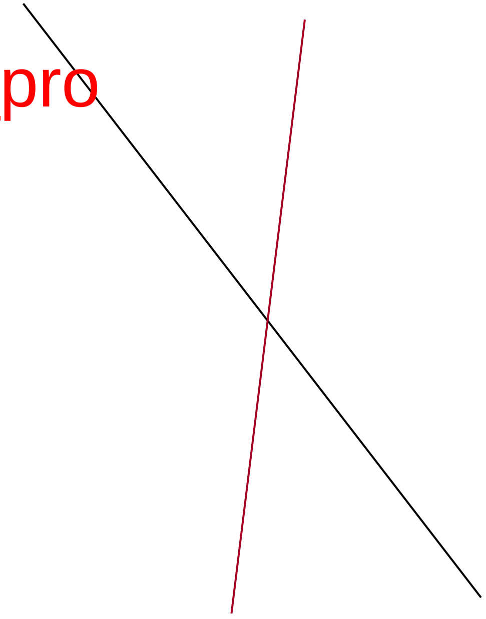
  - Understand the final solution (in the dual form)
    - Generalizes well to Kernel functions
  - SVM + Kernels

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

Linear classifiers: Which Hyperplane?

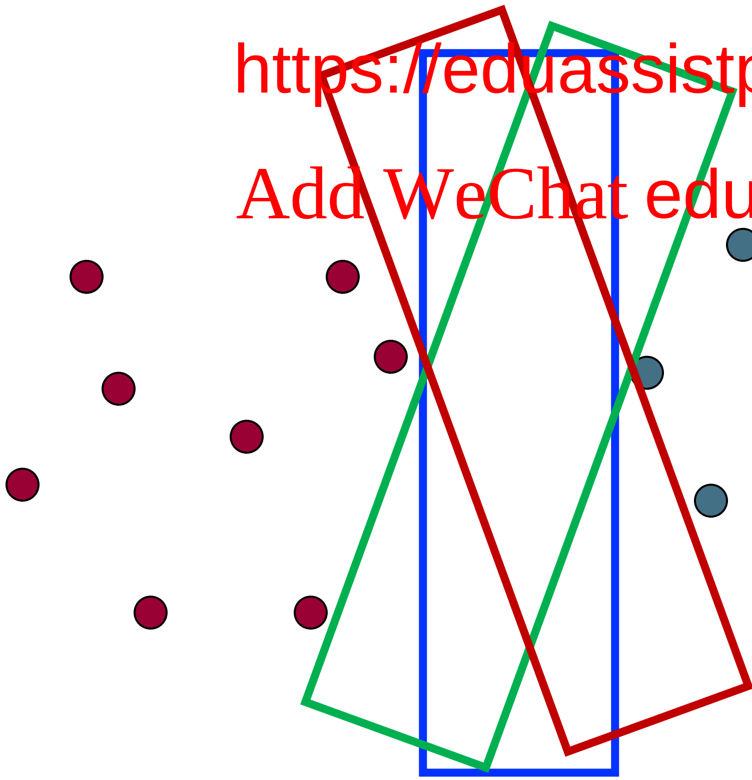
This line represents the decision boundary: $ax + by - c = 0$

- Lots of possible solutions for *a, b, c.*
- Some methods find a separating hyperplane, but not the optimal one [according to some crite 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



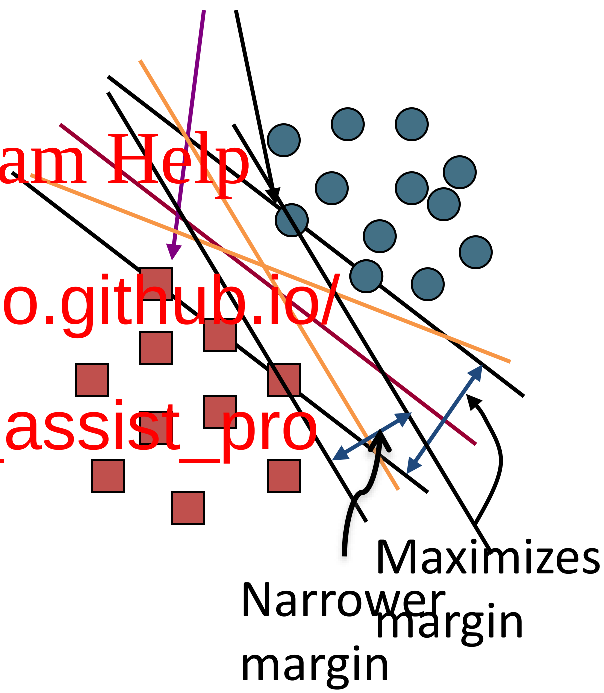
Another intuition

- 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 fun
  specified by a su
  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 d

