More Large-Scale Machine Learning

Perceptrons
Support-Vector Machines

Jeffrey D. Ullman
Stanford University

The Perceptron

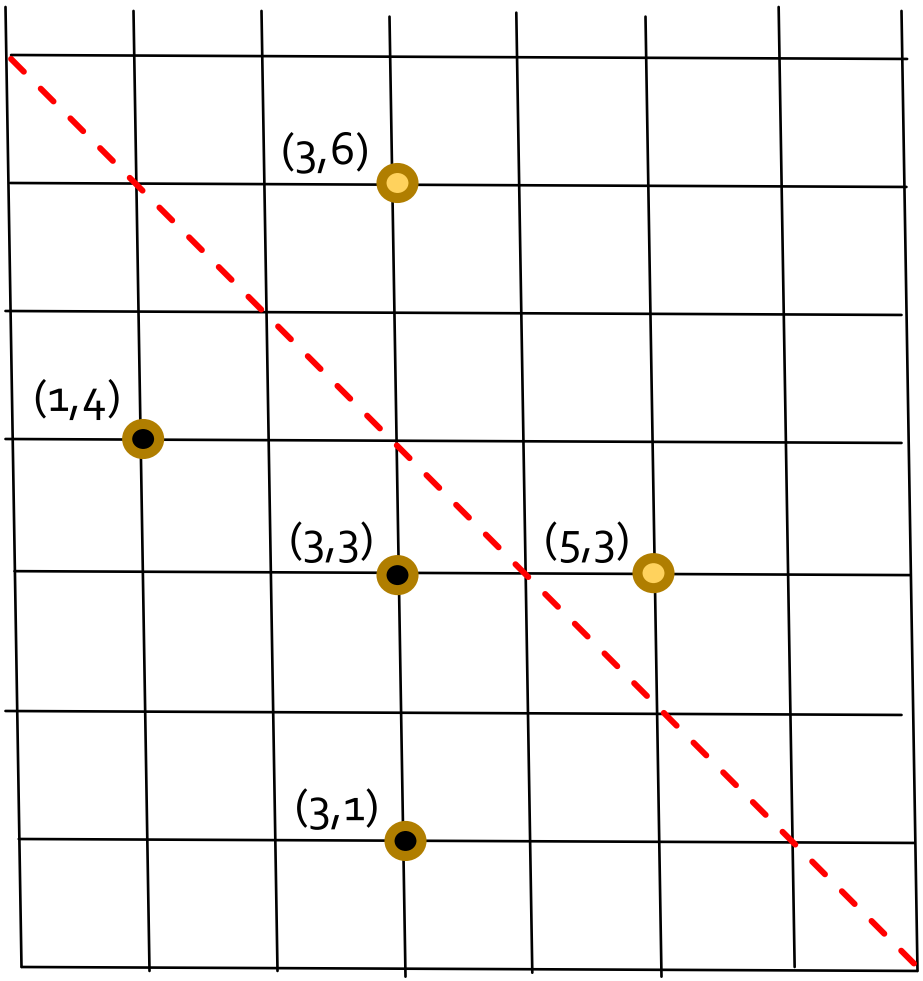
- Given a set of training points (**x**, y), where:
  1. **x** is a real-valued vector of d dimensions, and
  2. y is a binary decision +1 or -1,

a perceptron tries to find a linear separator between the positive and negative inputs.

Linear Separators

- A *linear separator* is a d-dimensional vector **w** and a *threshold* θ such that the *hyperplane* defined by **w** and θ separates the positive and negative examples.
- More precisely: given input **x**, this linear separator returns +1 if $\mathbf{x}.\mathbf{w} > \theta$ and returns -1 if not.
- Think of the i-th component of **w** as the *weight* given to the i-th dimension of the input vectors.

Example: Linear Separator

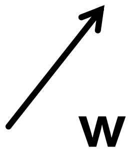


Black points = -1

Gold points = +1

w = (1,1)

$\theta = 7$



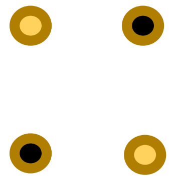
Hyperplane **x**.**w** = θ

If **x** = (a,b),

then a+b = 7

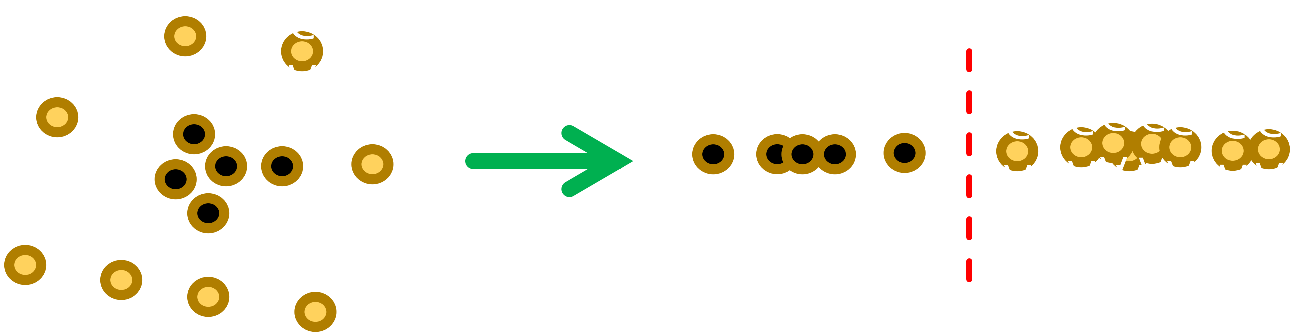
Goal: Finding w and θ

- Possibly **w** and θ do not exist, since there is no guarantee that the points are linearly separable.
- Example:



Kernel Functions Can Linearize

- Sometimes, we can transform points that are not linearly separable into a space where they are linearly separable.
- Example: Remember the clustering problem of concentric circles?
- Mapping points to their radii gives us a 1-dimensional space where they are separable.



