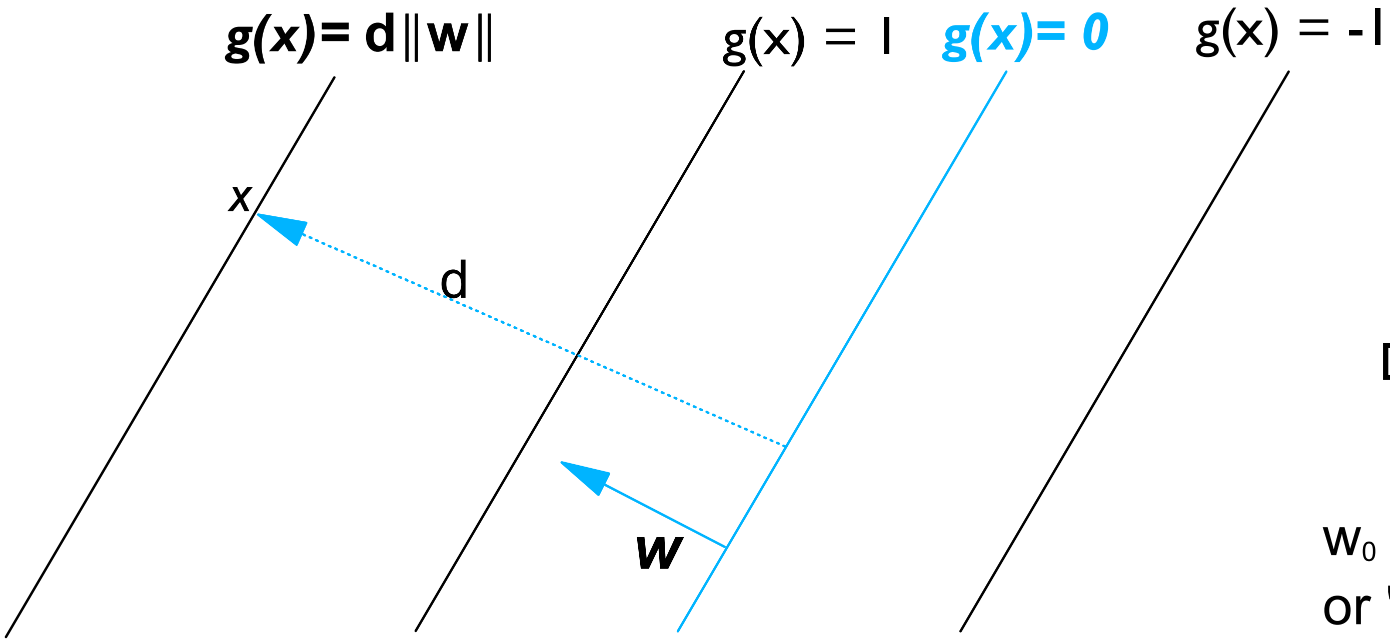
Linear Discriminants

- $x = (x_1, \ldots, x_d)$ = vector of attributes (features)
- $w = (w_1, \ldots, w_d)$ = weight vector
- $w \bullet x = \Sigma_1^d w_i x_i$

  $= wx^t$

  (or $w^t x$ if the vectors are column vectors, as in Duda, Hart & Stork)
- **Linear discriminant** is a function of the form:
  - $g(x) = w \bullet x + w_0 = \Sigma_1^d w_i x_i + w_0$
- w is normal to the **hyperplane** H defined by:
  - $H = \{x: g(x)=0\}$
  - Proof:
    - x_1, x_2 in $H \Rightarrow w \bullet (x_1 - x_2) = g(x_1) - w_0 - (g(x_2) - w_0) = 0$

Hyperplanes



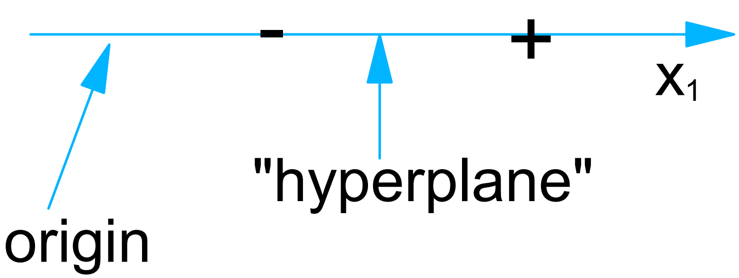
Distance of H from origin
$= |w_0| / \|w\|$

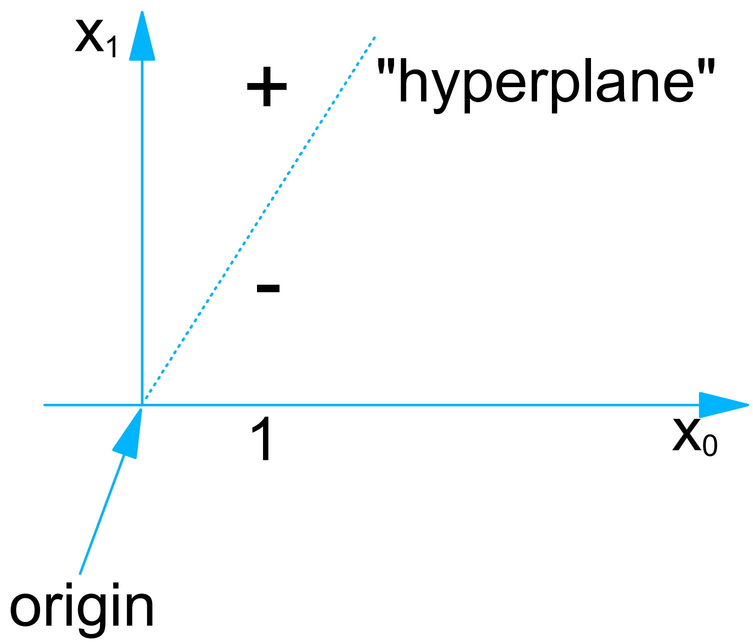
w_0 is called "bias" (confusing!) or "threshold weight"

