CSE 575: Statistical Machine Learning

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Instance-based Learning

1-Nearest Neighbor

Four things make a memory based learner:

1. *A distance metric*

   Euclidian (and many more)

2. *How many nearby neighbors to look at?*

   One

1. *A weighting function (optional)*

   Unused

2. *How to fit with the local points?*

   Just predict the same output as the nearest neighbor.

Consistency of 1-NN

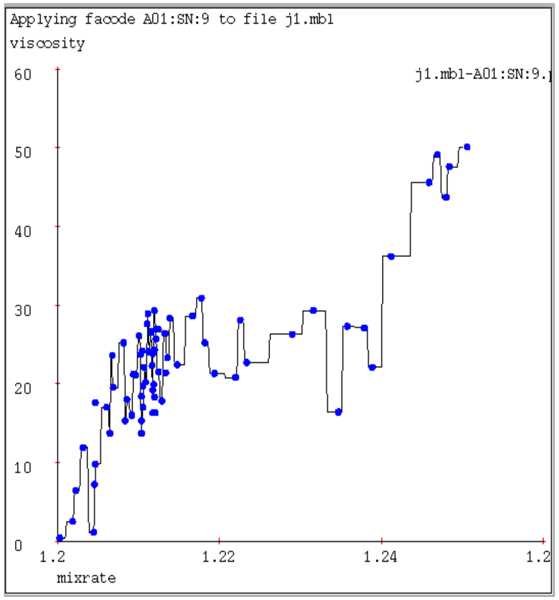
- Consider an estimator f_n trained on n examples
  - e.g., 1-NN, regression, ...
- Estimator is *consistent* if true error goes to zero as amount of data increases
  - e.g., for no noise data, consistent if:

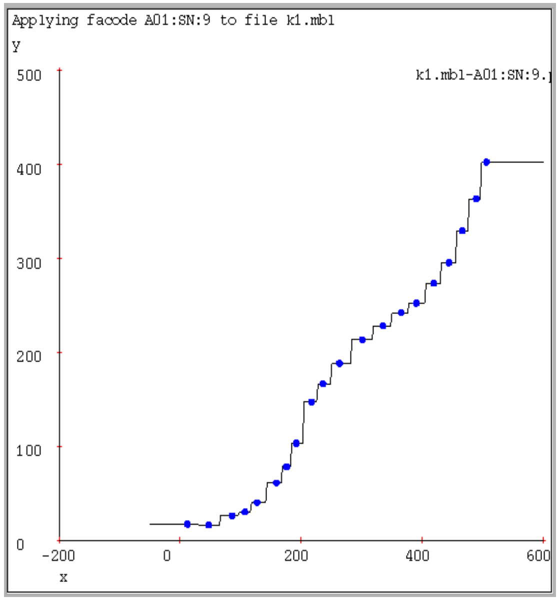
$$\lim_{n \to \infty} MSE(f_n) = 0$$

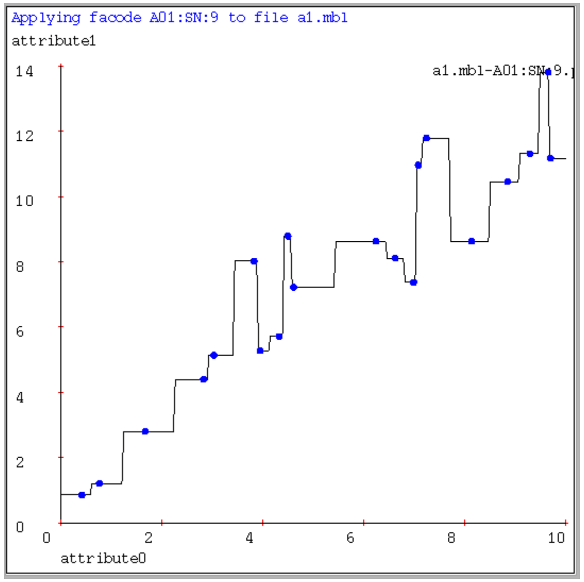
- Regression is not consistent!
  - Representation bias
- **1-NN is consistent** (under some mild fineprint)

What about variance???

1-NN overfits?







k-Nearest Neighbor

Four things make a memory based learner:

1. *A distance metric*

   Euclidian (and many more)

2. *How many nearby neighbors to look at?*

   k

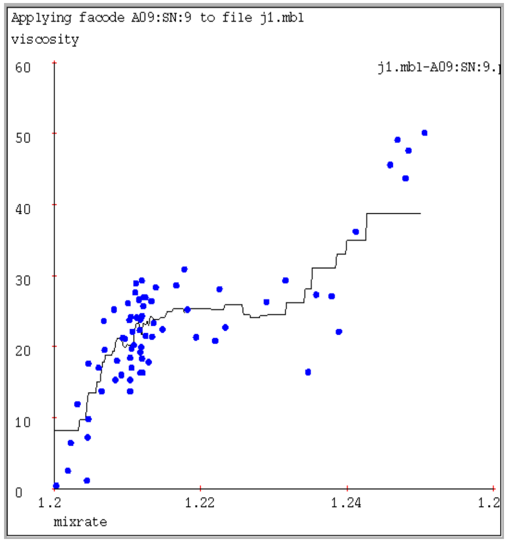
1. *A weighting function (optional)*

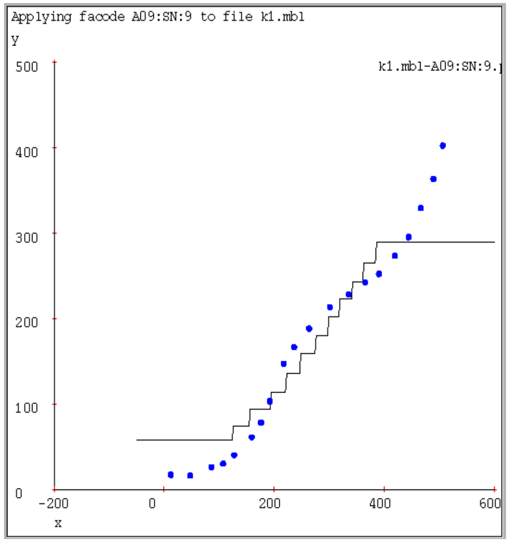
   Unused

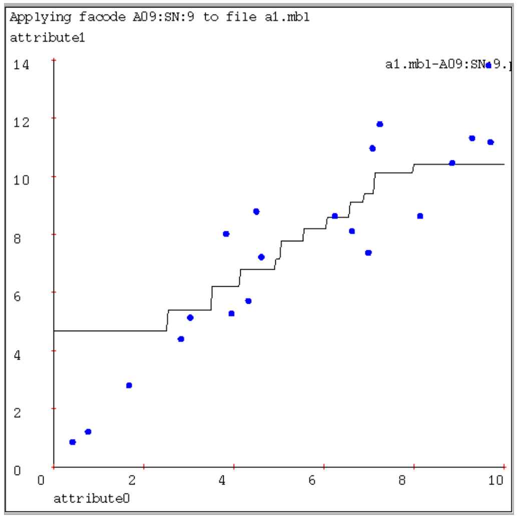
2. *How to fit with the local points?*

   Just predict the average output among the k nearest neighbors.

k-Nearest Neighbor (here k=9)







K-nearest neighbor for function fitting smooth away noise, but there are clear deficiencies.

