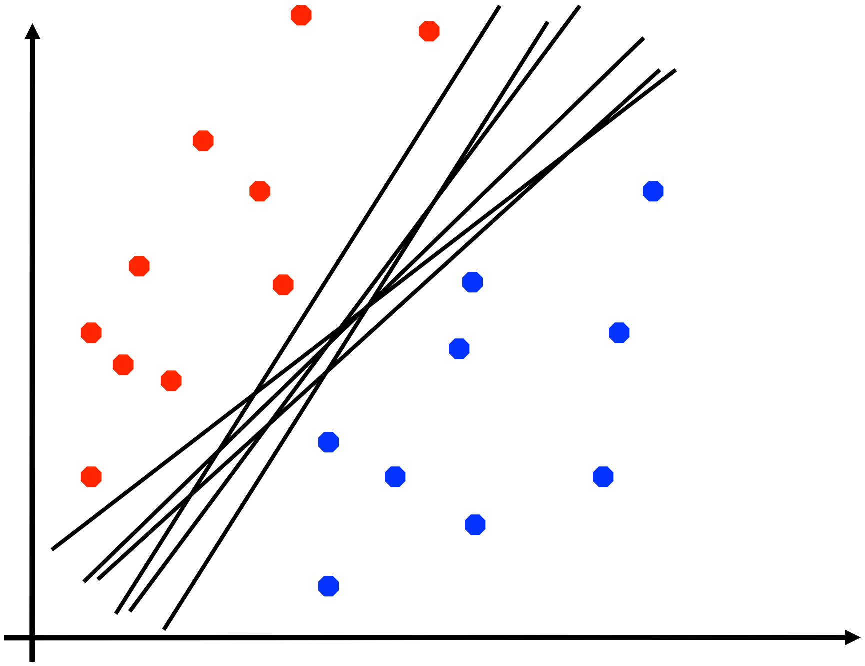
Machine Learning
Support Vector Machines (SVMs), Part 1

Slides adapted from David Sontag, who adapted from Luke Zettlemoyer, Vibhav Gogate, and Carlos Guestrin

Linear Separators

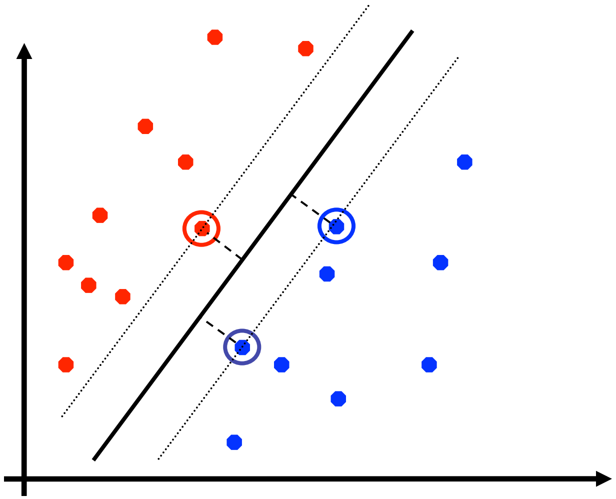
- If training data is linearly separable, perceptron is guaranteed to find *some* linear separator
- Which of these is **optimal**? How do we define optimal?



Support Vector Machine (SVM)

- SVMs (Vapnik, 1990's) choose the linear separator with the **largest margin**

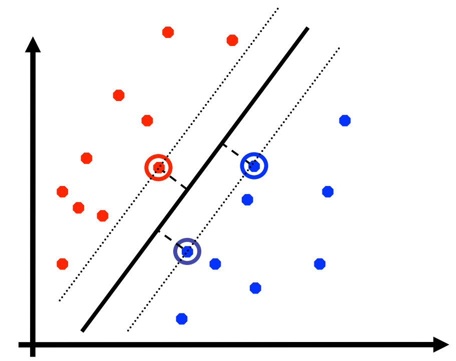
Robust to outliers!



V. Vapnik

- Good according to intuition, theory, practice
- SVM became famous when, using images as input, it gave accuracy comparable to neural-network in a handwriting recognition task

Support vector machines: 3 key ideas



1. Use **optimization** to find solution with largest margin

2. Seek **large margin** separator while allowing for some test errors

3. Use **kernel trick** to make large non-linear feature spaces computationally efficient

Optimization Problem

- Assume for now data is linearly separable
- Goal: Formulate the max margin problem as a tractable optimization problem:
  - Maximize an objective function subject to constraints, giving optimal **w** and b.