- Classifier is:
  i
- Functional margin of $\mathbf{x}_i$ is:

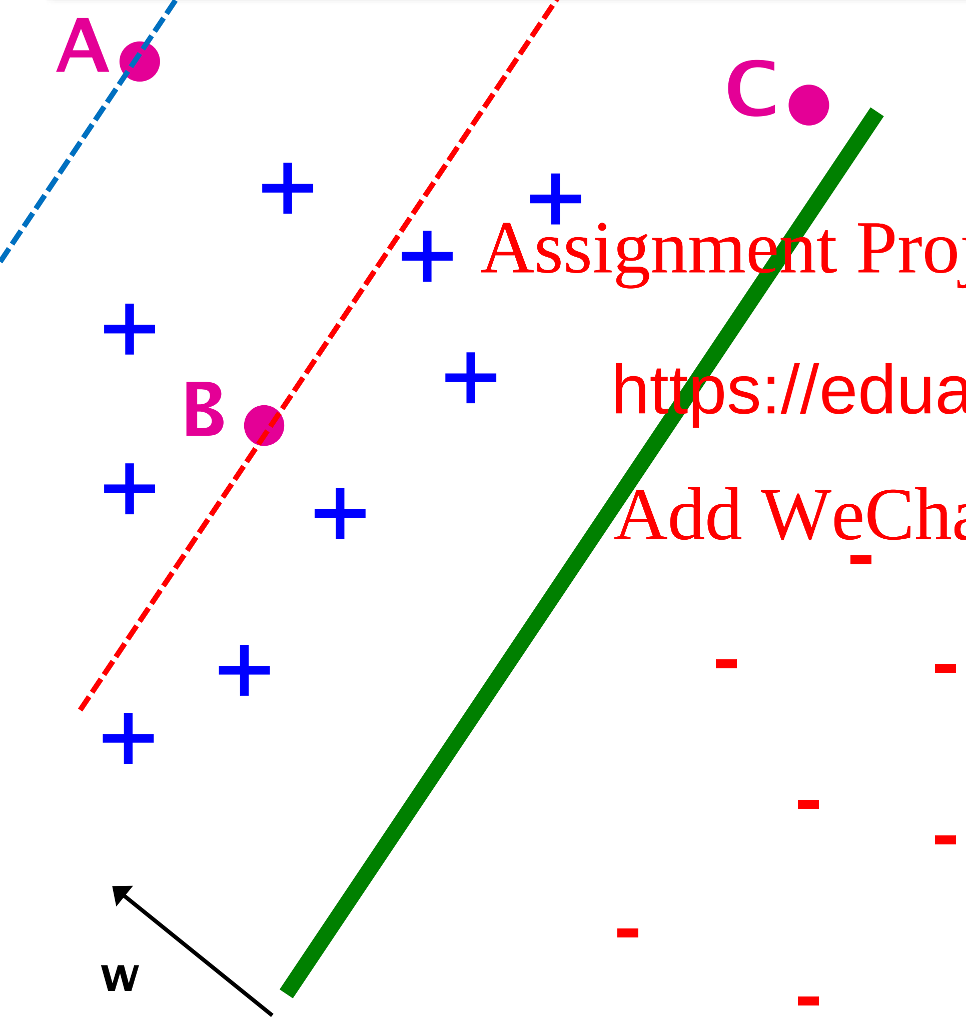
  - But note that we can increase this margin simply by scaling **w**, **b**....
- Functional margin of dataset is twice the minimum functional margin for any point
  - The factor of 2 comes from measuring the whole width of the margin