- Use g as a classifier: x is classified +1 if $g(x)>0$ i.e. $\Sigma_1^d w_i x_i > -w_0$
  -1 if $g(x)<0$ i.e. $\Sigma_1^d w_i x_i < -w_0$
- Thus the classifier is Sign(g(x))
- Extend from binary case (2 classes) to mulitiple classes later.

Threshold is an Extra Weight

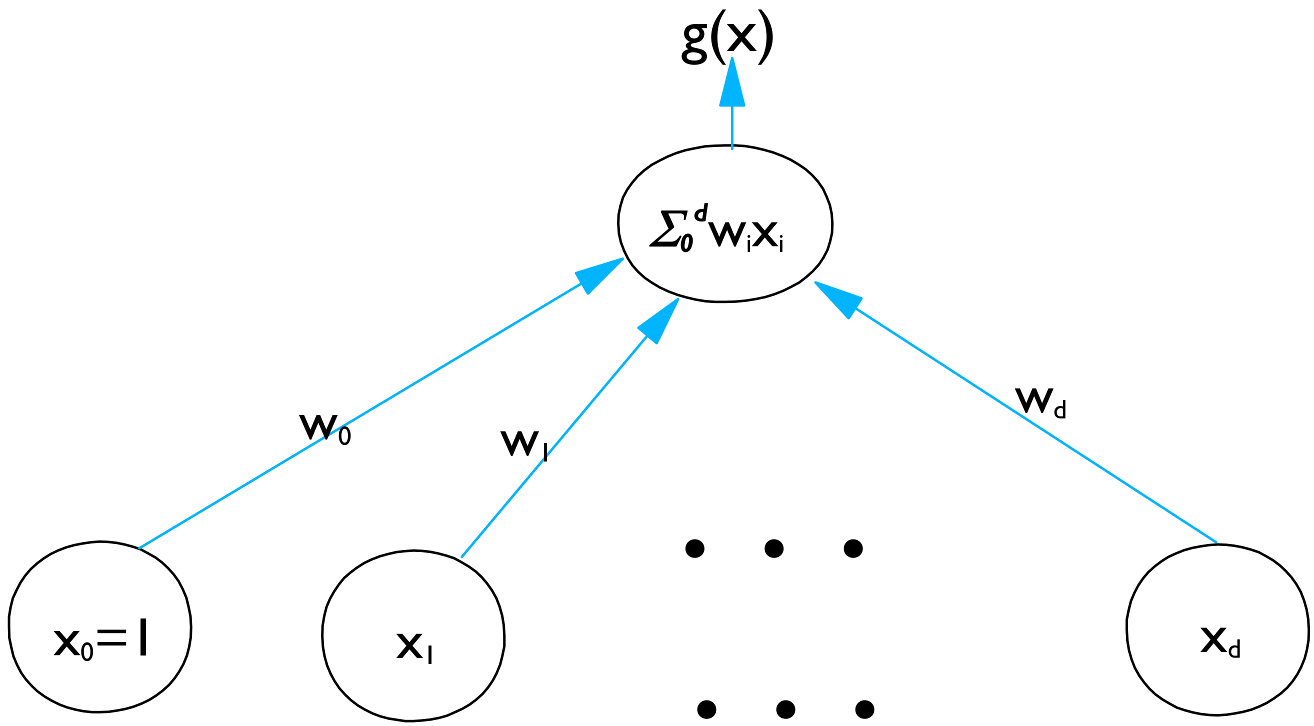
- w_0 can be incorporated into w by setting x_0=1
  - Then $g(x) = w \bullet x = \Sigma_0^d w_i x_i$
- Example:
  - d=1, "hyperplane" is just a point separating +ve from -ve points
  - Embed the points into d=2 space by making their first component 1
  - "hyperplane" passes through origin