Going to show for SVM

Minimize over **w**, b:

$$\mathbf{w}\bullet\mathbf{w} + C\,\Sigma_i \max(\,0,\ 1 - y^{(i)}\,(\mathbf{w}\bullet\mathbf{x}^{(i)}+b)\,)$$

- C is a positive constant. Use the C that gives lowest validation error
- For given C, can find optimal **w**,b using a variation of gradient descent

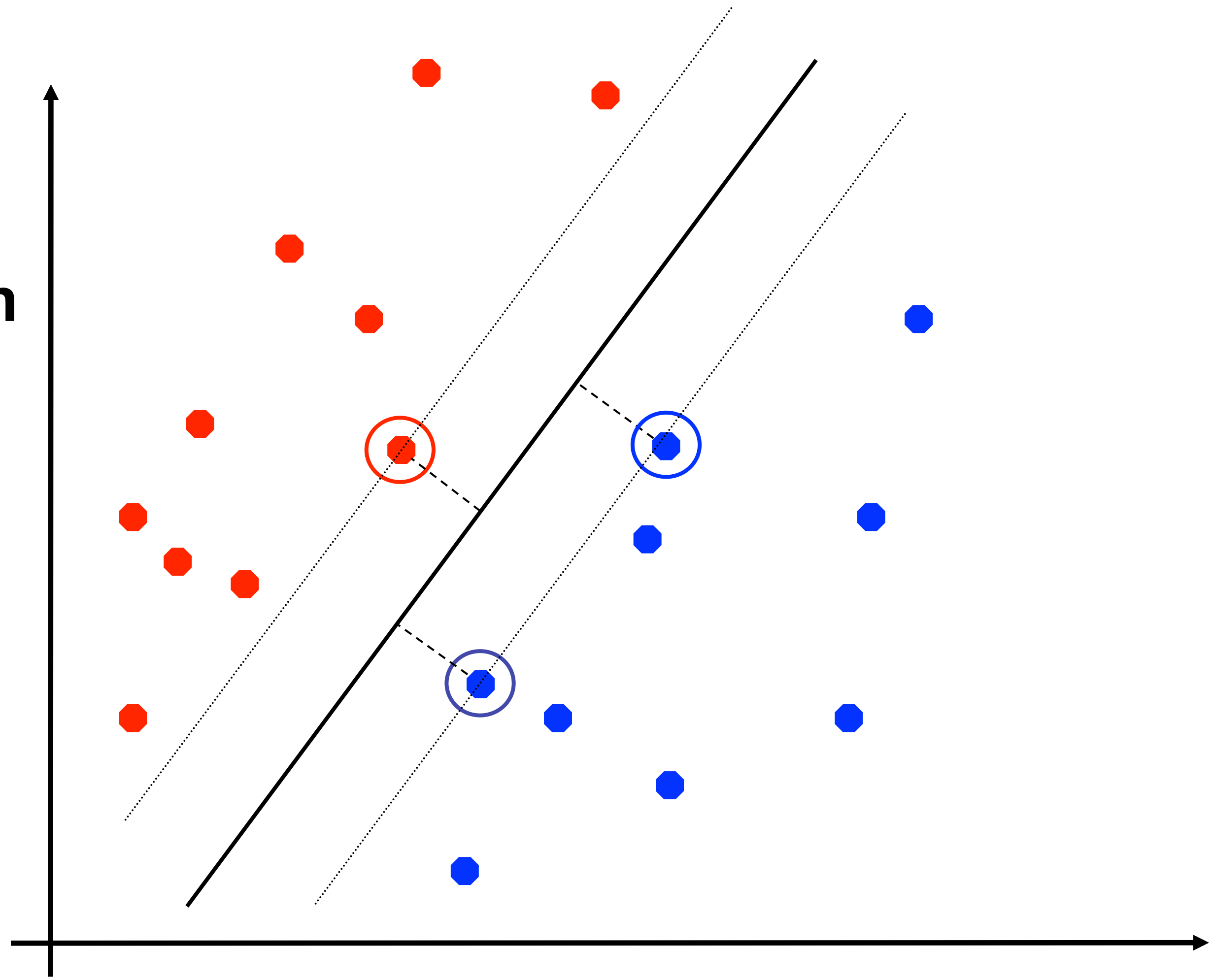
A Few Words About Linear Programming

- Class of constrained optimization problems
- Examples given on board
- Well studied, can solve problems with millions of variables and constraints
  - Many software packages, textbooks