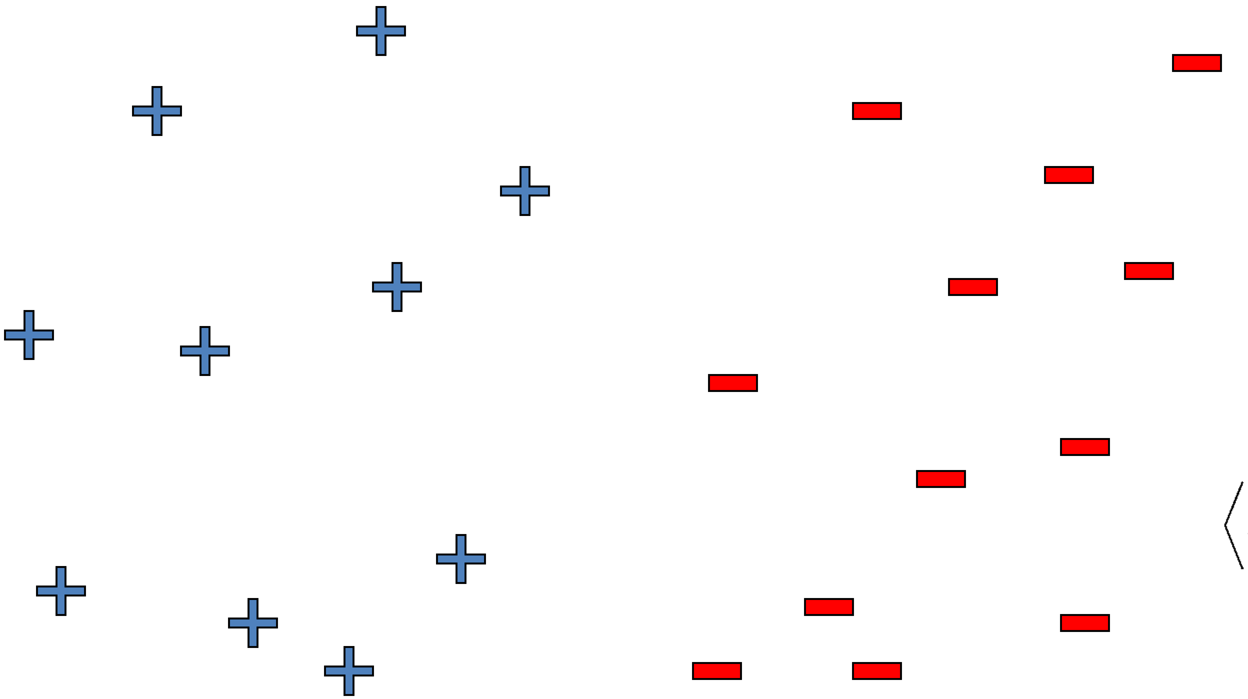
What can we do about all the discontinuities that k-NN gives us?

Curse of dimensionality for instance-based learning

- Must store and retrieve all data!
  - Most real work done during testing
  - For every test sample, must search through all dataset – very slow!
  - There are fast methods for dealing with large datasets, e.g., tree-based methods, hashing methods,
- Instance-based learning often poor with noisy or irrelevant features

Support Vector Machines

Linear classifiers – Which line is better?



Data:

$$\left\langle x_1^{(1)}, \ldots, x_1^{(m)}, y_1 \right\rangle$$
$$\vdots$$
$$\left\langle x_n^{(1)}, \ldots, x_n^{(m)}, y_n \right\rangle$$

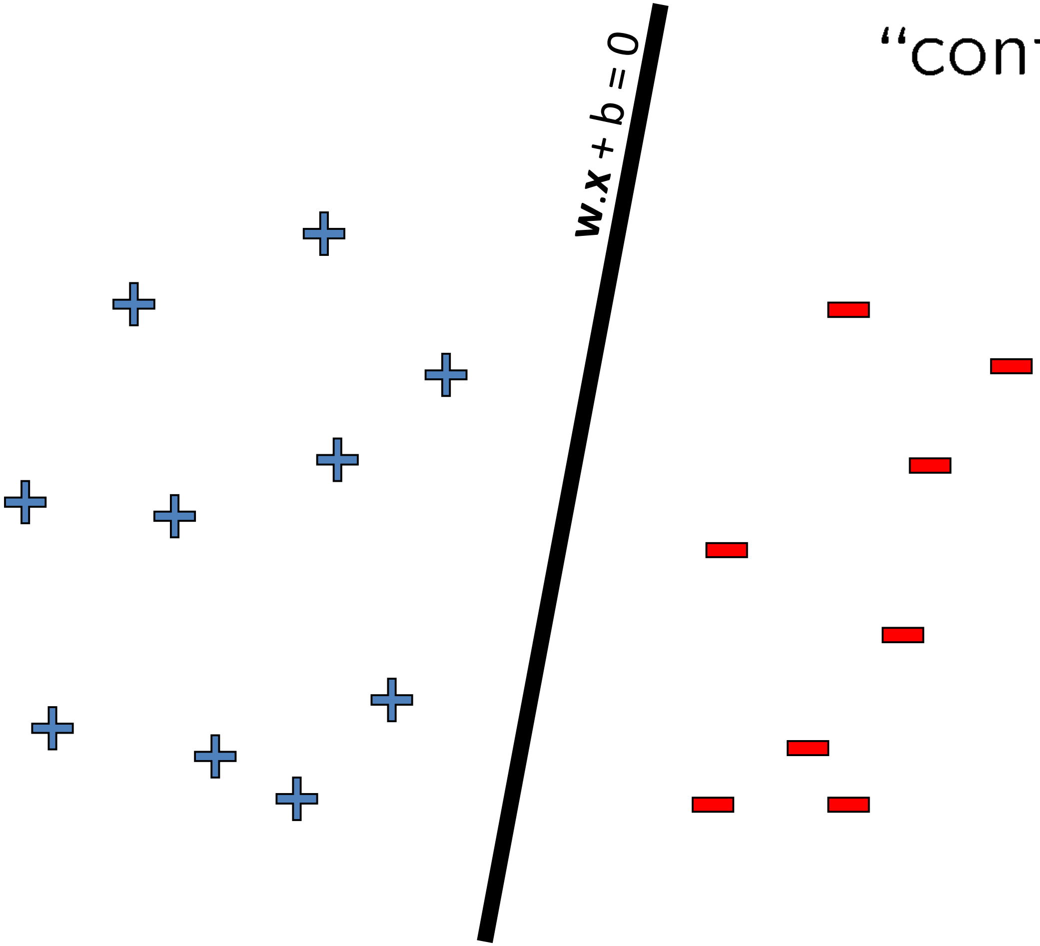
Example i:

$\left\langle x_i^{(1)}, \ldots, x_i^{(m)} \right\rangle$ — m features

$y_i \in \{-1, +1\}$ — class

$\mathbf{w}.\mathbf{x} = \sum_j w^{(j)} x^{(j)}$

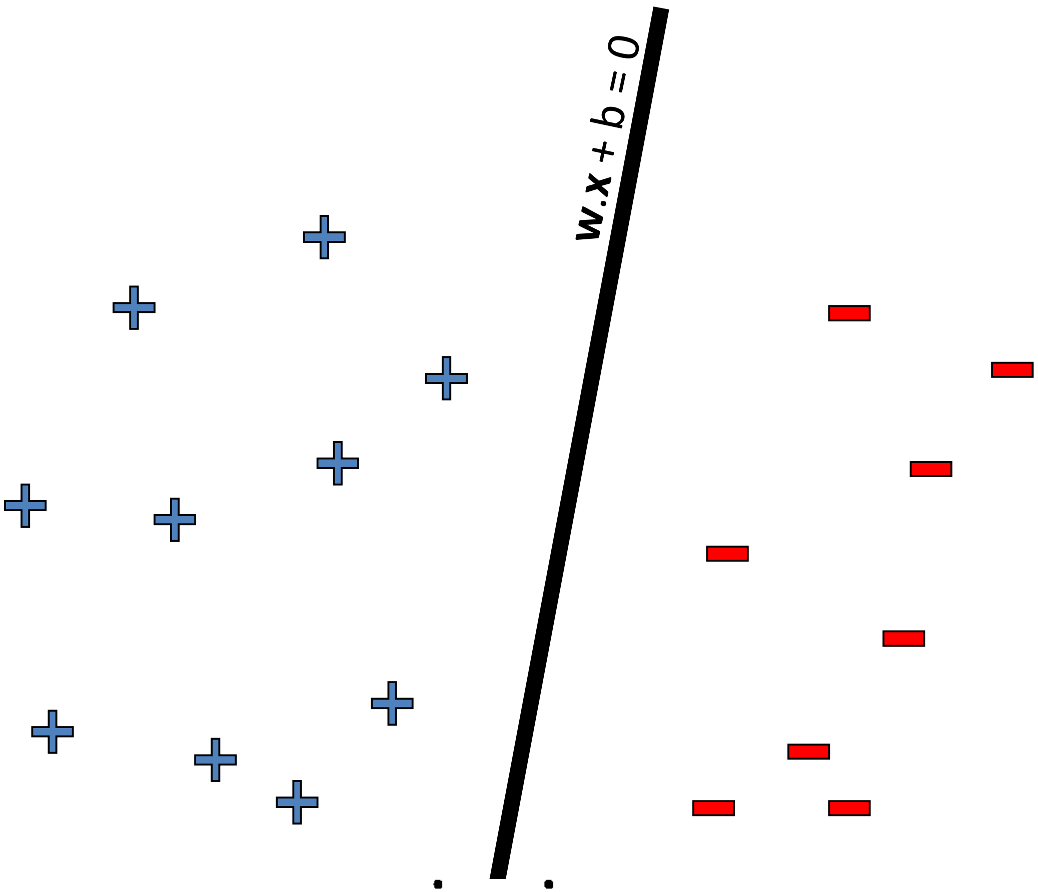
Pick the one with the largest margin!



"confidence" $= \left(\mathbf{w}.\mathbf{x}_j + b\right) y_j$

$\mathbf{w}.\mathbf{x} = \sum_j w^{(j)} x^{(j)}$

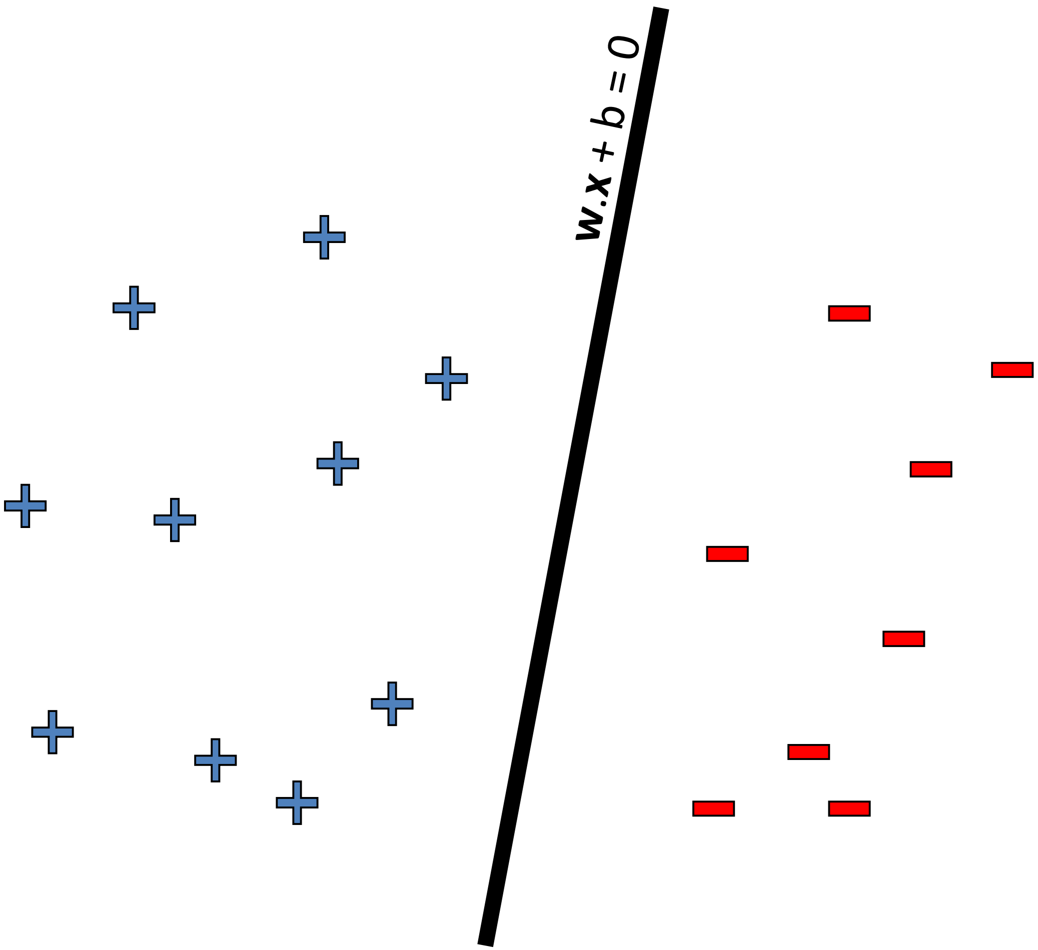
Maximize the margin



$$\text{maximize}_{\gamma,\mathbf{w},b} \quad \gamma$$

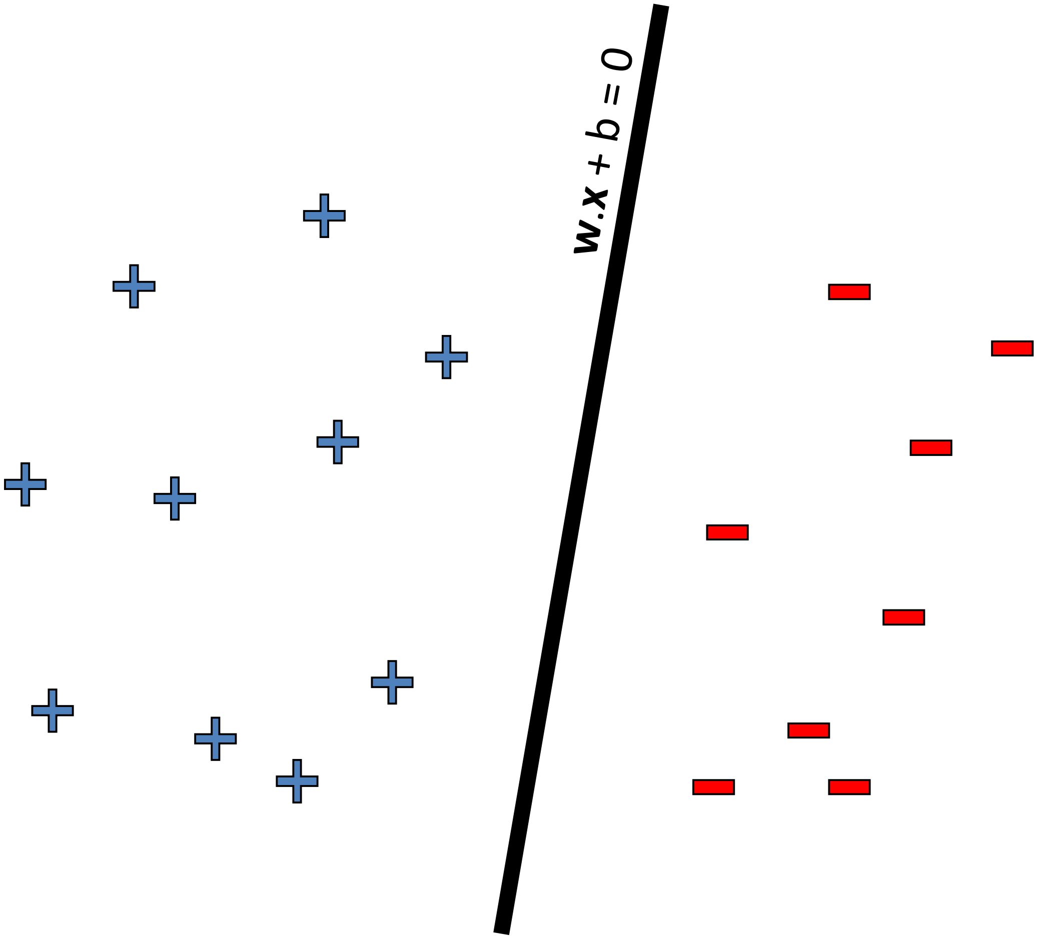
$$\big(\mathbf{w}.\mathbf{x}_j + b\big)\, y_j \geq \gamma,\ \ \forall j \in \text{Dataset}$$