Making the Threshold Zero

- A simplification: we can arrange that $\theta = 0$.
- Add a d+1-st dimension, whose value is -1 for all training points.
- If **x** is a d-dimensional input, let (**x**,-1) represent the extended (d+1)-dimensional vector.
- If **w** is the (unknown) normal to the separating hyperplane, and θ is the (unknown) threshold, let (**w**, θ) be **w** with an additional dimension with θ as the (unknown) d+1-st component.
- Then **x**.**w** > θ if and only if (**x**,-1).(**w**,θ) > 0.

Previous Example, Continued

- The positive training points (3,6) and (5,3) become (3,6,-1) and (5,3,-1).
- The negative training points (1,4), (3,3), and (3,1) become (1,4,-1), (3,3,-1), and (3,1,-1).
- Since we know **w** = (1,1) and θ = 7 separated the original points, then **w'** = (1,1,7) and θ = 0 will separate the new points.
- Example: (3,6,-1).(1,1,7) > 0 and (1,4,-1).(1,1,7) $\leq$ 0.

Training a Perceptron

- Assume threshold = 0.
- Pick a learning rate η, typically a small fraction.
- Start with **w** = (0, 0,…, 0).
- Consider each training example (**x**,y) in turn, until there are no misclassified points.
  - Use y = +1 for positive examples, y = -1 for negative.
- If **x**.**w** has a sign different from y, then this is a misclassified point.
  - Special case: also misclassified if **x.w** = 0.

Training – (2)

- If ($\mathbf{x}$,y) is misclassified, adjust $\mathbf{w}$ to accommodate $\mathbf{x}$ slightly.
- Replace $\mathbf{w}$ by $\mathbf{w}' = \mathbf{w} + \eta y\mathbf{x}$.
- Note $\mathbf{x}.\mathbf{w}' = \mathbf{x}.\mathbf{w} + \eta y|\mathbf{x}|^2$.
- That is, if y = +1, then the dot product of $\mathbf{x}$ with $\mathbf{w}'$, which was negative, has been increased by η times the square of the length of $\mathbf{x}$.
  - Similarly, if y = -1, the dot product has decreased.
  - May still have the wrong sign, but we're headed in the right direction.

Example: Training

Name	x	y
A	(1,4,-1)	-1
B	(3,3,-1)	-1
C	(3,1,-1)	-1
D	(3,6,-1)	+1
E	(5,3,-1)	+1

Let $\eta = 1/3$.

w = (0, 0, 0)

Use A: misclassified. New **w** =
(0, 0, 0) + (1/3)(-1)(1,4,-1) = (-1/3, -4/3, 1/3).

Use B: OK; Use C: OK.

Use D: misclassified. New **w** =
(-1/3, -4/3, 1/3) + (1/3)(+1)(3,6,-1) = (2/3, 2/3, 0).

Use E: OK.

Use A: misclassified. New **w** =
(2/3, 2/3, 0) + (1/3)(-1)(1,4,-1) = (1/3, -2/3, -1/3).

. . .