Maximize Margin Optimization Problem

For data point $\mathbf{x}^{(i)}$ let $\delta^{(i)}$ be the distance to the plane. The **margin** is $\delta := \min \delta^{(i)}$

We want to find a hyperplane (ie, $\mathbf{w}$ and b) that maximizes δ. To this end, let's calculate $\delta^{(i)}$

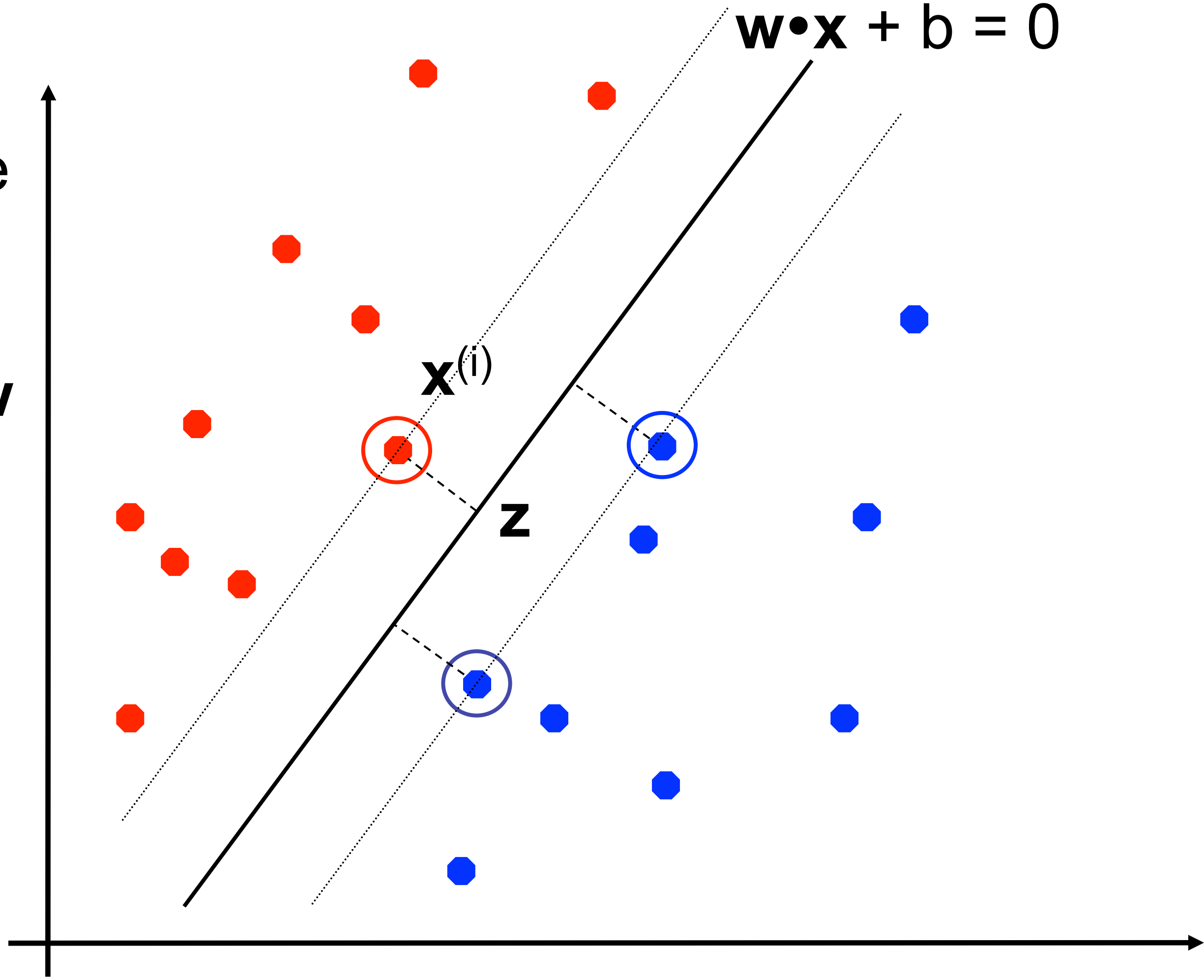


How can we calculate $\delta^{(i)}$?