But there are a many planes…



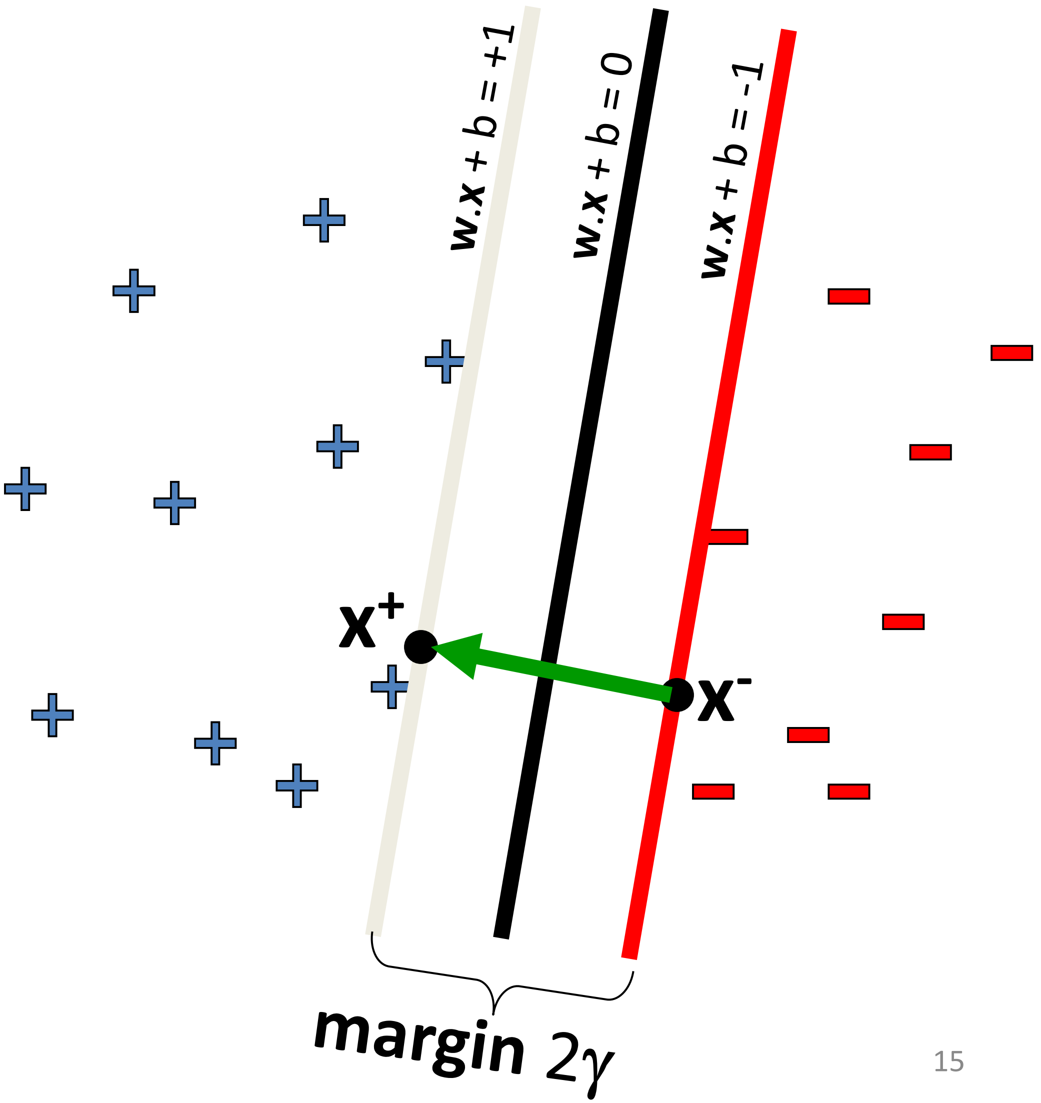
Review: Normal to a plane

$$\mathbf{x}_j = \bar{\mathbf{x}}_j + \lambda \frac{\mathbf{w}}{||\mathbf{w}||}$$