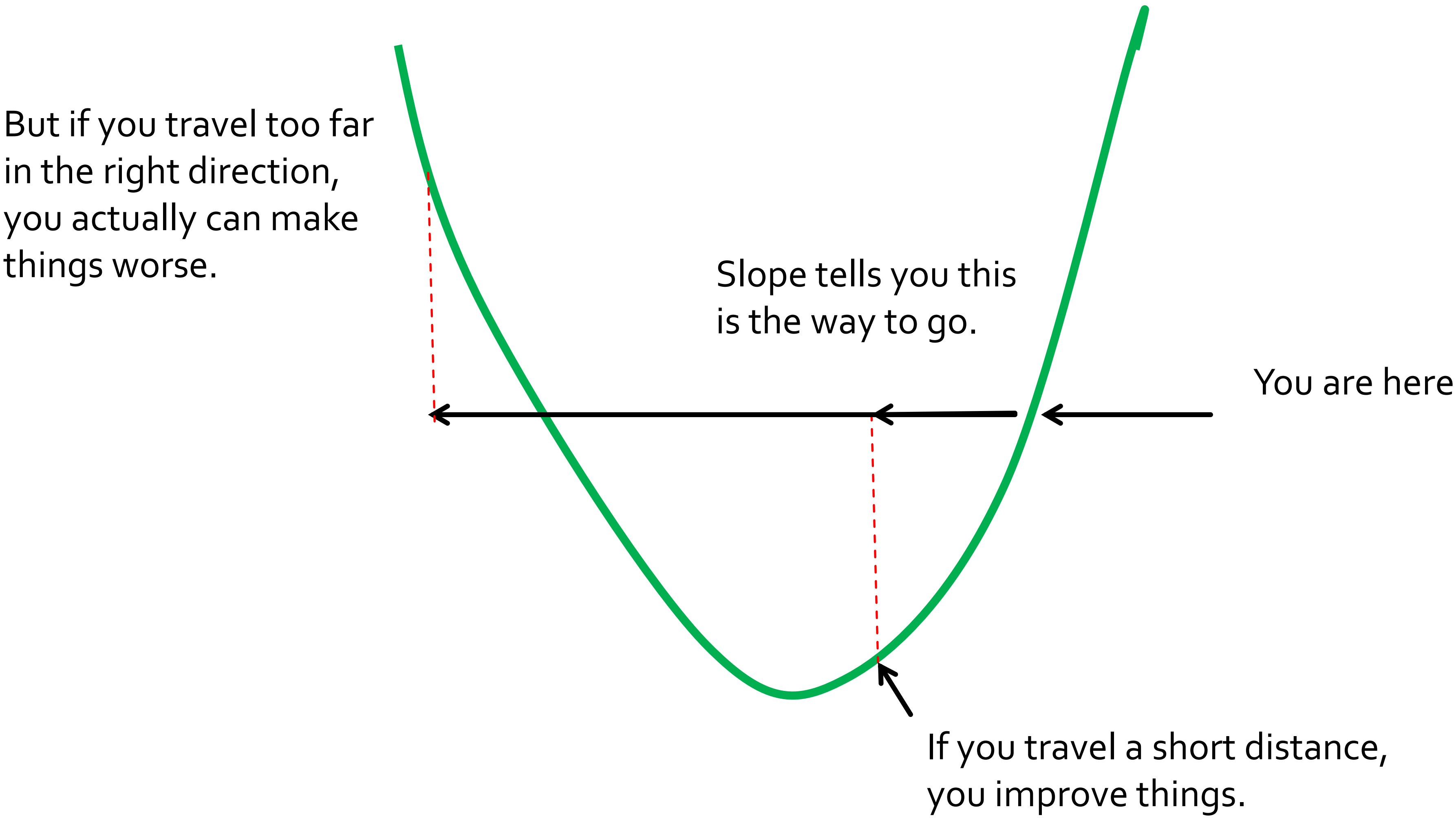
Parallelization

- Convergence is an inherently sequential process.
- We change **w** at each step, which can change:
  1. Which training points are misclassified.
  2. What the next vector **w’** is.
- However, if the learning rate is small, these changes are not great at each step.
- It is generally safe to process many training points at once, obtain the increments to **w** for each, and add them all at once.

Picking the Training Rate

- A very small training rate causes convergence to be slow.
- Too large a training rate can cause oscillation and may make convergence impossible, even if the training points are linearly separable.

The Problem With High Training Rate



The Winnow Algorithm

- Perceptron learning for binary training examples.
- Assume components of input vector **x** are 0 or 1; outputs y are -1 or +1.
- Uses a threshold θ, usually the number of dimensions of the input vector.
- Select a training rate $\eta < 1$.
- Initial weight vector **w** is (1, 1,…, 1).

Winnow Algorithm – (2)

- Visit each training example (**x**,y) in turn, until convergence.
- If **x.w** $> \theta$ and y = +1, or **x.w** $< \theta$ and y = -1, we're OK, so make no change to **w**.
- If **x.w** $\geq \theta$ and y = -1, lower each component of **w** where **x** has value 1.
  - More precisely: IF $x_i = 1$ THEN replace w_i by ηw_i.
- If **x.w** $\leq \theta$ and y = +1, raise each component of **w** where **x** has value 1.
  - More precisely: IF $x_i = 1$ THEN replace w_i by w_i/η.

Example: Winnow Algorithm

Viewer	Star Wars	Martian	Aveng-ers	Titanic	Lake House	You've Got Mail	y
A	0	1	1	1	1	0	+1
B	1	1	1	0	0	0	+1
C	0	1	0	1	1	0	-1
D	0	0	0	1	0	1	-1
E	1	0	1	0	0	1	+1

Goal is to classify "Scifi" viewers (+1) versus "Romance" (-1).
Initial w = (1, 1, 1, 1, 1, 1).
Threshold: $\theta = 6$.
Use $\eta = 1/2$.

Example: Winnow – (2)

	S	M	A	T	L	Y	y
A	0	1	1	1	1	0	+1
B	1	1	1	0	0	0	+1
C	0	1	0	1	1	0	-1
D	0	0	0	1	0	1	-1
E	1	0	1	0	0	1	+1

w = (1, 1, 1, 1, 1, 1).

Use A: misclassified. **x**.**w** = 4 ≤ 6.
New **w** = (1, 2, 2, 2, 2, 1).

Use B: misclassified. **x**.**w** = 5 ≤ 6.
New **w** = (2, 4, 4, 2, 2, 1).

Use C: misclassified. **x**.**w** = 8 > 6.
New **w** = (2, 2, 4, 1, 1, 1).

Now, D, E, A, B, C are all OK, so done.