Quiz: find $\delta^{(i)}$ in terms of **w**, b, and $\mathbf{x}^{(i)}$

- Let **z** be point on plane nearest to $\mathbf{x}^{(i)}$
- $\delta^{(i)} = |\mathbf{x}^{(i)} - \mathbf{z}\,|$
- (Assume first $\mathbf{x}^{(i)}$ and **w** on same side of plane.)
- Note **w** and $\mathbf{x}^{(i)} - \mathbf{z}$ point in same direction
- $(\mathbf{x}^{(i)} - \mathbf{z}) / \delta^{(i)} = \mathbf{w}/||\mathbf{w}||$

- Since **z** is on plane:
$\mathbf{w}\bullet\mathbf{z} + b = 0$



Complete quiz!

Answer:

$$\delta^{(i)} = y^{(i)}(\mathbf{w} \bullet \mathbf{x}^{(i)} + b)/|\mathbf{w}|$$

Thus if:

$$y^{(i)}(\mathbf{w} \bullet \mathbf{x}^{(i)} + b)/|\mathbf{w}| \geq \delta \quad \text{for all } i$$

then margin will be at least δ.

Margin Optimization Problem

Therefore, to maximize the margin, want to choose **w** and b to

maximize δ

subject to:

$$y^{(i)}(\mathbf{w}\bullet\mathbf{x}^{(i)} + b)/|\mathbf{w}| \geq \delta \quad \text{for all } i = 1,\ldots,m$$

Problem: Constraints are nonlinear. Difficult to solve.

Convert to Tractable Problem

Claim: If data is linearly separable, there exists $\mathbf{w}$, b such that:

- for all positive examples ($y^{(i)} = 1$):

  $\mathbf{w} \bullet \mathbf{x}^{(i)} + b \geq 1$

- for all negative examples ($y^{(i)} = -1$):

  $\mathbf{w} \bullet \mathbf{x}^{(i)} + b \leq -1$

Prove it now !

Thus, $y^{(i)} (\mathbf{w} \bullet \mathbf{x}^{(i)} + b) \geq 1$ for all $i = 1,2,\ldots,m$

Maximum Margin: Tractable

Theorem: Let **w**, b be an optimal solution to:

Minimize $||\mathbf{w}||^2 = w_1^2 + w_2^2 + \ldots + w_n^2$

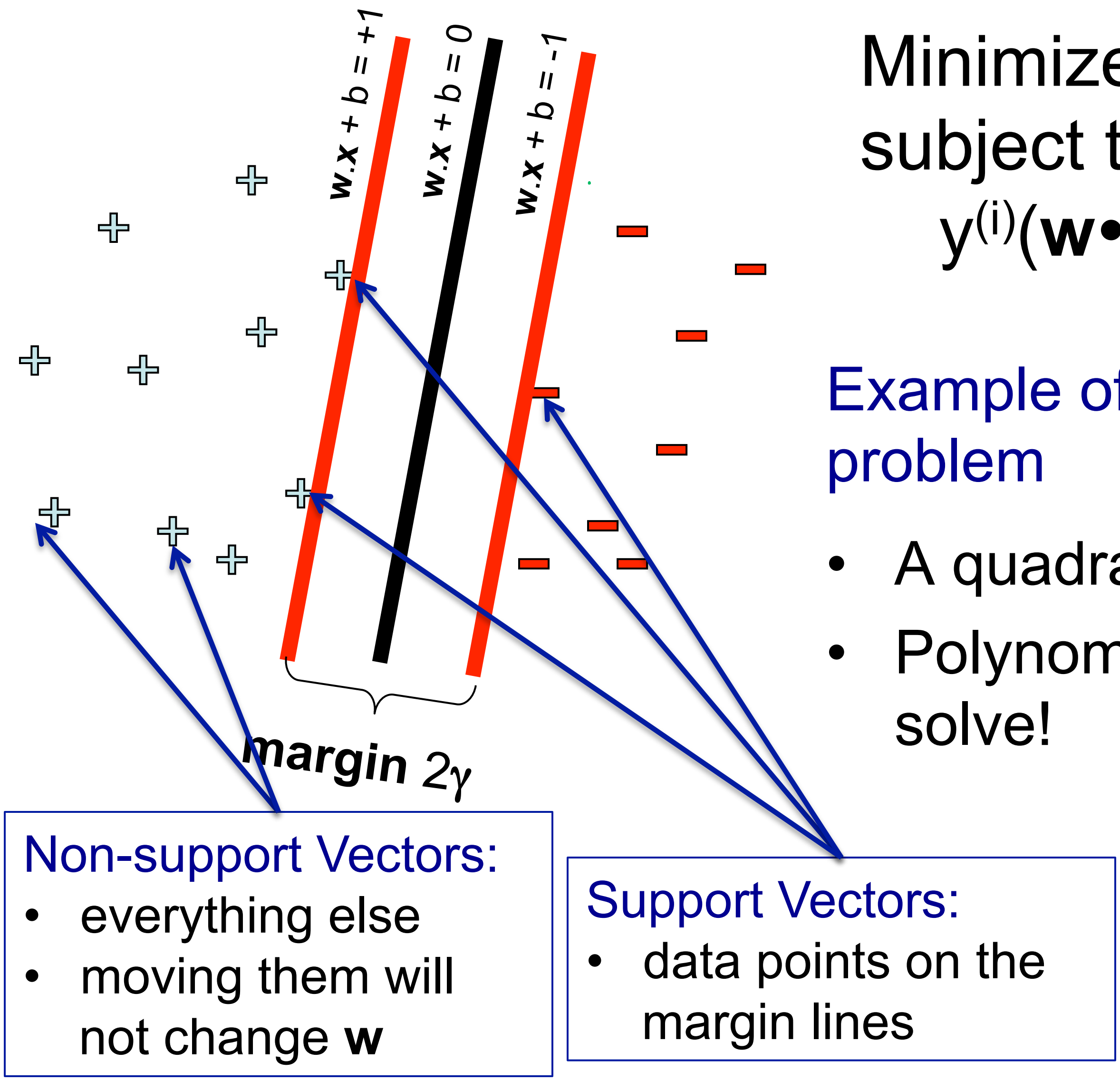
subject to:

$y^{(i)}(\mathbf{w} \bullet \mathbf{x}^{(i)} + b) \geq 1$ for all $i = 1, 2, \ldots, m$

Then $\mathbf{w} \bullet \mathbf{x} + b = 0$ is a hyperplane that provides the maximum margin.

Proof: Not hard. See notes by Andrew Ng.

(Hard margin) Support Vector Machines

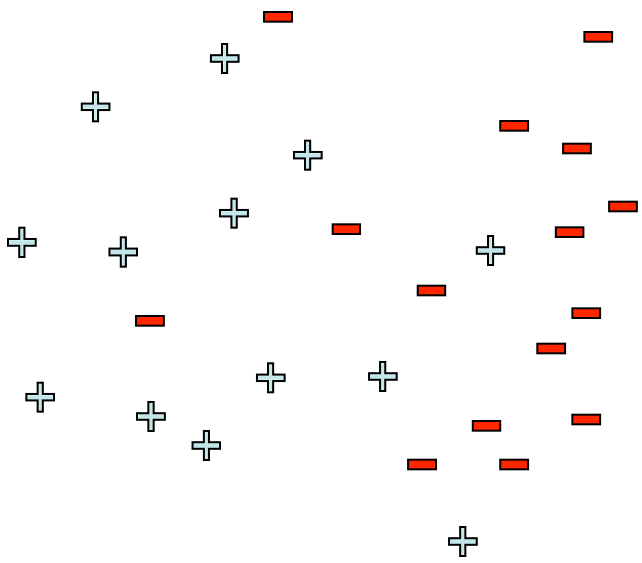


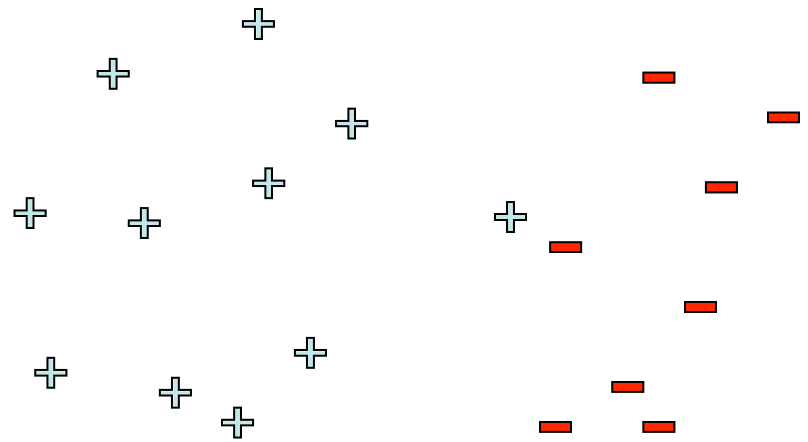
Minimize $||\mathbf{w}||^2$
subject to:
$$y^{(i)}(\mathbf{w} \bullet \mathbf{x}^{(i)} + b) \geq 1 \text{ for all } i$$

Example of a **convex optimization** problem

- A quadratic program
- Polynomial-time algorithms to solve!