NB: Not 1/0

NB: a common trick

$\mathbf{w}^T\mathbf{x}_i + b = 7.4$ $\mathbf{w}^T\mathbf{x}_i + b = 3.7$

Largest Margin

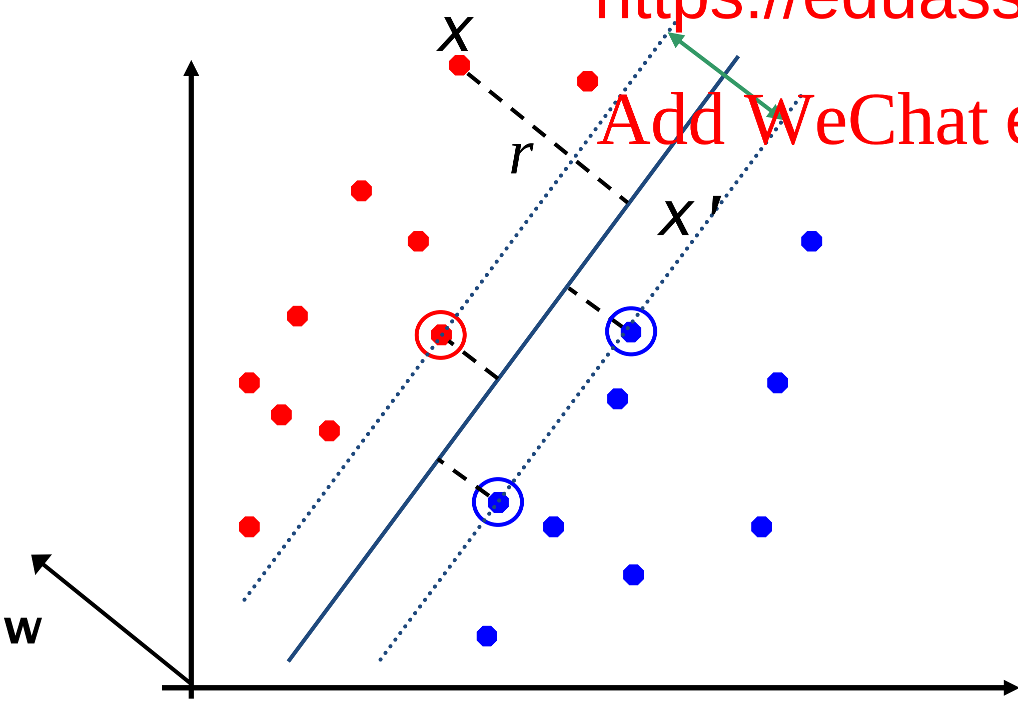


$\mathbf{w}^T\mathbf{x}_i + b = 0$

- 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 sep n between support vectors of classes.



ic der ding *r:*

x′ – **x** is perpendicular to
undary so parallel to **w**.
Unit vector is **w**/||**w**||, so line is
r**w**/||**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**