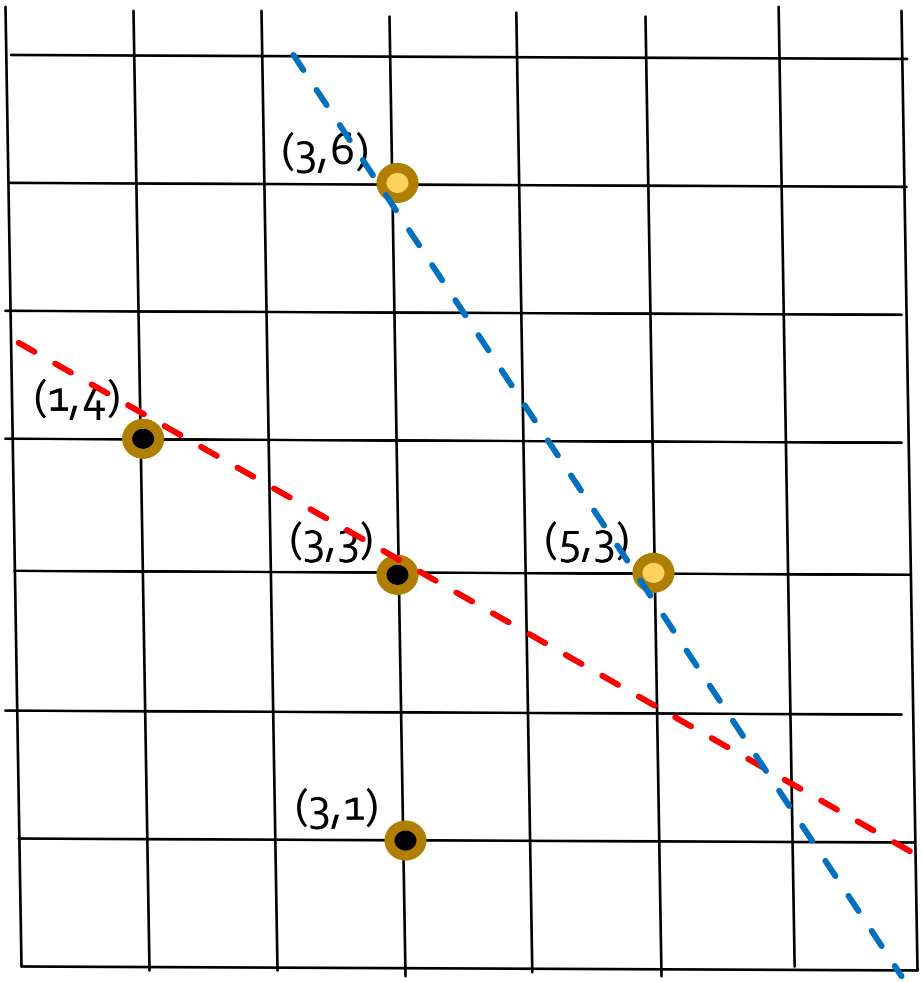
Support-Vector Machines

Problem with Perceptrons
Linearly Separable Data
Dealing with Nonseparable Data

Problems With Perceptrons

1. Not every dataset is linearly separable.
   - More common: a dataset is "almost" separable, but with a small fraction of the points on the wrong side of the boundary.
2. Perceptron design stops as soon as a linear separator is found.
   - May not be the best boundary for separating the data to which the perceptron is applied, even if the training data is a random sample from the full dataset.

Example: Problem



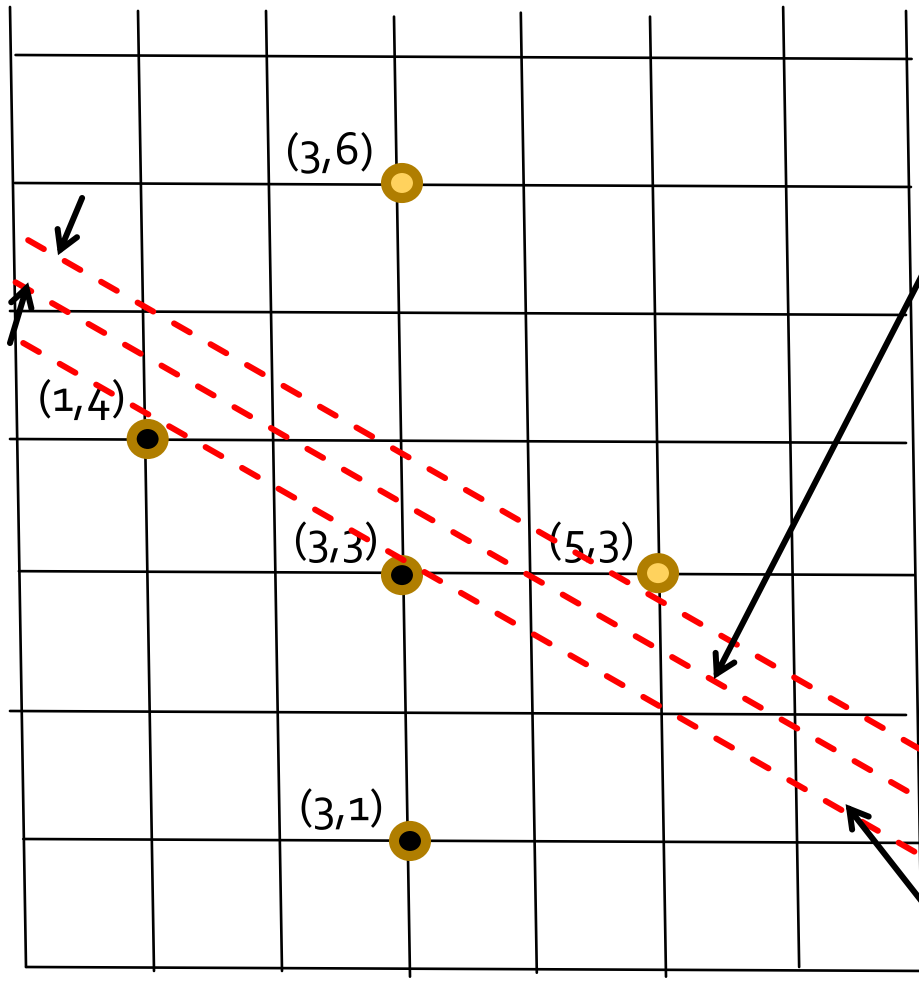
Either red or blue line separates training points. Can give different answers for many points.

Intuition Behind SVM

- By designing a better cost function, we can force the separating hyperplane to be as far as possible from the points in either class.
  - Reduces the likelihood that points in the test set will be misclassified.
- Later, we'll also consider picking a hyperplane for nonseparable data, in a way that minimizes the "damage."