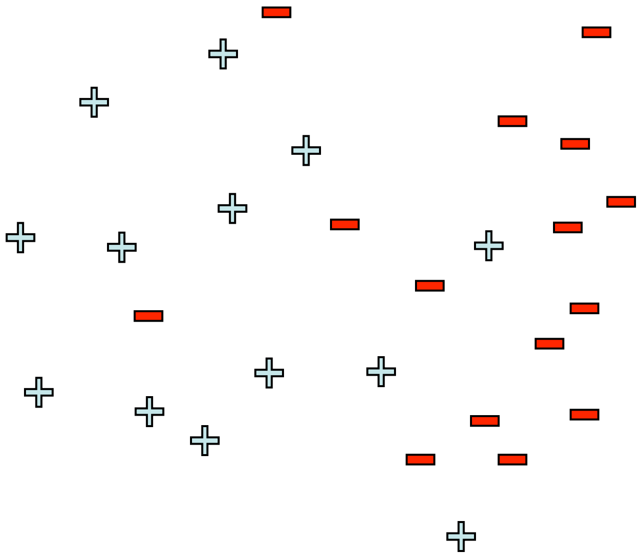
But what if you have:





non-separable <u>or</u> separable

Non-separable Data: 0-1 Loss

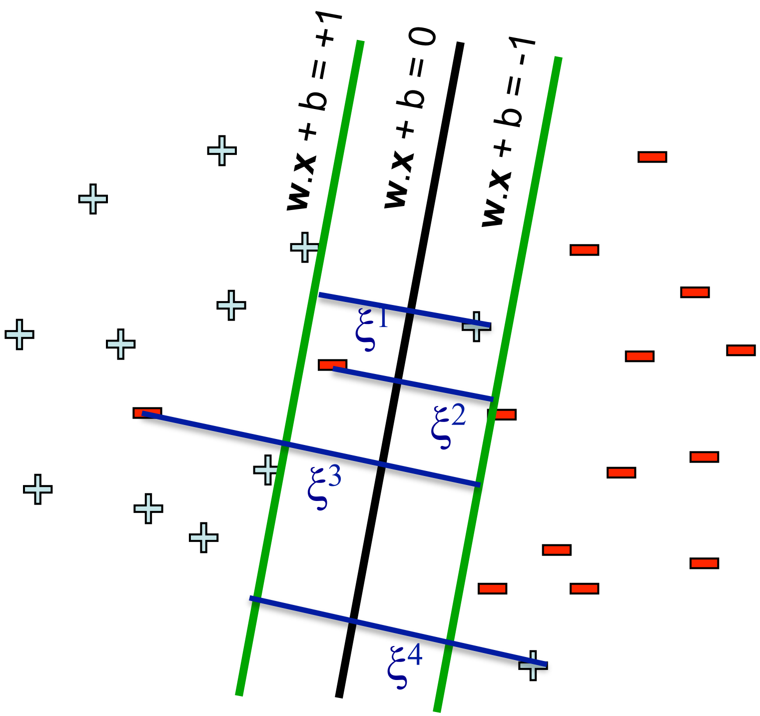


- Natural objective: Find hyperplane that violates as few constraints as possible. Mathematically, find **w**, b that minimizes

$$\sum_i 1(\, y^{(i)}(\mathbf{w} \bullet \mathbf{x}^{(i)} + b) < 0 \,)$$

- Called "0-1 loss"
- Unfortunately, this is an NP-hard problem.