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

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

scalar

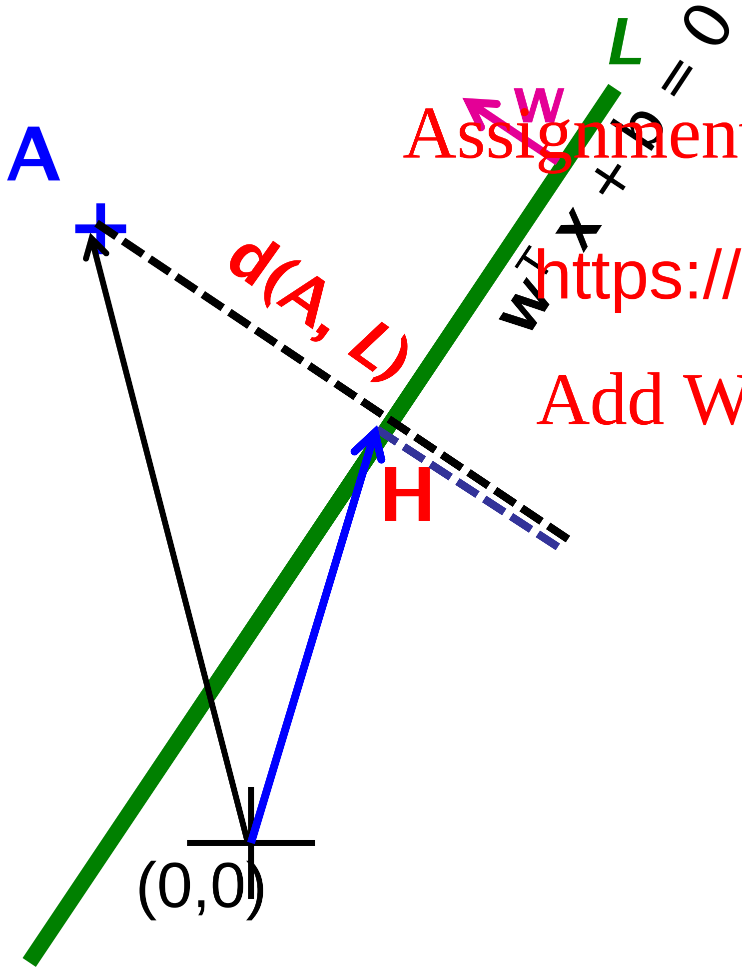
$\|A\| cos\theta$

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

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>

- H is on the line L, so

  b = 0

- (<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 $\{(\mathbf{x_i}, y_i)\}$

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

- For support vectors, the inequality be lity

- Then, since each example's distance f plane is

$$\frac{\quad T \quad}{\|\quad\|}$$

- The margin is:

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

Derivation of ρ

- **Hyperplane**

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

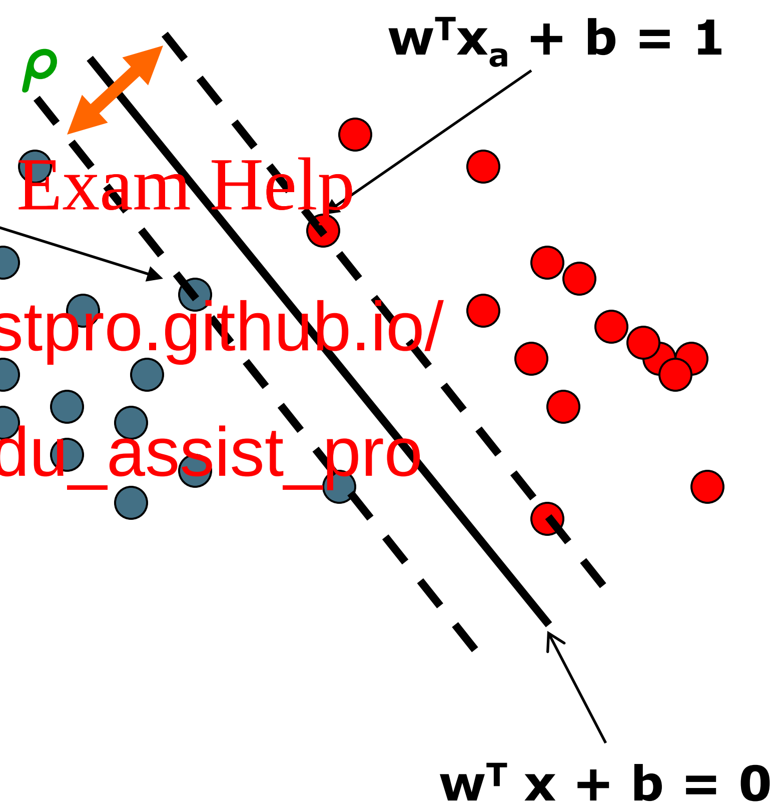
- **Extra scale constraint**:

  $\min_{i=1,\ldots,n} |w^T x_i + b| = 1$

- This implies:

  $w^T(x_a - x_b) = 2$

  $\rho = ||x_a - x_b||_2 = 2/||w||_2$



Solving the Optimization Problem

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

- This is now optimizi ... t to *linear* constraints

- Quadratic optimiza ... class of mathematical programming problem, and many (int ... ms exist for solving them (with many special ones built for SVM

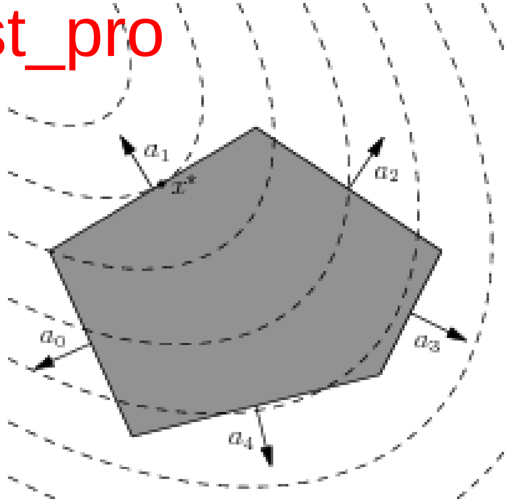
- The solution involves constructing a *dual problem* where a *Lagrange multiplier* α_i is associated with every constraint in the primary problem:

Find $\alpha_1 \ldots \alpha_N$ such that
$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^{\mathrm{T}}\mathbf{x_j}$ 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
$\mathbf{\Phi}(\mathbf{w}) = ½\, \mathbf{w}^T\mathbf{w}$ is minimized;
and for all $\{(\mathbf{x_i}, y_i)\}$: $y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

- What are fixe
- **Linear** constr s 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 fu

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

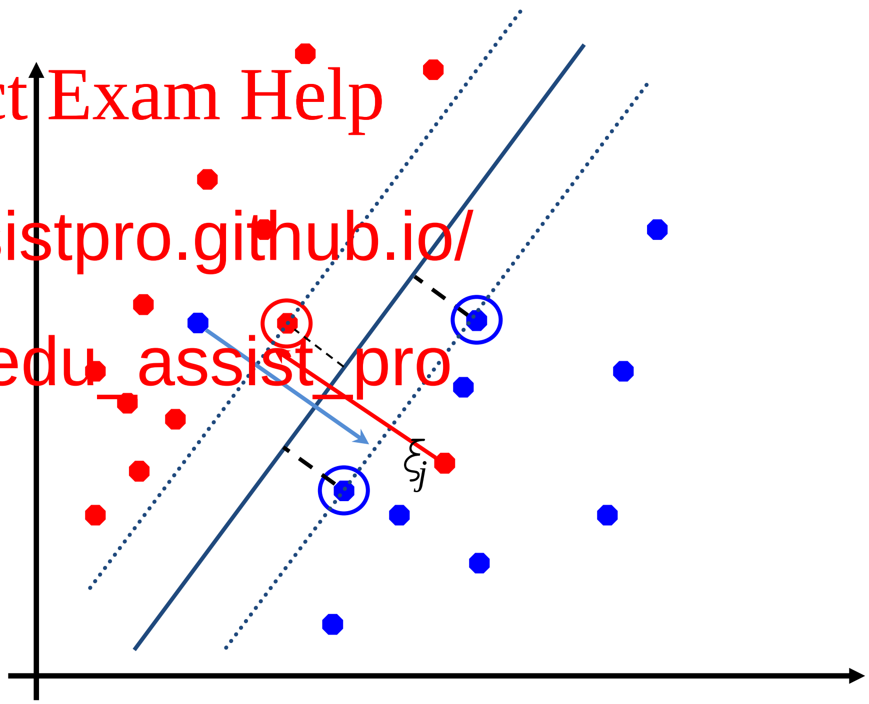
$$f(\mathbf{x}) = \sum_{sv \in SV} y_{sv} \cdot \alpha_{sv} \cdot \langle \mathbf{x}_{sv}, \mathbf{x} \rangle + b$$

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

  - Classification is based on the sign of f($\mathbf{x}$)
- Notice that it relies on an ***inner product*** between the test point $\mathbf{x}$ 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 misclass difficult or noi
- 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 $\{(\mathbf{x_i}, y_i)\}$
$y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1$

- The new formulation incorporating sla

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 $\{(\mathbf{x_i}, y_i)\}$
$y_i(\mathbf{w}^T\mathbf{x_i} + b) \geq 1 - \xi_i$ and $\xi_i \geq 0$ for all i