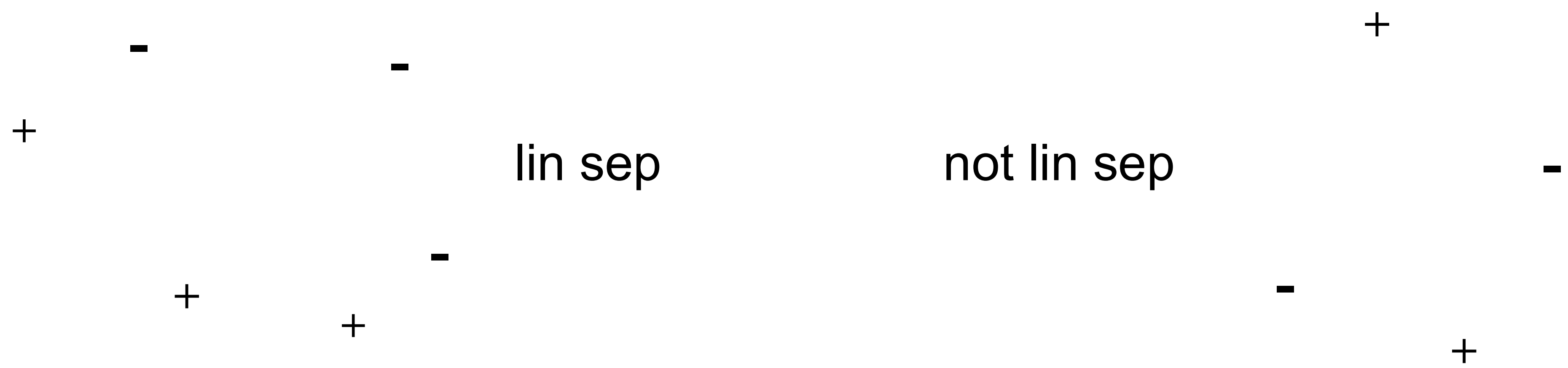
Perceptron

- Input is $x = (1, x_1, ..., x_d)$
- Weight vector $= (w_0, w_1, ..., w_d)$
- Output is $g(x) = w \bullet x = \Sigma_0^d w_i x_i$
- Classify using Sign(g(x))



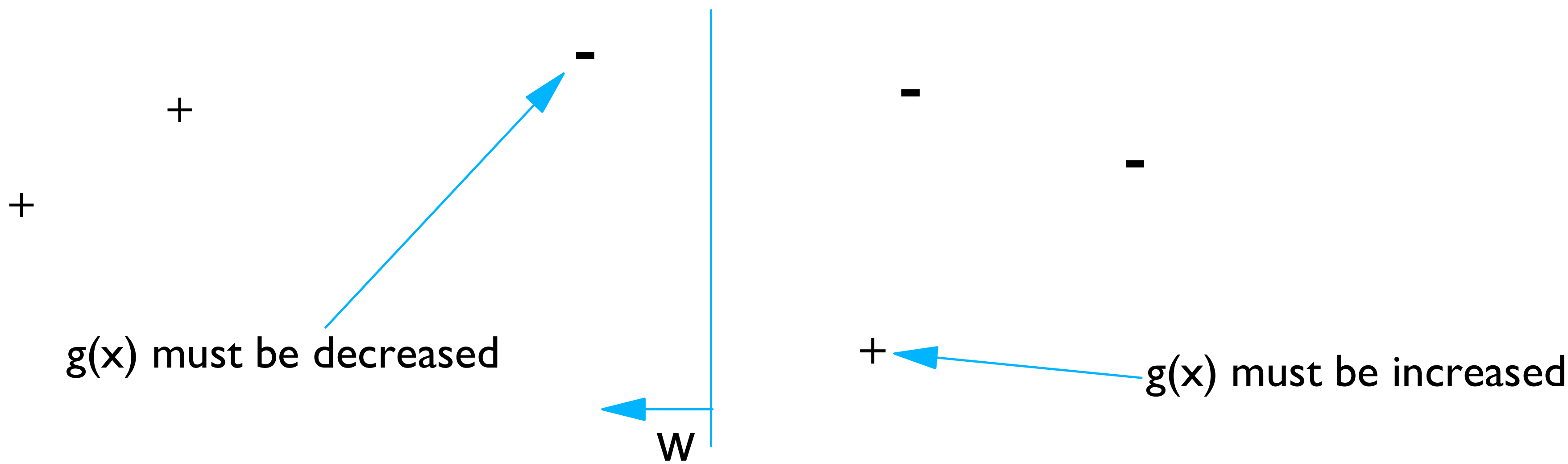
Linearly Separable

- Given: Training Sample T = $\{(x_1, y_1), \ldots, (x_n, y_n)\}$, where:
  - each x_i is a vector $x_i = (x_{i1}, \ldots, x_{id})$
  - each $y_i = \pm 1$
- T is ***linearly separable*** if there is a hyperplane separating the +ve points from the -ve points i.e. there exists w such that
  - $g(x_i) = w \bullet x_i > 0$ if and only if $y_i = +1$
  - i.e. $y_i(w \bullet x_i) > 0$ for all i



Finding a Weight Vector

- Hypothesis Space = all weight vectors (with d+1 coordinates)
- If w separates +ve from -ve points, so does aw for any a >0.
- How do we find a "good" weight vector w?
- Could try "all" w until find one
  - e.g. try all integer-valued w in order of increasing length.
- Better idea
  - repeatedly change w to correct the points it classifies incorrectly.