Instead consider following LP



$$\text{Minimize}_{\mathbf{w},b,\xi} \sum_i \xi^{(i)}$$

s.t.

$$(\mathbf{w} \cdot \mathbf{x}^{(i)} + b) y^{(i)} \geq 1 - \xi^{(i)} \text{ for all i}$$

"slack variables"

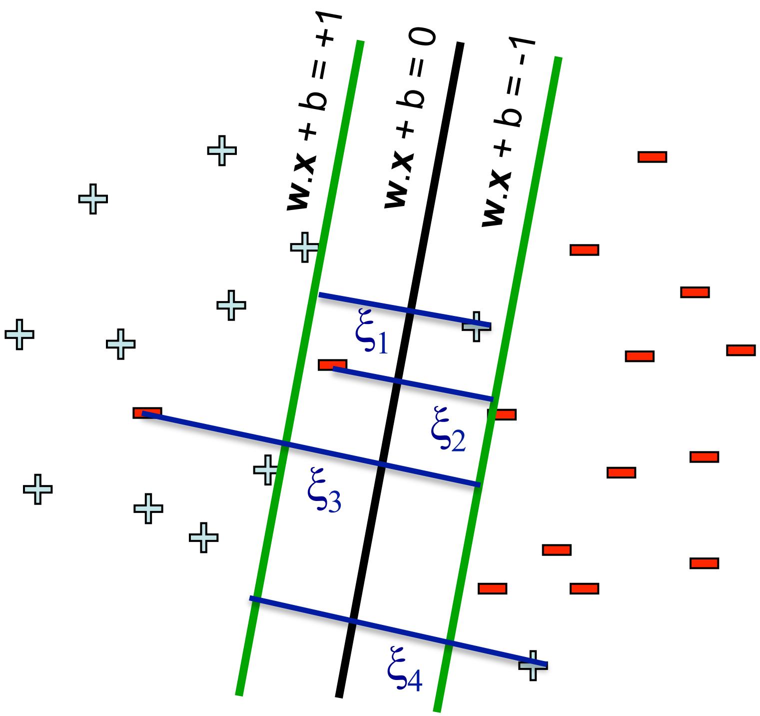
We now have a linear program, and can efficiently find its optimum

At optimal solution, for each data point:

- If $(\mathbf{w} \cdot \mathbf{x}^{(i)} + b) y^{(i)} \geq 1$, $\xi^{(i)} = 0$
- If $(\mathbf{w} \cdot \mathbf{x}^{(i)} + b) y^{(i)} < 1$, $\xi^{(i)} = 1 - (\mathbf{w} \cdot \mathbf{x}^{(i)} + b) y^{(i)}$ (constraint binding)

So $\xi^{(i)} = \max(0, 1 - (\mathbf{w} \cdot \mathbf{x}^{(i)} + b) y^{(i)})$

Equivalent Formulation



Original LP formulation:

$$\text{Minimize}_{\mathbf{w},b,\xi} \ \Sigma_i \ \xi^{(i)}$$

s.t.

$$(\mathbf{w}\bullet\mathbf{x}^{(i)}+b)y^{(i)} \geq 1 - \xi^{(i)} \text{ for all } i$$

Equivalent "hinge-loss" formulation:

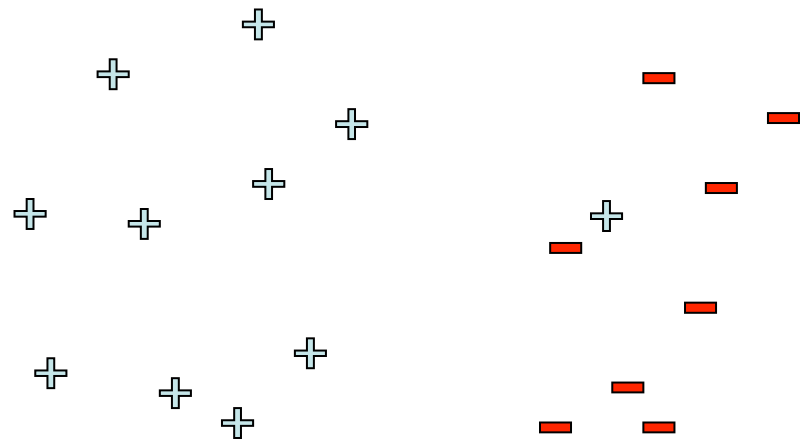
$$\text{Min} \ \ \Sigma_i \max(\ 0,\ 1 - (\mathbf{w}\bullet\mathbf{x}^{(i)}+b)y^{(i)}\ )$$

Compare with 0-1 loss:

$$\text{Min} \ \Sigma_i \ 1(\ y^{(i)}(\mathbf{w}\bullet\mathbf{x}^{(i)}+b) < 0\ )$$

In homework, you will show that max(0, 1 - ($\mathbf{w}\bullet\mathbf{x}^{(i)}$+b)$y^{(i)}$) is a tight upper bound for 1($y^{(i)}$($\mathbf{w}\bullet\mathbf{x}^{(i)}$+b) < 0). So minimizing the hinge loss should make 0-1 loss small (original goal). So original LP (equiv to minimizing hinge loss) should be a good heuristic.