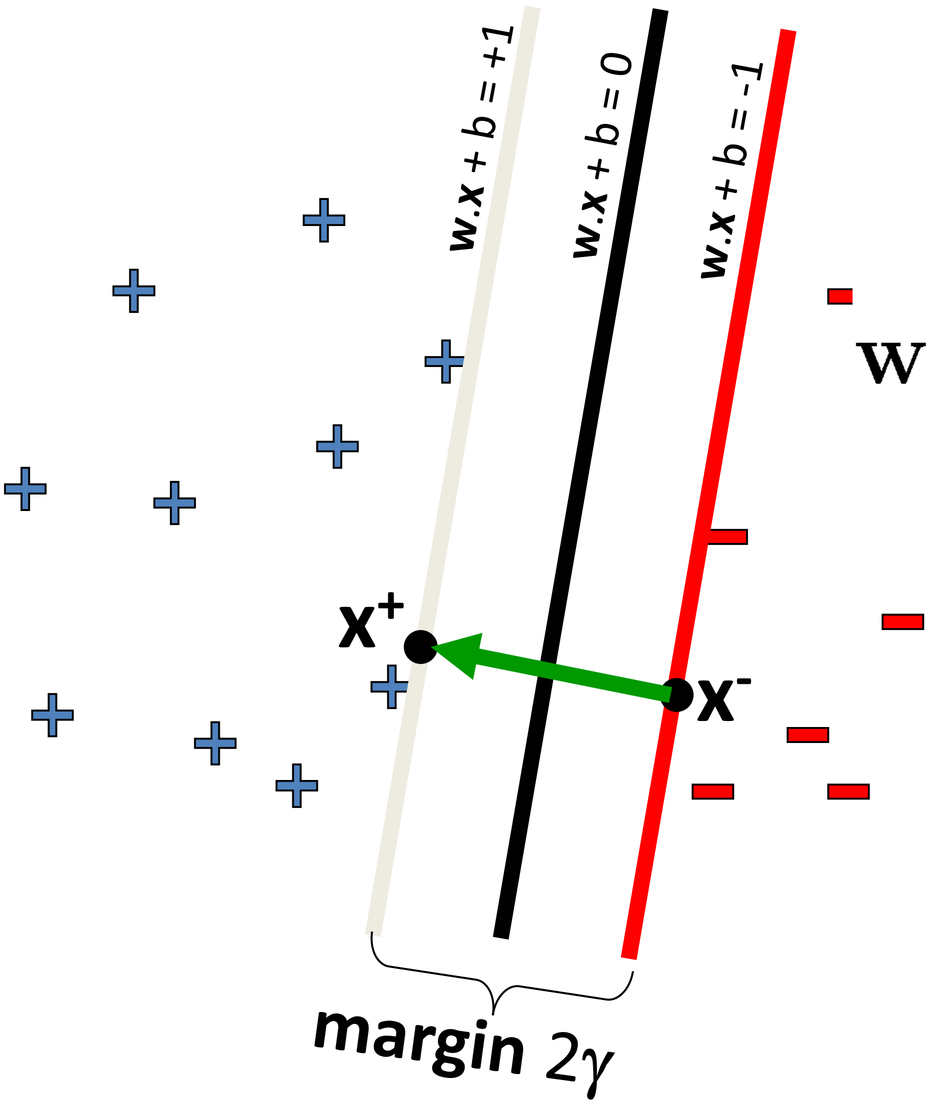


Normalized margin – Canonical hyperplanes

$$\mathbf{x}_j = \bar{\mathbf{x}}_j + \lambda \frac{\mathbf{w}}{||\mathbf{w}||}$$



Normalized margin – Canonical hyperplanes



$$\mathbf{x}^+ = \mathbf{x}^- + \lambda \frac{\mathbf{w}}{||\mathbf{w}||}$$

$$\mathbf{w}.\mathbf{x}^+ + b = 1$$

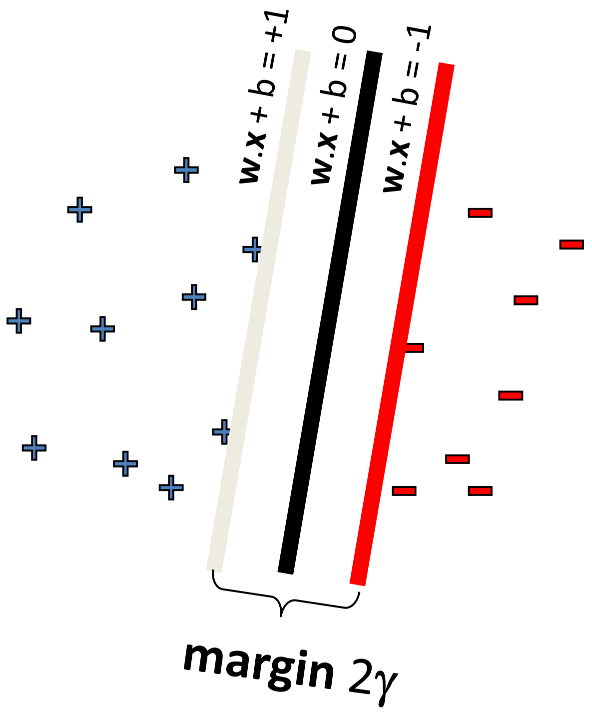
$$\mathbf{w}.(\mathbf{x}^- + \lambda \frac{\mathbf{w}}{||\mathbf{w}||}) + b = 1$$

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

$$\gamma = \frac{1}{\sqrt{\mathbf{w}.\mathbf{w}}}$$

Margin maximization using canonical hyperplanes

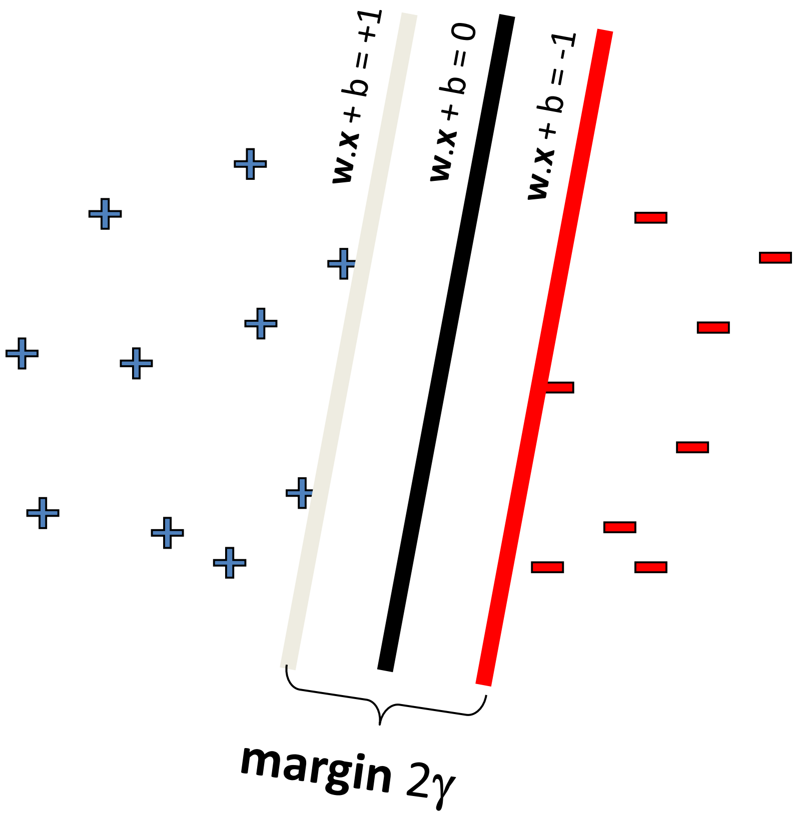
$$\gamma = \frac{1}{\sqrt{\mathbf{w}.\mathbf{w}}}$$



$$\text{maximize}_{\gamma,\mathbf{w},b} \quad \gamma$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq \gamma, \ \forall j \in \text{Dataset}$$

$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \forall j \in \text{Dataset}$$

Support Vector Machines (SVMs)



$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \forall j$$

- Solve efficiently by quadratic programming (QP)
  - Well-studied algorithms
- Hyperplane defined by support vectors

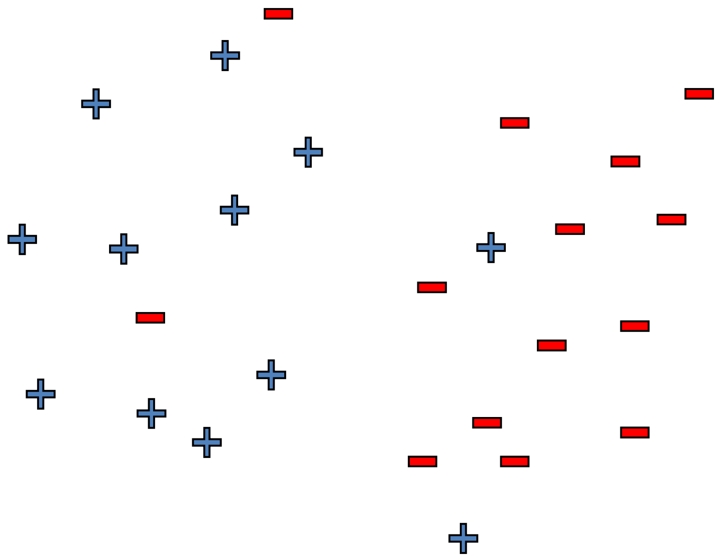
What if the data is not linearly separable?