Example: One Candidate

Margin γ

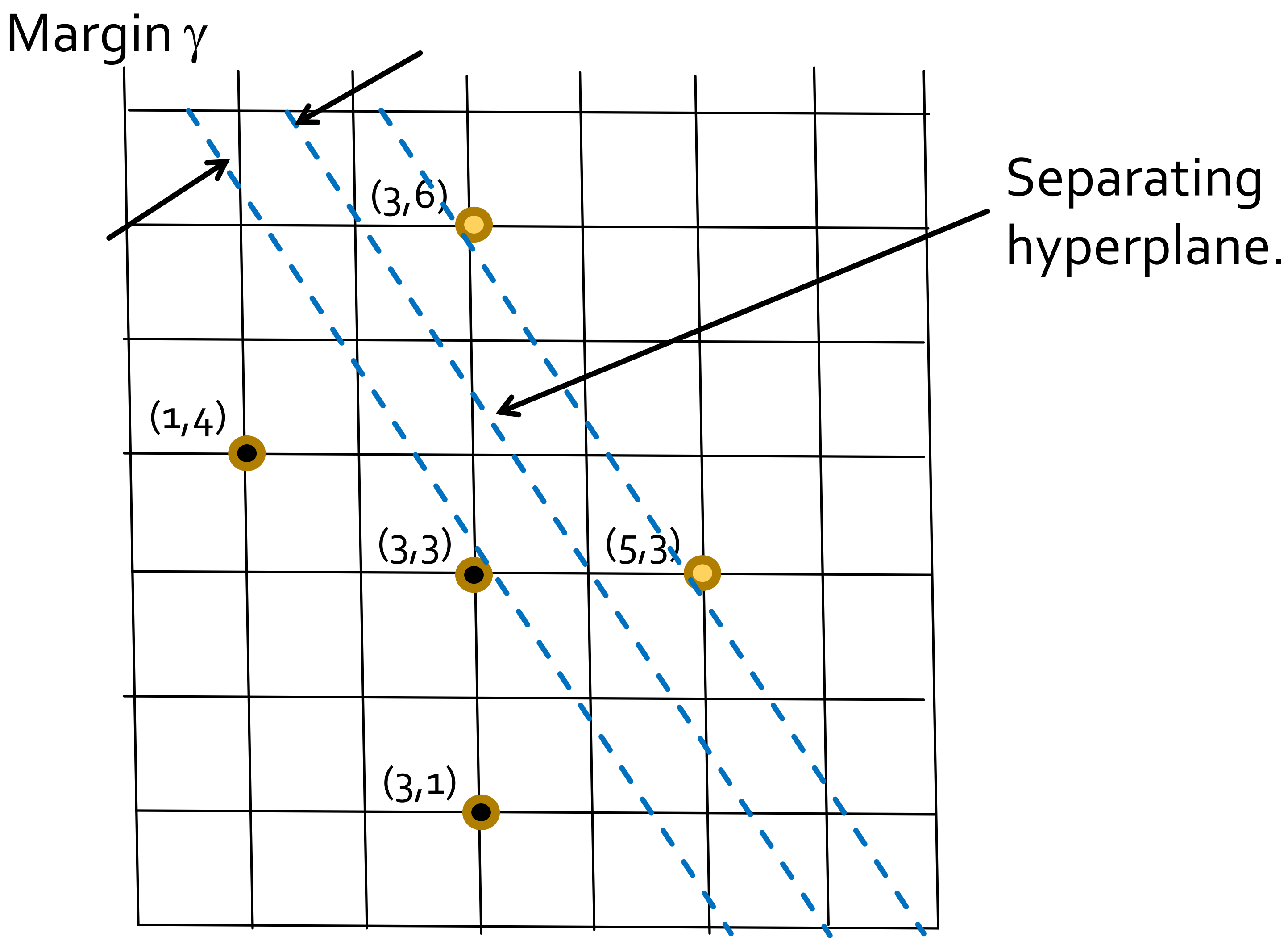


Separating hyperplane.

(1,4), (3,3), and (5,3) are the *support vectors*, limiting the margin for this choice of hyperplane.

Call these the "upper" and "lower" hyperplanes.