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

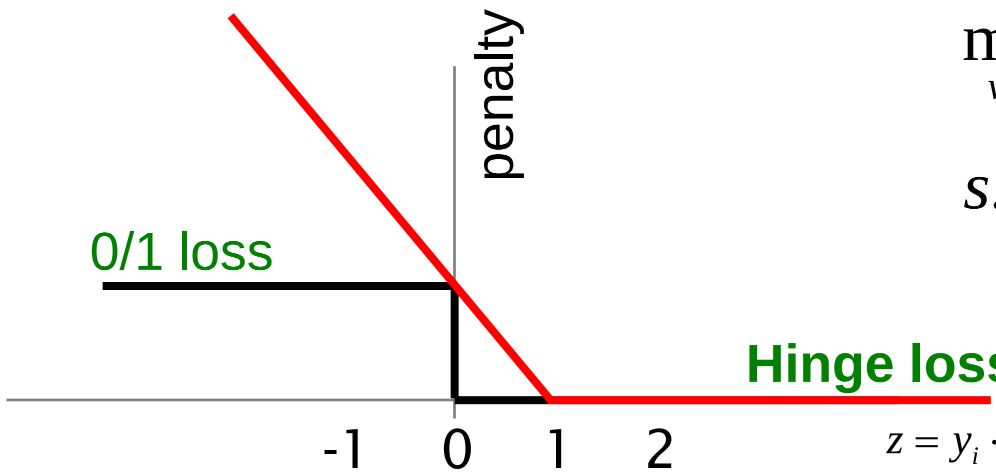
Alternative View

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

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

Hyper-para

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



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

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

Hinge loss: max{0, 1-z}

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

[Optional]

Soft Margin Classification – Solution

- The dual problem for soft margin classification:

Find $\alpha_1 \ldots \alpha_N$ such that

$\mathbf{Q}(\boldsymbol{\alpha}) = \Sigma\alpha_i - ½\Sigma\Sigma\alpha_i\alpha_j y_i y_j \mathbf{x_i}^T\mathbf{x_j}$ is maximized and

(1) $\Sigma\alpha_i y_i = 0$

(2) $0 \leq \alpha_i \leq C$ fo

- Neither slack variables ξ_i nor their Lagrang ear 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!

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

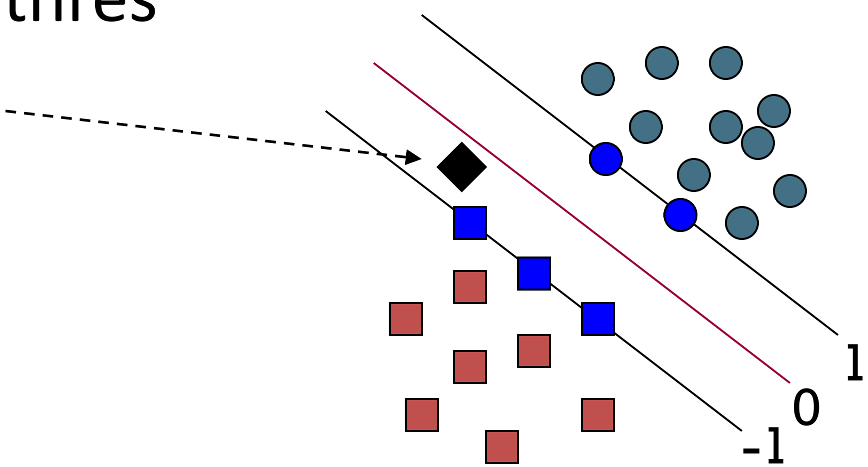
Classification with SVMs

- Given a new point $\mathbf{x}$, we can score its projection onto the hyperplane normal:
  - I.e., compute score: $\mathbf{w}^T\mathbf{x} + b = \Sigma\alpha y_i \mathbf{x}_i^T\mathbf{x} + b$
    - Decide clas
  - Can set confidence thres

Score > t: yes

Score < -t: no

Else: don't know



Linear SVMs: Summary

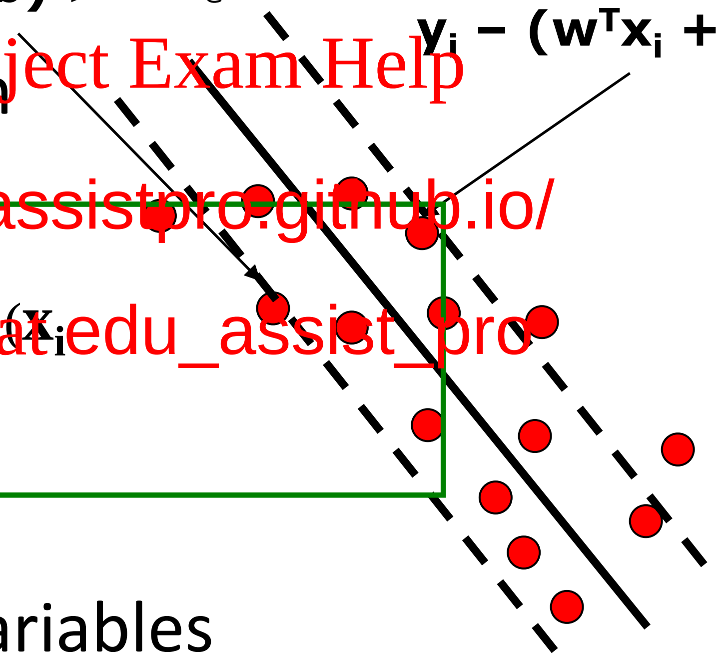
- The classifier is a *separating hyperplane.*
- The most "important" training points are the support vectors; they define the hyperplane.
- Quadratic optimiza ... ich training points $\mathbf{x}_i$ are **support vectors** wit ... ers α_i.
- Both in the dual formulation of the pr ... he solution, training 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