Use features of features of features of features….

(x, x^2)

What if the data is still not linearly separable?

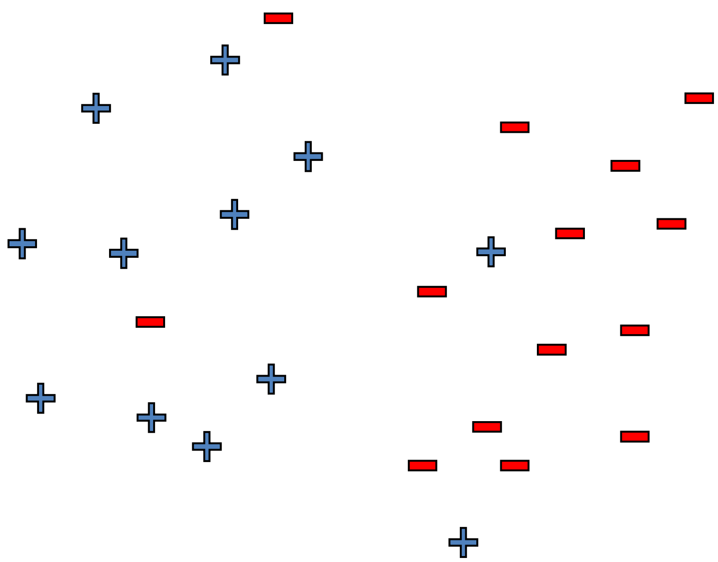
$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 \qquad ,\forall j$$



- Minimize **w.w** and number of training mistakes
  - Tradeoff two criteria?
- Tradeoff #(mistakes) and **w.w**
  - 0/1 loss
  - Slack penalty *C*
  - Not QP anymore
  - Also doesn’t distinguish near misses and really bad mistakes

Slack variables – Hinge loss

$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 \qquad ,\forall j$$



- If margin ≥ 1, don’t care
- If margin < 1, pay linear penalty

Side note: What's the difference between SVMs and logistic regression?

SVM:

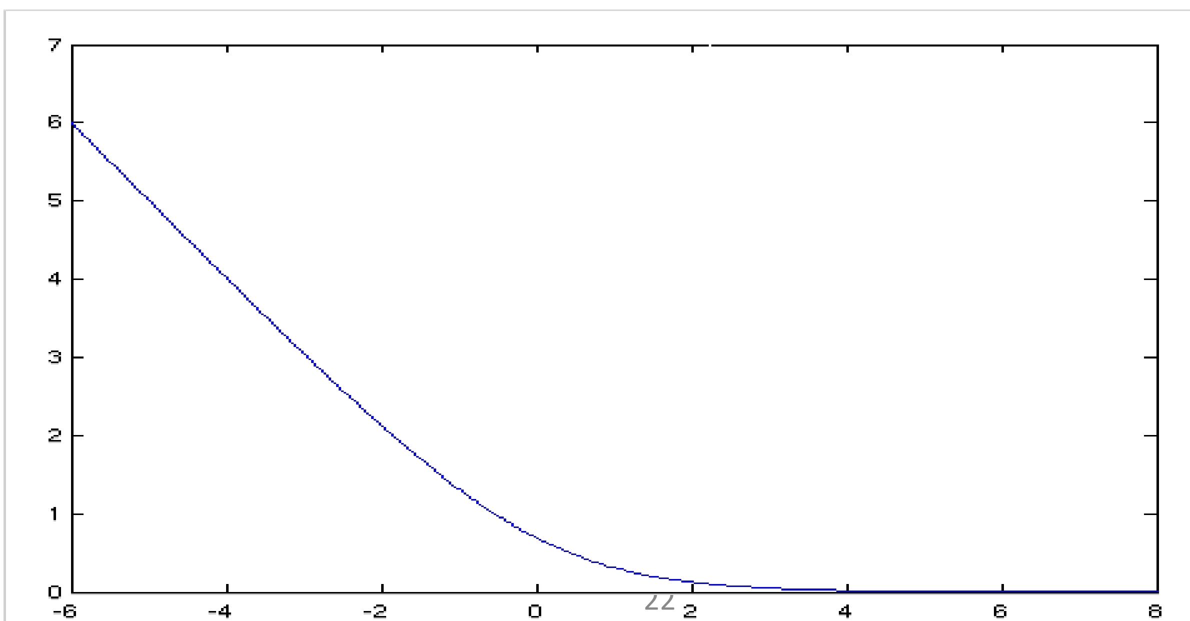
$$\text{minimize}_{\mathbf{w},b} \quad \mathbf{w}.\mathbf{w} + C \sum_j \xi_j$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j, \ \forall j$$
$$\xi_j \geq 0, \ \forall j$$

Logistic regression:

$$P(Y = 1 \mid x, \mathbf{w}) \ = \ \frac{1}{1 + e^{-(\mathbf{w}.\mathbf{x}+b)}}$$

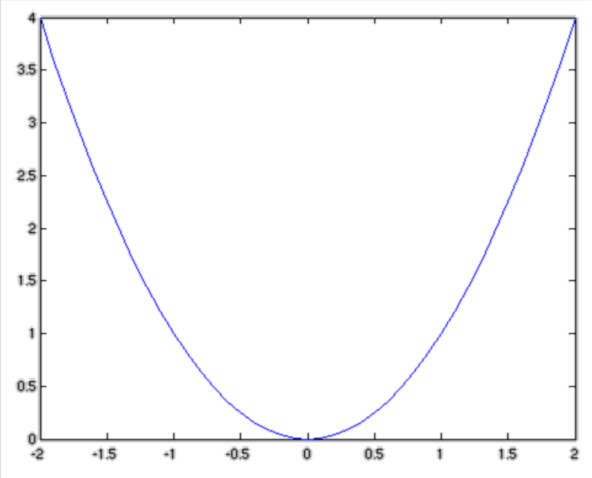
Log loss:

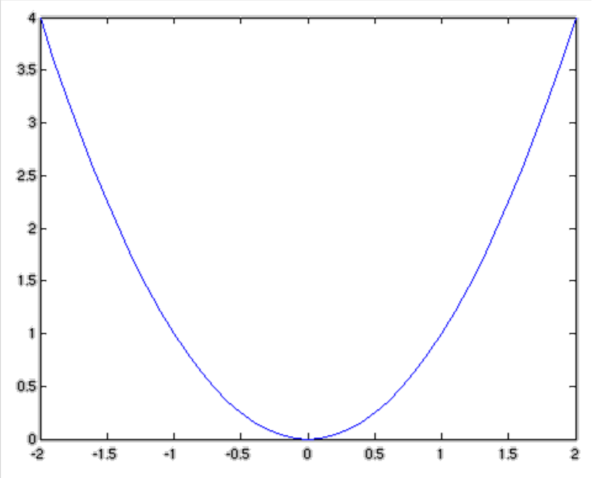
$$-\ln P(Y = 1 \mid x, \mathbf{w}) \ = \ \ln\left(1 + e^{-(\mathbf{w}.\mathbf{x}+b)}\right)$$