Example: Hyperplane With Larger γ



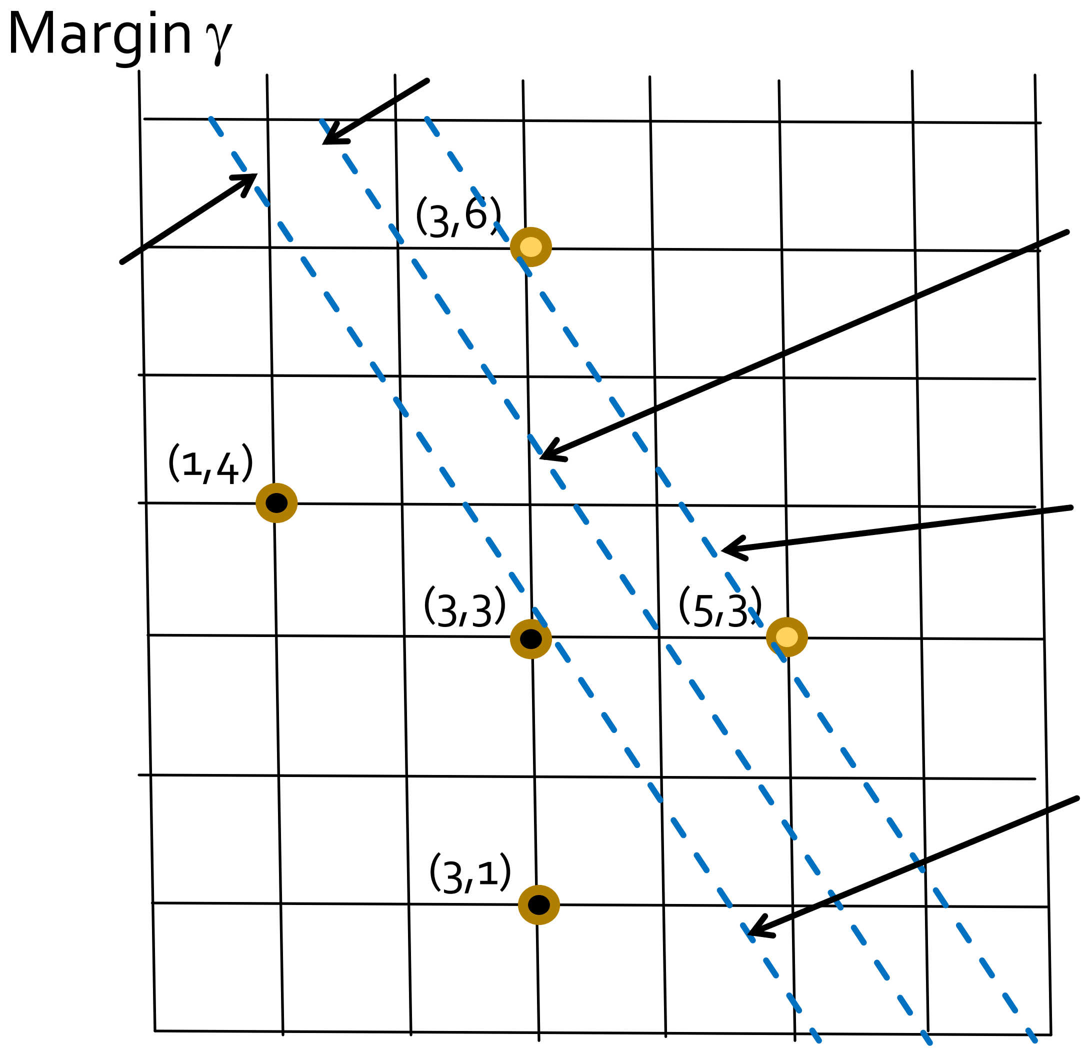
Maximizing γ

- Let weight vector **w** be the (unknown) normal to the best hyperplane, and b an (unknown) constant.
- We would like to find **w** and b that maximizes γ subject to the constraint that for each training example (**x**,y), we have y(**w**.**x** + b) $\geq \gamma$.
  - That is, if y = +1, then point **x** is at least γ above the separating hyperplane, and if y = -1, then **x** is at least γ below.
- Problem: scale of **w** and b.
  - Double **w** and b and we can double γ.

Maximizing γ – (2)

- Solution: require $|\mathbf{w}|$ to be the unit of length for γ.
- Equivalent formulation: require that the constant terms in the upper and lower hyperplanes (those that are parallel to the separating hyperplanes, but just touch the support vectors) be b+1 and b-1.
- The problem of maximizing γ, computed in units of $|\mathbf{w}|$, turns out to be equivalent to minimizing $|\mathbf{w}|$ subject to the constraint that all points are outside the upper and lower hyperplanes.

Example: Unit Separation



Separating hyperplane
w.**x**+b = 0.

Upper hyperplane
w.**x**+b = 1.

Lower hyperplane
w.**x**+b = -1.

Example: Constraints

- Consider the running example, with positive points (3,6) and (5,3), and with negative points (1,4), (3,3), and (3,1).
- Let **w** = (u,v).
- Then we must minimize |**w**| subject to:
  - $3u + 6v + b \geq 1$.
  - $5u + 3v + b \geq 1$.
  - $u + 4v + b \leq -1$.
  - $3u + 3v + b \leq -1$.
  - $3u + v + b \leq -1$.

Solving the Constraints

- This is almost a linear program.
- Difference: the objective function sqrt(u^2+v^2) is not linear.
- Cheat: if we believe the blue hyperplane with support vectors (3,6), (5,3), and (3,3) is the best we can do, then we know that the normal to this hyperplane has $v = 2u/3$, and we only have to minimize u.