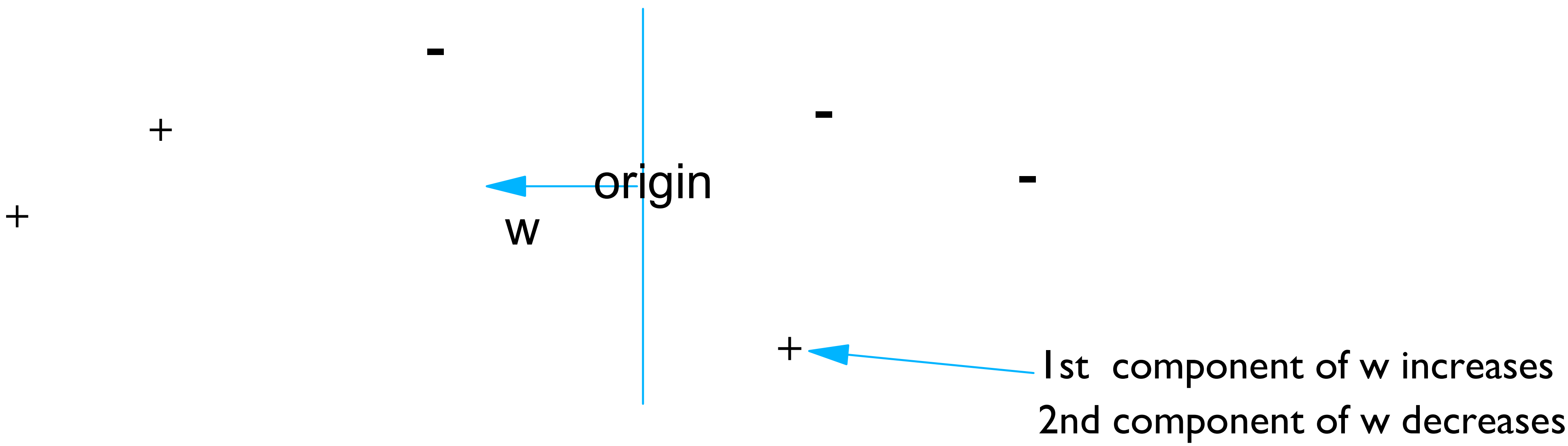


Updating the Weights

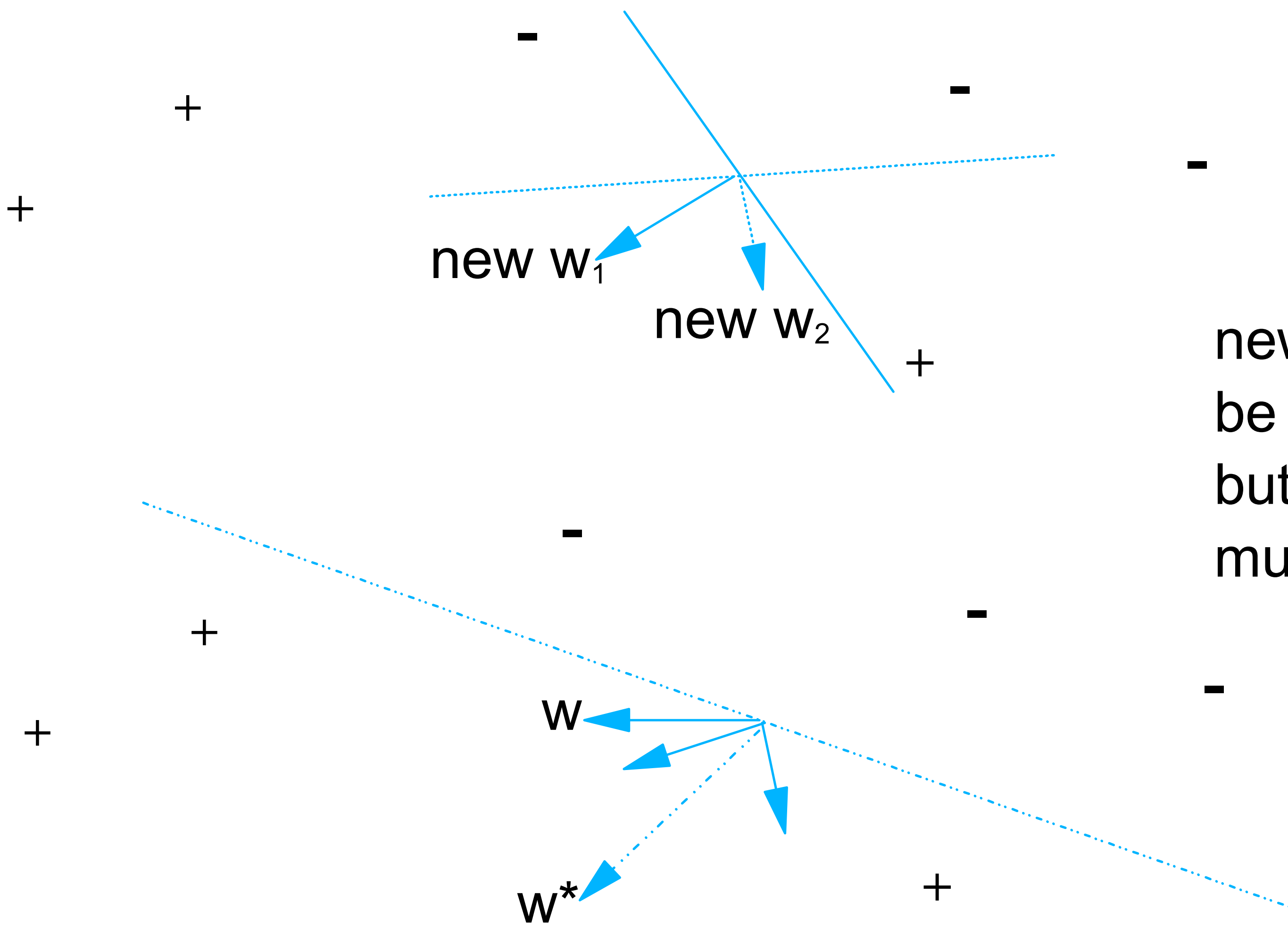
- If a +ve point x_r is incorrectly classified i.e. $w \bullet x_r < 0$, then:
  - INCREASE $w \bullet x_r$ by:
    - increasing w_i if $x_{ri} > 0$
    - decreasing w_i if $x_{ri} < 0$
- If a -ve point x_r is incorrectly classified i.e. $w \bullet x_r > 0$, then:
  - DECREASE $w \bullet x_f$ by:
    - increasing w_i if $x_{ri} < 0$
    - decreasing w_i if $x_{ri} > 0$
- For both +ve and -ve points, do:
  - $w \leftarrow w + y_r x_r$ if x_r is incorrectly classified
- NOTE: A point x_r is **classified correctly** if and only if
  - $y_r(w \bullet x_r) > 0$
- Notational "trick" used by some texts:
  - multiply -ve points by -1
  - can express formulas more simply (without y_i)