Now have two LP formulations. Which is better?



Hard-margin SVM

Minimize $||\mathbf{w}||^2$
subject to:
$y^{(i)}(\mathbf{w} \bullet \mathbf{x}^{(i)} + b) \geq 1$ for all i

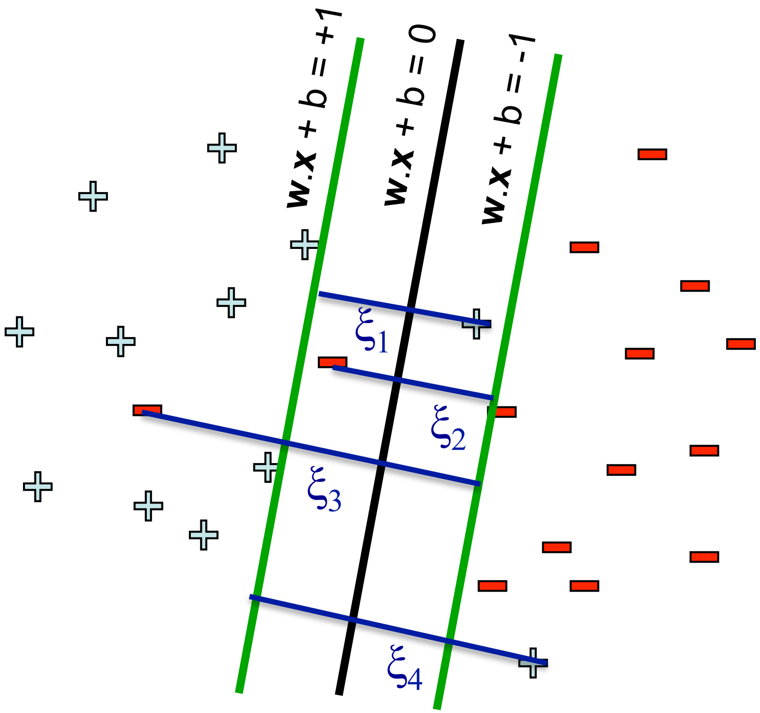
Good for finding wide margin. But will not have a feasible solution if data is not linearly separable.

0-1 loss (bounded) SVM

Minimize$_{\mathbf{w},b,\xi}$ $\Sigma_i\ \xi^{(i)}$
subject to
$(\mathbf{w} \bullet \mathbf{x}^{(i)}+b)y^{(i)} \geq 1 - \xi^{(i)}$ for all i

Focuses on region where the data doesn't linearly separate. May ignore the big picture and overfit the problematic data.

"Soft margin SVM"



Minimize$_{\mathbf{w},b,\xi}$ $\mathbf{w \bullet w} + C\ \Sigma_i\ \xi^{(i)}$
subject to
$(\mathbf{w \bullet x}^{(i)}+b)y^{(i)} \geq 1 - \xi^{(i)}$ for all i

Slack penalty $C > 0$:

- Want to find **w**, b so that the the margin is large and the # of errors is small.
- Want large margin to prevent overfitting.
- Solve optimization problem for different values of C. Choose the C that gives the smallest validation error.

Cross validation

- Divide labeled examples into 10 parts.
  - For each part
    - Use that part for validation, other 9 parts for training (optimization problem). Obtain validation error.
  - Calculate the average validation error over the 10 parts.
- Do for each C.
- Choose the C that has the lowest average validation error.

Summary: SVM Soft-Margin Optimization Problem

Minimize$_{\mathbf{w},b,\xi}$ $\mathbf{w}\bullet\mathbf{w} + C \, \Sigma_i \, \xi^{(i)}$
subject to
$(\mathbf{w}\bullet\mathbf{x}^{(i)}+b)y^{(i)} \geq 1 - \xi^{(i)}$ for all i

Or equivalently, the non-linear unconstrained problem:

Minimize$_{\mathbf{w},b}$ $\mathbf{w}\bullet\mathbf{w} + C \, \Sigma_i \max(\, 0, 1 - y^{(i)} \, (\mathbf{w}\bullet\mathbf{x}^{(i)}+b))$

regularization