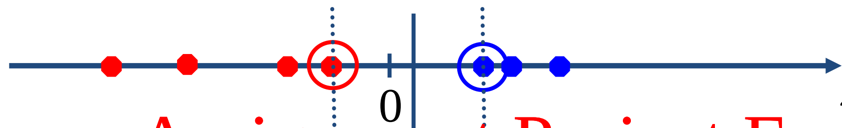


Find **w** and b such that
$\mathbf{\Phi}(\mathbf{w}) = \frac{1}{2}\, \mathbf{w}^T\mathbf{w}$ is minimized and for all $\{(\mathbf{x_i}$
$y_i - (\mathbf{w}^T\mathbf{x_i} + \mathrm{b}) \geq -\ \varepsilon$
$y_i - (\mathbf{w}^T\mathbf{x_i} + \mathrm{b}) \leq \varepsilon$

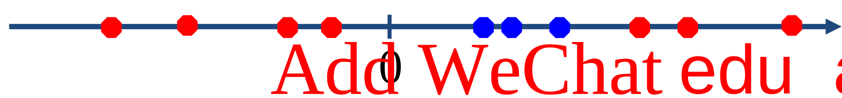
- We can introduce slack variables
  - Similar to soft margin loss function

Non-linear SVMs

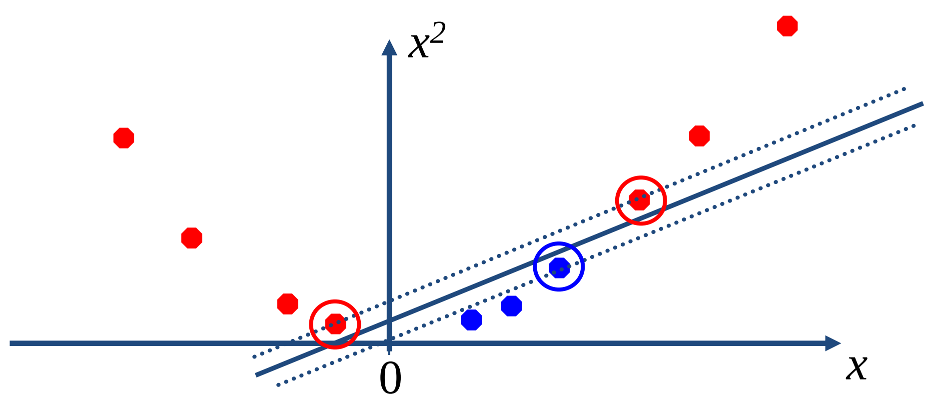
- Datasets that are linearly separable (with some noise) work out great:



- But what are we go oo hard?