Perceptron Algorithm

- Algorithm:
  - w=0
  - Repeat until all points x_i are correctly classified
    - If x_r is incorrectly classified, do $w \leftarrow w + y_r x_r$
  - Output w



Intuition behind Convergence



new w is not guaranteed to be closer to w* than w was, but will be closer to some multiple of w*

Perceptron Convergence Proof

- Proposition: If the training set is linearly separable, the perceptron algorithm converges to a solution vector in a finite number of steps.

Proof

- Let w* be some solution vector i.e. $y_i(w^* \bullet x_i) > 0$ for all i (Eqn 1)
  - w* exists because the sample is linearly separable
  - $a w^*$ is a solution vector for any $a > 0$.
- The update is:
  - $w(k+1) = w(k) + y_r x_r$ if x_r is misclassified
- We want to show that:
  - $|w(k+1) - a w^*|^2 \leq |w(k) - a w^*|^2 - c$ for some constant c>0
- We have:
  - $|w(k+1) - a w^*|^2 = |w(k) - a w^* + y_r x_r|^2 = (w(k) - a w^* + y_r x_r) \bullet (w(k) - a w^* + y_r x_r)$

    $= |w(k) - a w^*|^2 + 2(w(k) - a w^*) \bullet y_r x_r + |y_r x_r|^2$
- Since $w(k) \bullet y_r x_r < 0$ because x_r was misclassified, we have:
  - $|w(k+1) - a w^*|^2 \leq |w(k) - a w^*|^2 - 2 a y_r (w^* \bullet x_r) + |y_r x_r|^2$ (Eqn 2)

Convergence Proof (contd)

- Since $y_r(w^*\bullet x_r) > 0$ from (Eqn 1), our goal is:

  pick a so large that $-2ay_r(w^*\bullet x_r) + |y_r x_r|^2 < -c$ for some constant $c>0$
- Let $\beta = \max_i |y_i x_i| = \max_i |x_i|$

  $\gamma = \min_i y_r(w^*\bullet x_r) > 0$ (Neither β nor γ depend on k!)
- Then:
  - $-2ay_r(w^*\bullet x_r) + |y_r x_r|^2 < -2a\gamma + \beta^2$
- Pick $a = \beta^2/\gamma$
- Then:
  - $-2ay_r(w^*\bullet x_r) + |y_r x_r|^2 < -2\beta^2 + \beta^2 = -\beta^2$

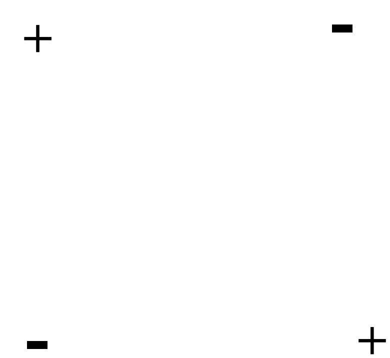
    and so, from (Eqn 2)
  - $|w(k+1)-aw^*|^2 \leq |w(k)-aw^*|^2 - \beta^2$
- Since squared distances are never negative, this decrease must eventually stop; i.e. the update rule "$w(k+1) = w(k) + y_r x_r$ if x_r is misclassified" stops changing w - at that point $w(k) = aw^*$ for some a and so w(k) separates the training points.
- Same proof (different notation!) as in Duda, Hart & Stork, pg 230-232

Perceptron Algorithm (Details)

- Implementing the algorithm in practice:
  - Need to cycle through examples multiple times
  - Update w after each cycle, not every example ("batch perceptron")
  - ***Learning Rate*** η
    - $w \leftarrow w + \eta y_r x_r$
    - small η gives slow convergence
    - large η may cause overshoot
    - η can be updated each iteration, want $\eta = \eta(k) \to 0$ as iteration $k \to \infty$
      - $\eta(k) = \eta(1)/k$
      - Decrease $\eta(k)$ if performance improves on k^{th} step