Solving the Constraints if $v = 2u/3$

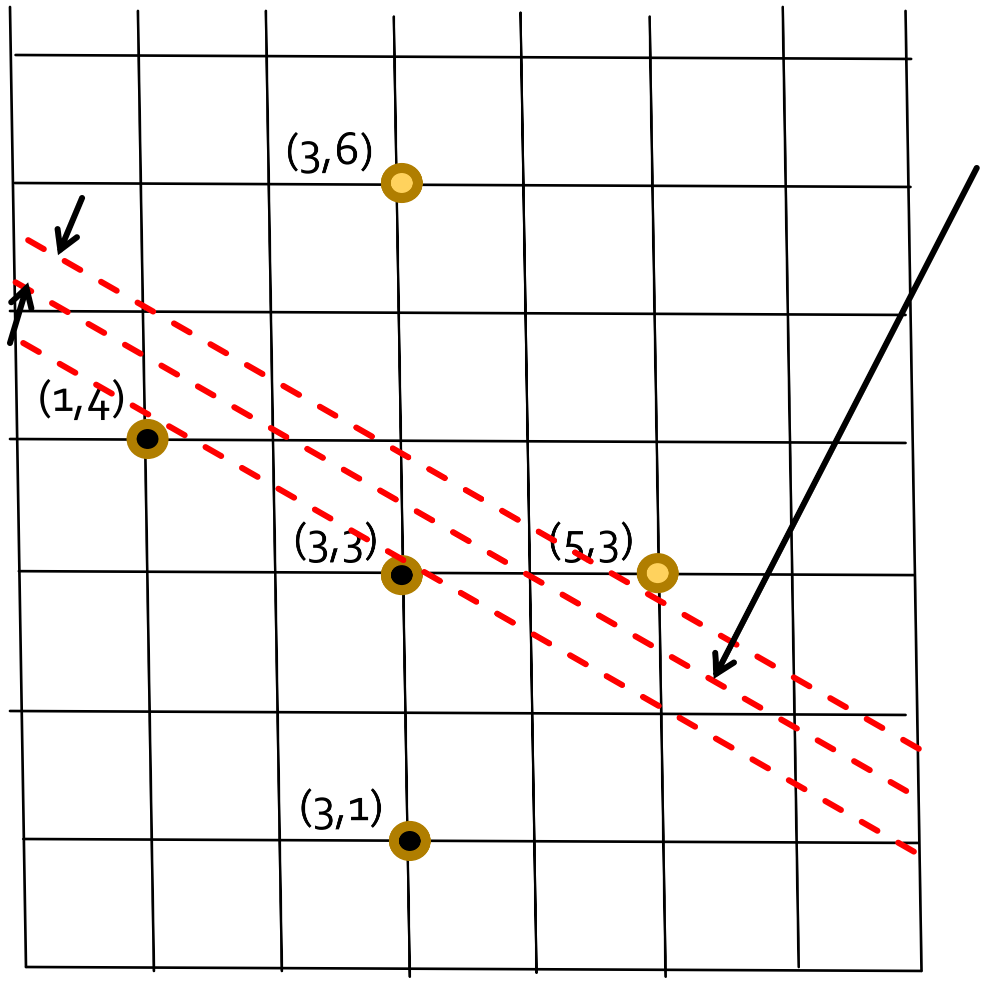
Point	Constraint	If $v = 2u/3$
(3,6)	$3u + 6v + b \geq 1$	$\mathbf{7u + b \geq 1}$
(5,3)	$5u + 3v + b \geq 1$	$\mathbf{7u + b \geq 1}$
(1,4)	$u + 4v + b \leq -1$	$11u/3 + b \leq -1$
(3,3)	$3u + 3v + b \leq -1$	$\mathbf{5u + b \leq -1}$
(3,1)	$3u + v + b \leq -1$	$11u/3 + b \leq -1$

Constraints of support vectors are hardest to satisfy. Smallest u is when $u = 1$, $v = 2/3$, $b = -6$.

$|\mathbf{w}| = \text{sqrt}(1^2 + (2/3)^2) = 1.202.$

Remember This Hyperplane With a Smaller Margin?

Margin γ



Separating hyperplane.

The normal to the hyperplane, **w**, has slope 2, so v = 2u.

Here's What Happens if v = 2u

Point	Constraint	If v = 2u
(3,6)	$3u + 6v + b \geq 1$	$15u + b \geq 1$
(5,3)	$5u + 3v + b \geq 1$	$\mathbf{11u + b \geq 1}$
(1,4)	$u + 4v + b \leq -1$	$\mathbf{9u + b \leq -1}$
(3,3)	$3u + 3v + b \leq -1$	$\mathbf{9u + b \leq -1}$
(3,1)	$3u + v + b \leq -1$	$5u + b \leq -1$

Constraints of support vectors are hardest to satisfy.
Smallest u is when
$u = 1$, $v = 2$, $b = -10$.

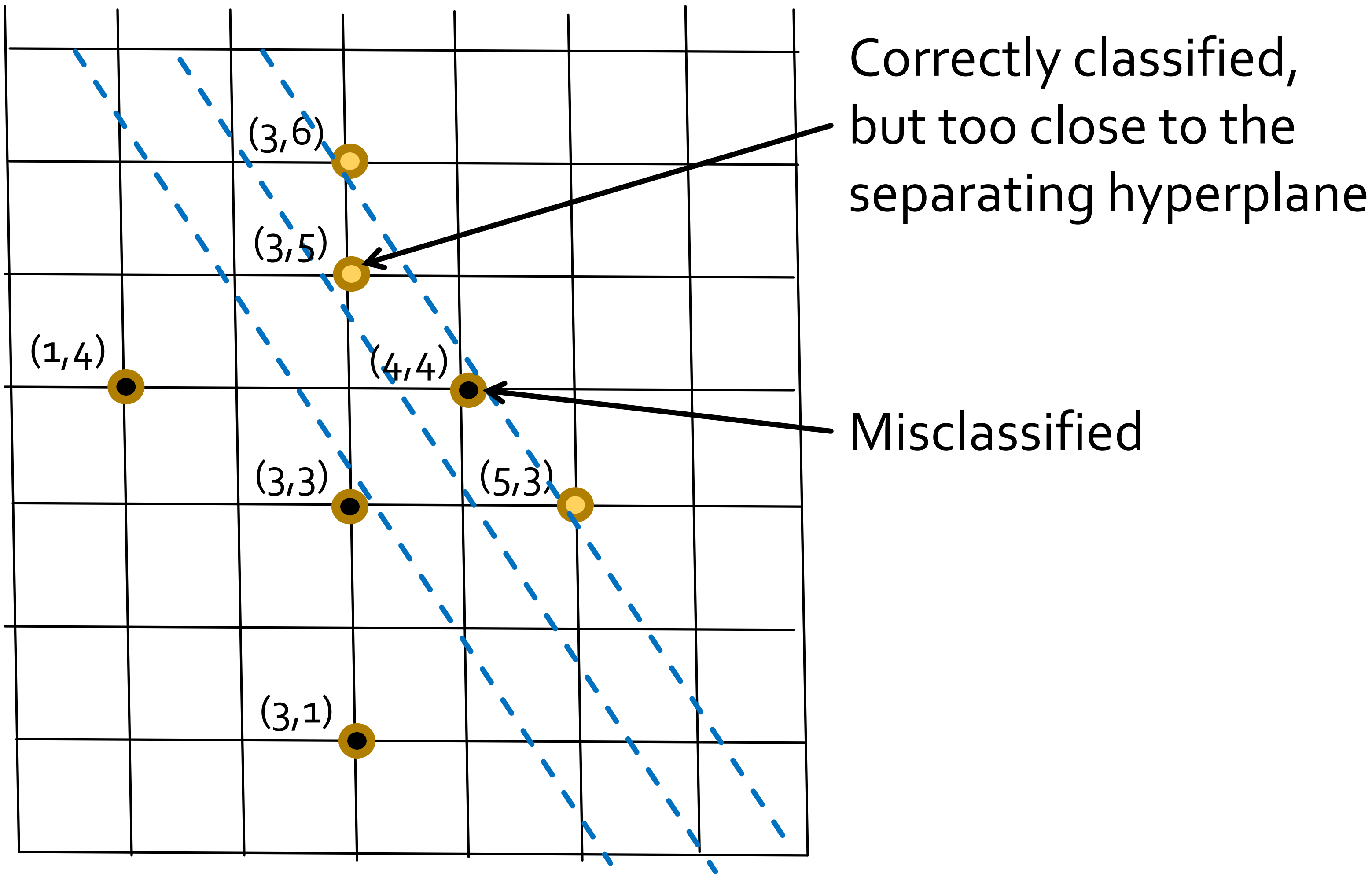
$|\mathbf{w}| = \text{sqrt}(1^2 + 2^2) = 2.236$.