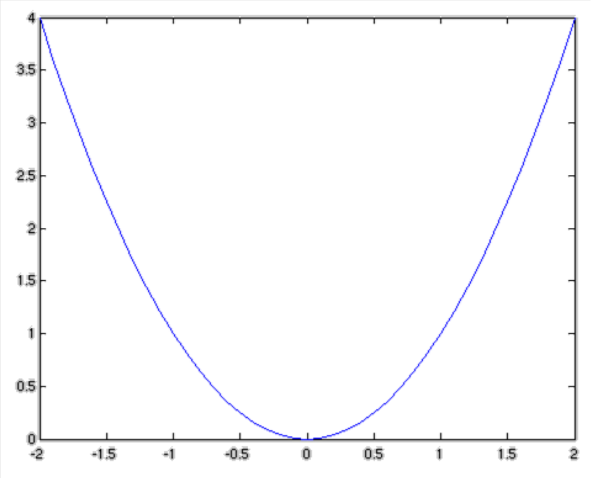


Constrained optimization

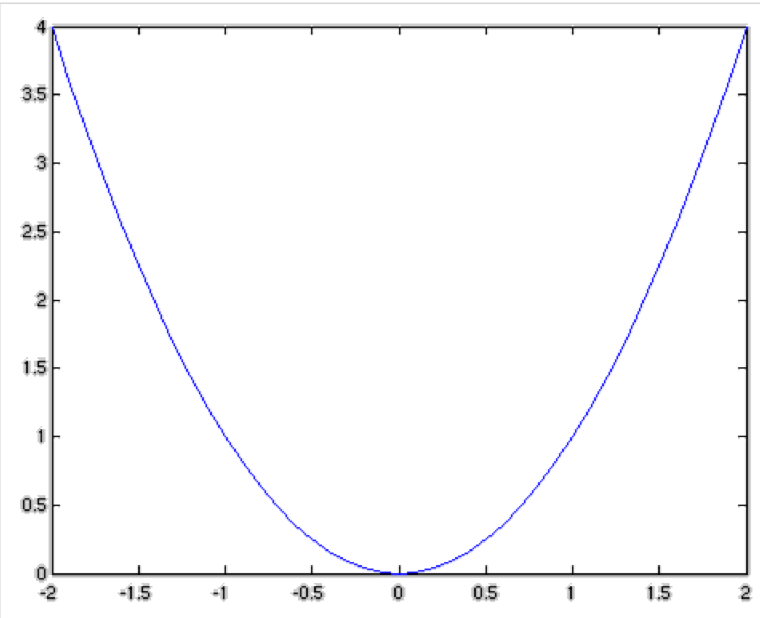
$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq b$$







Lagrange multipliers – Dual variables



$$\min_x \; x^2$$
$$\text{s.t.} \quad x \geq b$$

Moving the constraint to objective function

Lagrangian:

$$L(x, \alpha) = x^2 - \alpha(x - b)$$
$$\text{s.t.} \quad \alpha \geq 0$$

Solve:

$$\min_x \max_\alpha \; L(x, \alpha)$$
$$\text{s.t.} \quad \alpha \geq 0$$

Dual SVM derivation (1) – the linearly separable case

$$\text{minimize}_{\mathbf{w},b} \quad \frac{1}{2}\mathbf{w}.\mathbf{w}$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1,\ \forall j$$

Dual SVM derivation (2) – the linearly separable case

$$L(\mathbf{w}, \alpha) = \frac{1}{2}\mathbf{w}.\mathbf{w} - \sum_j \alpha_j \left[\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j - 1\right]$$

$$\alpha_j \geq 0, \ \forall j$$

$$\mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

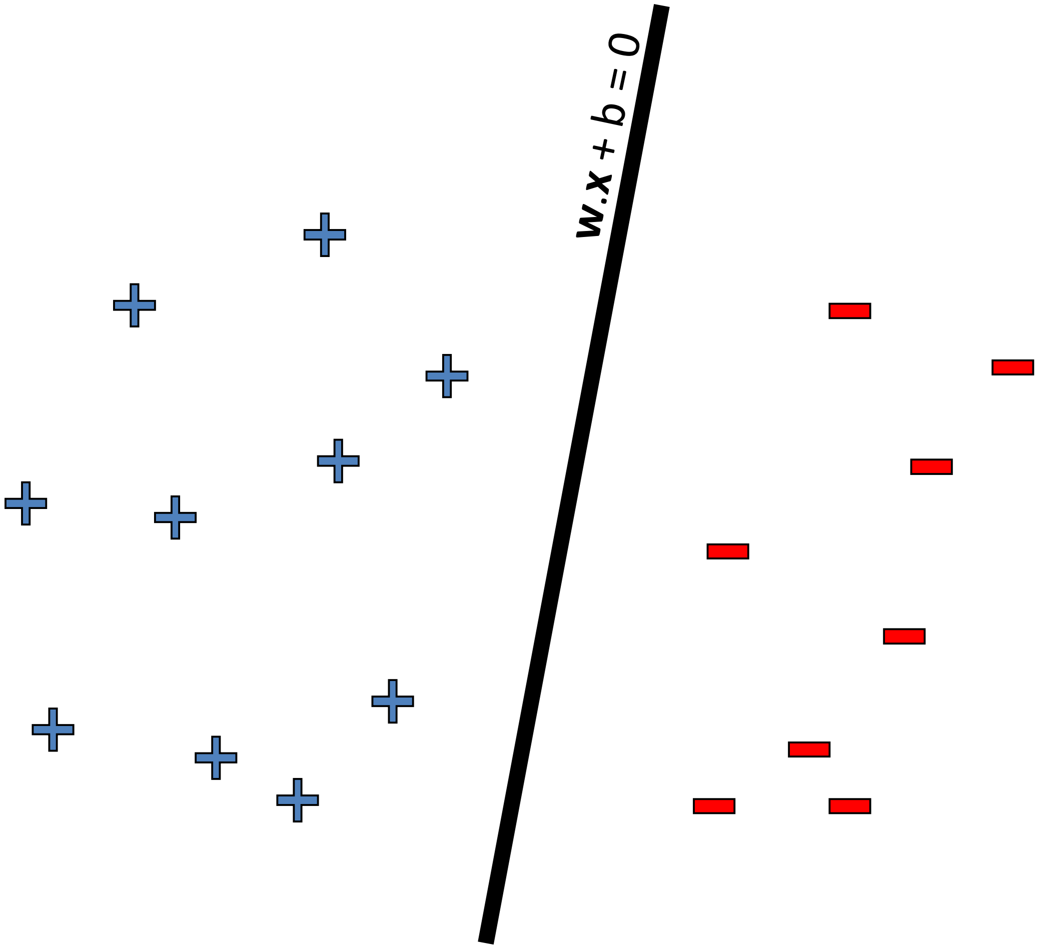
$$\text{minimize}_{\mathbf{w}} \quad \frac{1}{2}\mathbf{w}.\mathbf{w}$$

$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \forall j$$

$$b = y_k - \mathbf{w}.\mathbf{x}_k$$

for any k where $\alpha_k > 0$

Dual SVM interpretation



$$\mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

Dual SVM formulation – the linearly separable case

maximize$_\alpha$ $\sum_i \alpha_i - \frac{1}{2}\sum_{i,j}\alpha_i\alpha_j y_i y_j \mathbf{x}_i\mathbf{x}_j$

$\sum_i \alpha_i y_i = 0$
$\alpha_i \geq 0$

$$\boxed{\begin{array}{l} \mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i \\ b = y_k - \mathbf{w}.\mathbf{x}_k \\ \text{for any } k \text{ where } \alpha_k > 0 \end{array}}$$

Dual SVM derivation – the non-separable case

$$\text{minimize}_{\mathbf{w},b} \quad \frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_j \xi_j$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j,\ \forall j$$
$$\xi_j \geq 0,\ \forall j$$