Non Linearly-Separable

- Perceptron Algorithm does not converge if training set is not linearly separable
  - Cannot learn X-OR or any non-linearly separable concept.
  - Pointed out by Minsky & Papert (1969) - set back research for many years
- Linearly Separable training sample $\nRightarrow$ underlying concept is linearly separable
  - As d, the number of dimensions, increases, random training set is increasingly likely to be linearly separable
- In practice, try get low error if not lin sep.
- Heuristics:
  - Terminate when (length of) w stops fluctuating
  - Average recent w's
  - Choice of learning rate



X-OR

Gradient Descent

- Suppose J is some function of the weight w which we want to minimize.
- Gradient Descent searches iteratively for this minimum by moving from the current choice of w in the direction of J's ***steepest descent***:
  - $w \leftarrow w - \eta \nabla J(w)$,
    - where ∇J is the vector $(\partial J/\partial w_0, \partial J/\partial w_1, ..., \partial J/w_d)$
  - Terminate when $|\eta \nabla J(w)|$ is sufficiently small
- Example: $J(w) = -\Sigma_M y_i(w \bullet x_i)$
  - where the sum is ONLY over the set M of x_i misclassified by this hyperplane
  - $y_i(w \bullet x_i) < 0$ if x_i is misclassified, so $J(w) >= 0$, we would like to minimize J.
- Since $y_i(w \bullet x_i) = y_i(w_1 x_{i1} + ... + w_d x_{id})$,

  $\partial J/\partial w_r = -\Sigma_M y_i x_{ir}$

  $\nabla J = -\Sigma_M y_i x_i$

  and gradient descent becomes:

  $w \leftarrow w + \eta \Sigma_M y_i x_i$ ("batch perceptron")
- Thus Perceptron Algorithm does ***gradient descent search in weight space***.

Least-Mean-Squared

- $J(w)$ = Squared Error$(w) = 0.5\Sigma_1^n (y_i-(w\bullet x_i))^2$
- Since $y_i-(w\bullet x_i) = y_i-(w_1x_{i1}+ \ldots +w_dx_{id})$,

  $\partial J/\partial w_r = 0.5\Sigma_1^n 2(y_i-(w\bullet x_i))(-x_{ir})$

  $\nabla J = -\Sigma_1^n (y_i-(w\bullet x_i))x_i$

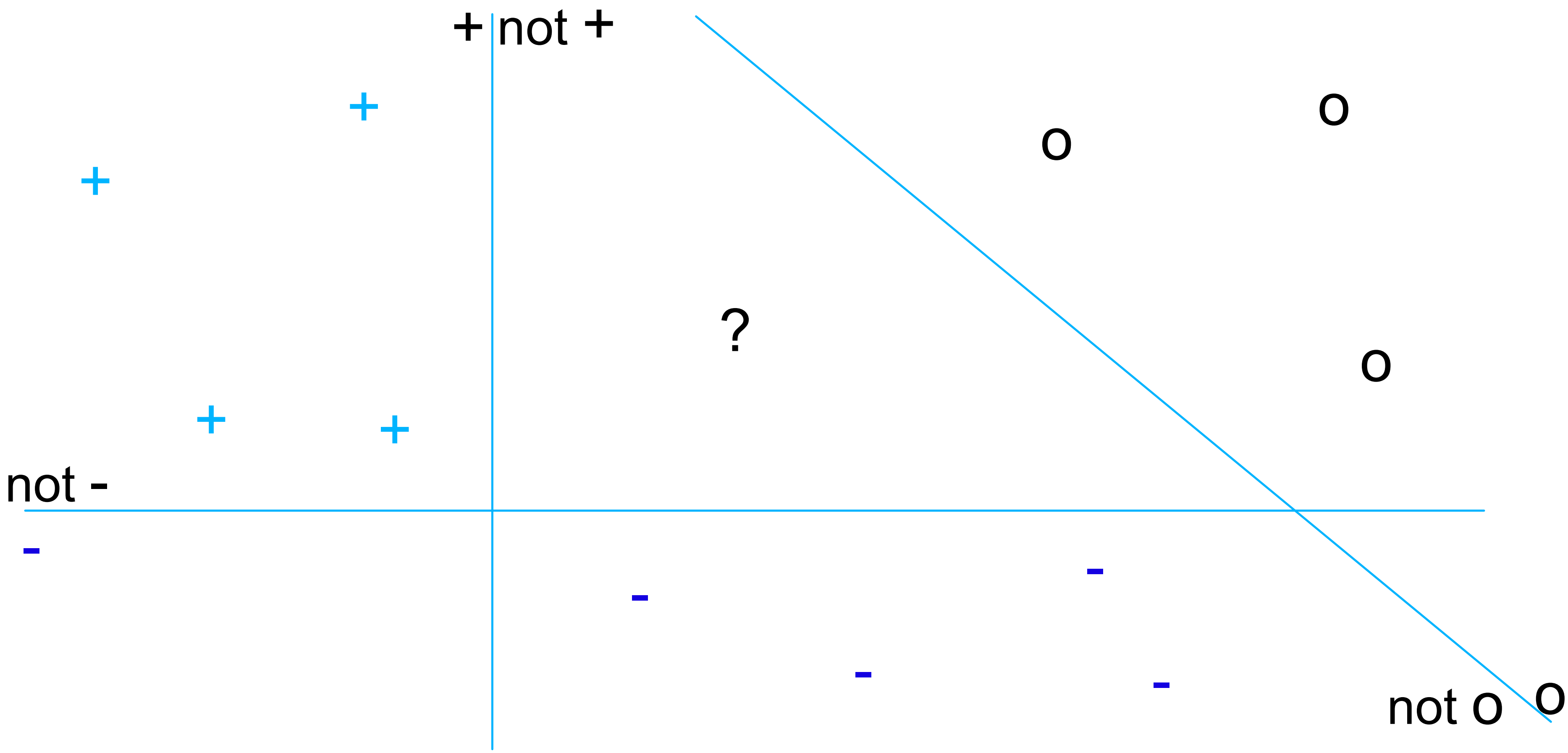
  $w \leftarrow w + \eta\Sigma_1^n(y_i-(w\bullet x_i))x_i$
- For faster convergence, consider the samples one-by-one:

  $w \leftarrow w + \eta(y_i-(w\bullet x_i))x_i$
  - the LMS (or Delta or Widrow-Hoff) learning rule.
  - same algorithm (different notation!) as Duda, Hart and Stork, pg 246.
  - basis of backpropagation algorithm for training neural networks.
- LMS rule converges asymptotically to the weight vector yielding minimum squared error whether or not the training sample is linearly separable.
- However, minimizing the error does NOT necessarily minimize the number of misclassified examples.

Multiple Classes

- Suppose there are n classes c_1, ..., c_n
- (1) 1 vs rest
  - Use 1 linear discriminant for each class c_i, where points in c_i are +ve, all points not in c_i are -ve.
  - Need n linear discriminants
  - Assign ambiguous elements to nearest class
- (2) pairwise
  - Use 1 linear discriminant for each pair of classes
  - Need n(n-1)/2 linear discriminants
  - Assign points to class that gets most votes
  - Assign ambiguous elements to nearest class
- (3) linear machine
  - Use $g_i(x) = w_i x^t + w_{i0}$ for i=1 to n; Assign x to c_i if $g_i(x) > g_j(x)$ for all $j \neq i$
  - Need n linear discriminants
  - No ambiguous elements

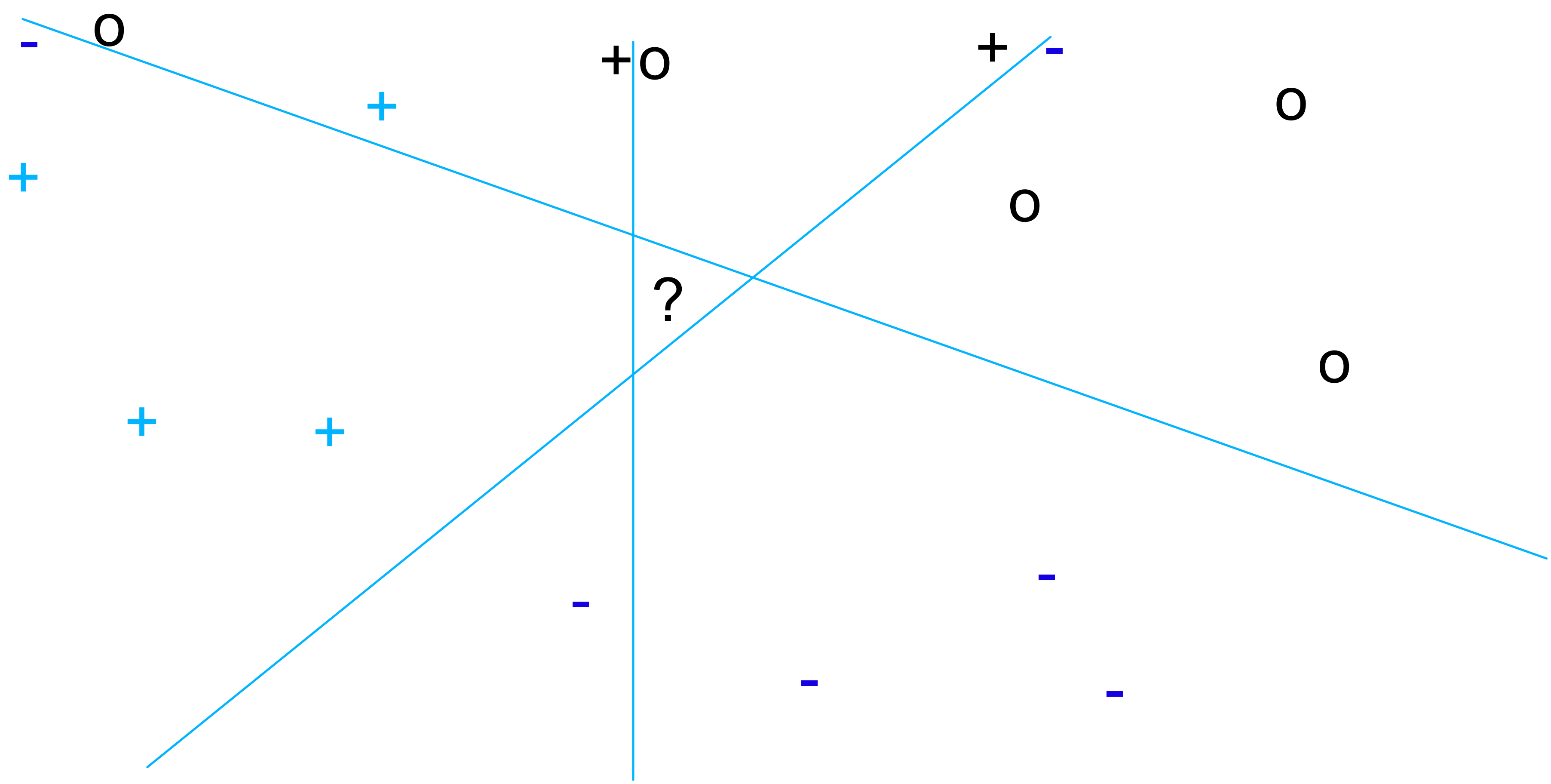
Multiple classes (1 vs rest)