Since we want the minimum $|\mathbf{w}|$, we prefer the previous hyperplane.

Did That Look Too Easy?

- 2 dimensions is not that hard.
- In general there are d+1 support vectors for d-dimensional data.
- Support vectors must lie on the convex hulls of the sets of positive and negative points.
- Once you find a candidate separating hyperplane and its parallel upper and lower hyperplanes, you can calculate $|\mathbf{w}|$ for that candidate.
- But there is a more general approach, next.

Nonseparable Data



New Goal

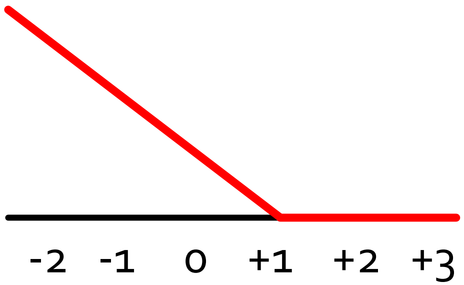
- We'll still assume that we want a "separating" hyperplane **w**.**x** + b = 0 defined by normal vector **w** and constant b.
- And to establish the length of **w**, we take the upper and lower hyperplanes to be **w**.**x** + b = +1 and **w**.**x** + b = -1.
- Allow points to be inside the upper and lower hyperplanes, or even entirely on the wrong side of the separator.

New Goal – (2)

- Minimize a cost function that includes:
  1. The square of the length of **w** (to encourage a small |**w**|), and
  2. A term that penalizes points that are either:
     a. On the right side of the separator, but on the wrong side of the upper or lower hyperplanes.
     b. On the wrong side of the separator.
- The term (2) is *hinge loss* =
  - 0 if point is on the right side of the upper or lower hyperplane.
  - Otherwise linear in the amount of "wrong."

Hinge Loss Function

- Let **w**.**x** + b = 0 be the separating hyperplane, and let (**x**, y) be a training example.
- The hinge loss for this point is
  max(0, 1 – y(**w**.**x** + b)).



- Example: If y = +1 and **w**.**x** + b = 2, loss = 0.
  - Point **x** is properly classified and beyond the upper hyperplane.
- Example: If y = +1 and **w**.**x** + b = 1/3, loss = 2/3.
  - Point **x** is properly classified but not beyond the upper hyperplane.
- Example: If y = -1 and **w**.**x** + b = 2, loss = 3.
  - Point **x** is completely misclassified.

Expression to Be Minimized

- Let there be n training examples ($\mathbf{x}_i$, y_i).
- The cost expression:

$$f(\mathbf{w}, b) = |\mathbf{w}|^2/2 + C\ \Sigma_{j=1,\ldots,n} \max(0, 1 - y_j(\mathbf{w}.\mathbf{x}_j + b))$$

  - C is a constant to be chosen.
- Solve by gradient descent.
- Remember, $\mathbf{w} = (w_1, w_2, \ldots, w_d)$ and each $\mathbf{x}_j = (x_{j1}, x_{j2}, \ldots, x_{jd})$.
- Take partial derivatives with respect to each w_i.
- First term has derivative w_i.
  - Which, BTW, is why we divided by 2 for convenience.

Gradient Descent – (2)

- The second term $C\,\Sigma_{j=1,\ldots,n} \max(0, 1 - y_j(\mathbf{w}.\mathbf{x}_j + b))$ is trickier.
- There is one term in the partial derivative with respect to w_i for each j.
- If $y_j(\mathbf{w}.\mathbf{x}_j + b) \geq 1$, then this term is 0.
- But if not, then this term is $-Cy_jx_{ji}$.
- So given the current **w**, you need first to sort out which $\mathbf{x}_j$'s give 0 and which give $-Cy_jx_{ji}$ before you can compute the partial derivatives.