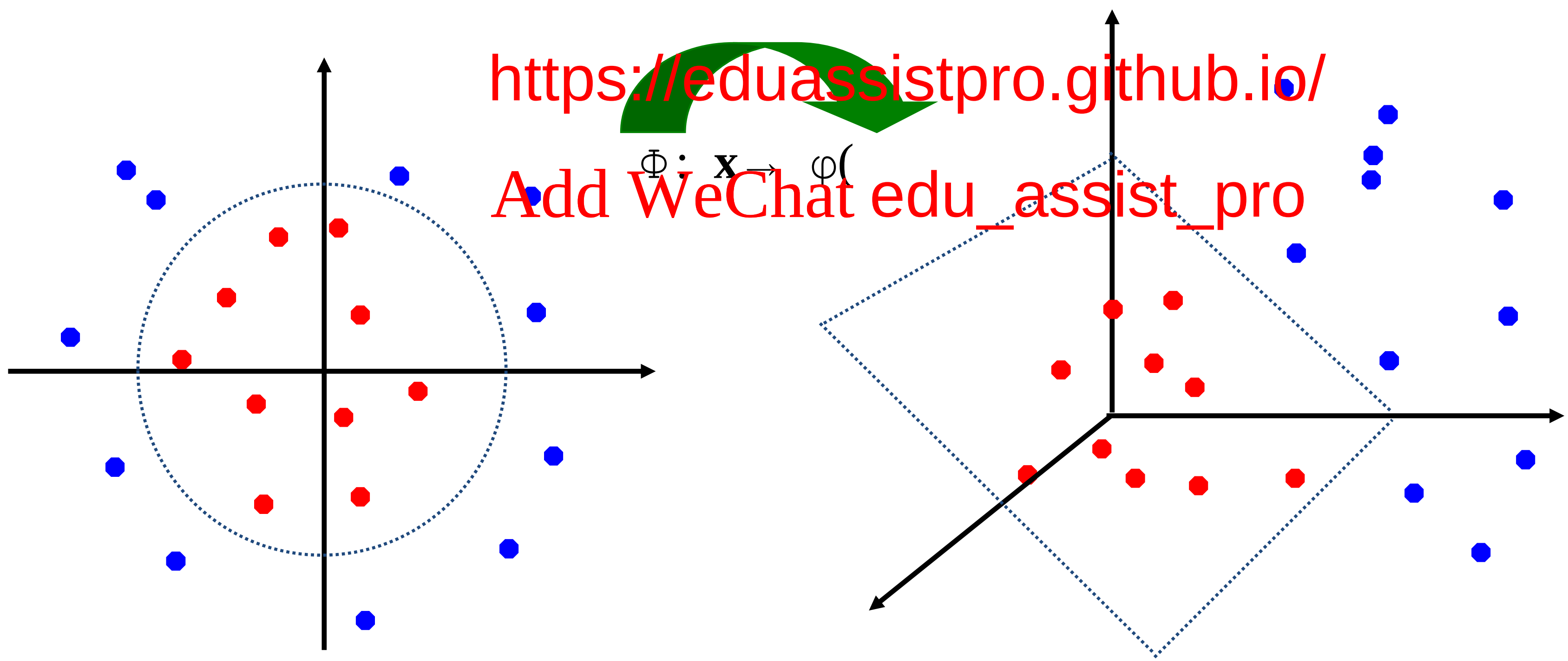
- How about … mapping data to a highe space:



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 transforma r product becomes:

- A *kernel function* is some functio ponds to an inner product in **some** expanded featu
  - 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

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

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-f nation indicates how much to spend
    - e.g., “travel rarely” AND ”high income mbinations
  - NLP, feature vector = 1[w ∈ x] ➔ c dicates two word co-occurrence (where phrase/multi-word expression (MWE) is just a special case)
- $\mathbf{x} \rightarrow \varphi(\mathbf{x})$, 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 ad terms, typically x_i * x_j, to still use linear reg 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 sub

  - inner product in that “enhanced” 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 kern

  - 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

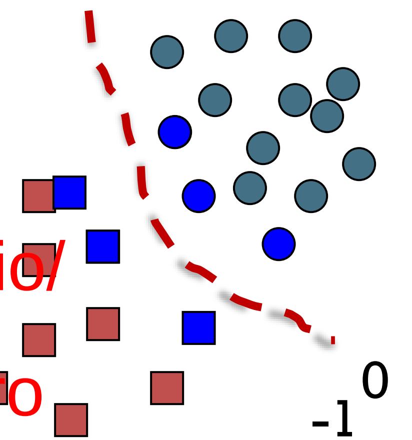
Classification with SVMs **with Kernels**

- 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 cl > 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 c samples
  - Can adapt to different objec rnel)
    - Any K(u, v) can be used if sym ous, 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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- T. Joachims, *Learning to Classify Text using Support Vector Machines*. Kluwer, 2002.
- Fan Li, Yiming Yang. 2003. A Loss Function Analysis for Classification Methods in Text Categorization. ICML 2003: 472-479.
- 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/