Use n linear discriminants for n classes

Ambiguous region (?) - use distance to nearest class

Multiple class (pairwise)



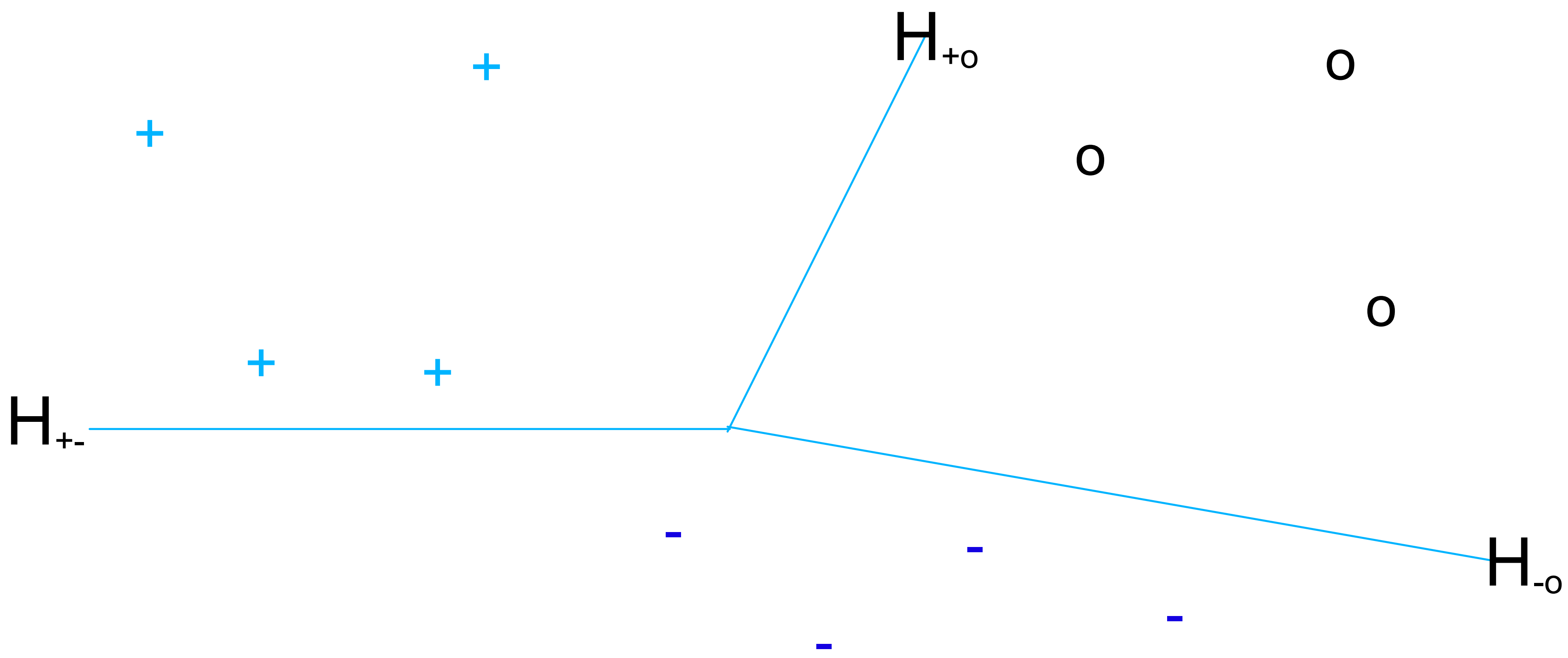
Use n(n-1)/2 linear discriminants for n classes

Ambiguous region (?) - use distance to nearest class

Linear Machine

- Define n linear discriminants:
  - $g_i(x) = w_i x^t + w_{i0}$ i=1 to n
    - Note typo in Duda Hart and Stork, pg 218! ($g_i(x) = w^t x_i + w_{i0}$)
- Assign x to class with largest value:
  - x belongs to c_i if $g_i(x) > g_j(x)$ for all $j \neq i$
- Divides space into n regions, where each g_i is largest
  - Regions are convex and single connected
  - No ambiguous region
- The boundary between any 2 contiguous regions is a hyperplane:
  - $H_{ij} = \{x: g_i(x) = g_j(x)\} = \{x: (w_i - w_j)x^t + w_{i0} - w_{j0} = 0\}$
  - Thus differences between weight vectors are normal to the boundaries
  - May not have all n(n-1)/2 boundaries
- How does the definition of linearly separable generalize to multiple classes? (See Homework)

Multiple classes (Linear machine)



Use n linear discriminants for n classes
No ambiguous region