Dual SVM formulation – the non-separable case

maximize$_\alpha$ $\sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j$

$\sum_i \alpha_i y_i = 0$
$C \geq \alpha_i \geq 0$

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

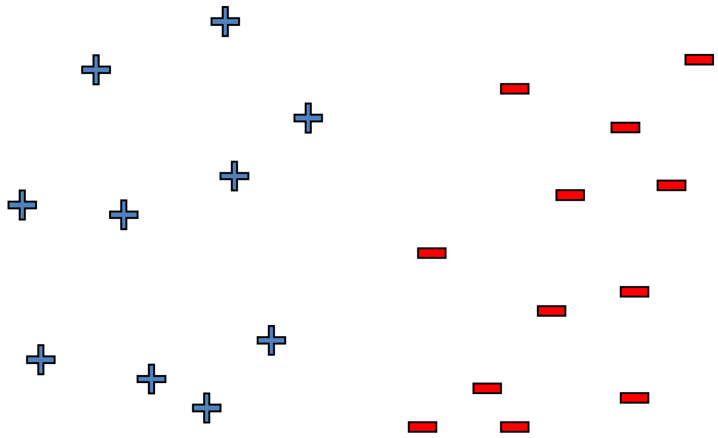
$$b = y_k - \mathbf{w}.\mathbf{x}_k$$

for any k where $C > \alpha_k > 0$

Why did we learn about the dual SVM?

- There are some quadratic programming algorithms that can solve the dual faster than the primal
- But, more importantly, the "**kernel trick**"!!!
  - Another little detour…

Reminder from last time: What if the data is not linearly separable?



Use features of features of features of features….

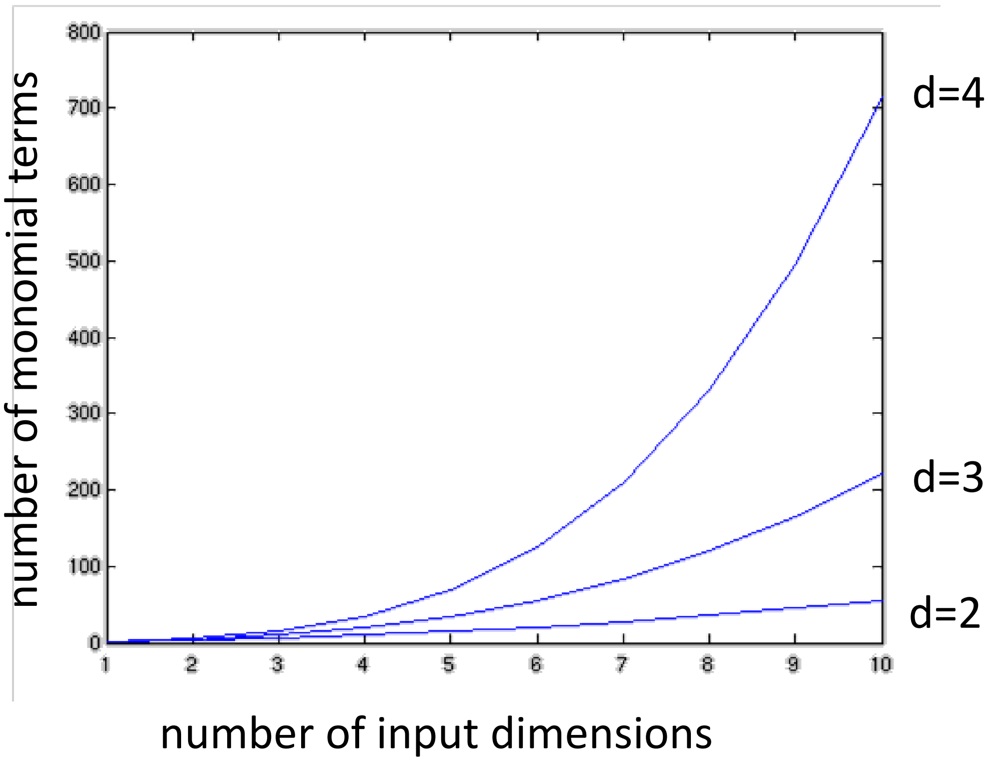
$$\Phi(\mathbf{x}) : R^m \mapsto F$$

Feature space can get really large really quickly!

Higher order polynomials

$$\text{num. terms} = \binom{d+m-1}{d} = \frac{(d+m-1)!}{d!(m-1)!}$$

m – input features
d – degree of polynomial



grows fast!
d = 6, m = 100
about 1.6 billion terms

Dual formulation only depends on dot-products, not on **w**!

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j$$

$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$
$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

Dot-product of polynomials

$$\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = \text{polynomials of degree d}$$

Finally: the "kernel trick"!

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i\alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$
$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

$$\boxed{\begin{array}{l} \mathbf{w} = \sum_i \alpha_i y_i \Phi(\mathbf{x}_i) \\ b = y_k - \mathbf{w}.\Phi(\mathbf{x}_k) \\ \text{for any } k \text{ where } C > \alpha_k > 0 \end{array}}$$

- Never represent features explicitly
  - Compute dot products in closed form
- Constant-time high-dimensional dot-products for many classes of features

- Very interesting theory – Reproducing Kernel Hilbert Spaces

Polynomial kernels

- All monomials of degree d in O(d) operations:

$$\Phi(\mathbf{u})\cdot\Phi(\mathbf{v}) = (\mathbf{u}\cdot\mathbf{v})^d = \text{polynomials of degree d}$$

- How about all monomials of degree up to d?
  - Solution 0:
  - Better solution:

Common kernels

- Polynomials of degree d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^d$$

- Polynomials of degree up to d

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^d$$

- Gaussian kernels

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||}{2\sigma^2}\right)$$

- Sigmoid

$$K(\mathbf{u}, \mathbf{v}) = \tanh(\eta \mathbf{u} \cdot \mathbf{v} + \nu)$$

Overfitting?

- Huge feature space with kernels, what about overfitting???
  - Maximizing margin leads to sparse set of support vectors
  - Some interesting theory says that SVMs search for simple hypothesis with large margin
  - Often robust to overfitting

What about at classification time

- For a new input **x**, if we need to represent Φ(**x**), we are in trouble!
- Recall classifier: sign(**w**.Φ(**x**)+b)
- Using kernels we are cool!

$$K(\mathbf{u}, \mathbf{v}) = \Phi(\mathbf{u}) \cdot \Phi(\mathbf{v})$$

$$\mathbf{w} = \sum_i \alpha_i y_i \Phi(\mathbf{x}_i)$$

$$b = y_k - \mathbf{w}.\Phi(\mathbf{x}_k)$$

for any k where $C > \alpha_k > 0$

SVMs with kernels

- Choose a set of features and kernel function
- Solve dual problem to obtain support vectors α_i
- At classification time, compute:

$$\mathbf{w} \cdot \Phi(\mathbf{x}) = \sum_i \alpha_i y_i K(\mathbf{x}, \mathbf{x}_i)$$

$$b = y_k - \sum_i \alpha_i y_i K(\mathbf{x}_k, \mathbf{x}_i)$$

for any k where $C > \alpha_k > 0$

Classify as

$$sign\left(\mathbf{w} \cdot \Phi(\mathbf{x}) + b\right)$$

What's the difference between SVMs and Logistic Regression?

	SVMs	Logistic Regression
Loss function	Hinge loss	Log-loss
High dimensional features with kernels	Yes!	Yes!
Solution sparse	Often yes!	Almost always no!
Semantics of output	"Margin"	Real probabilities