

ISE 599

Special Topics Applied Predictive Analytics

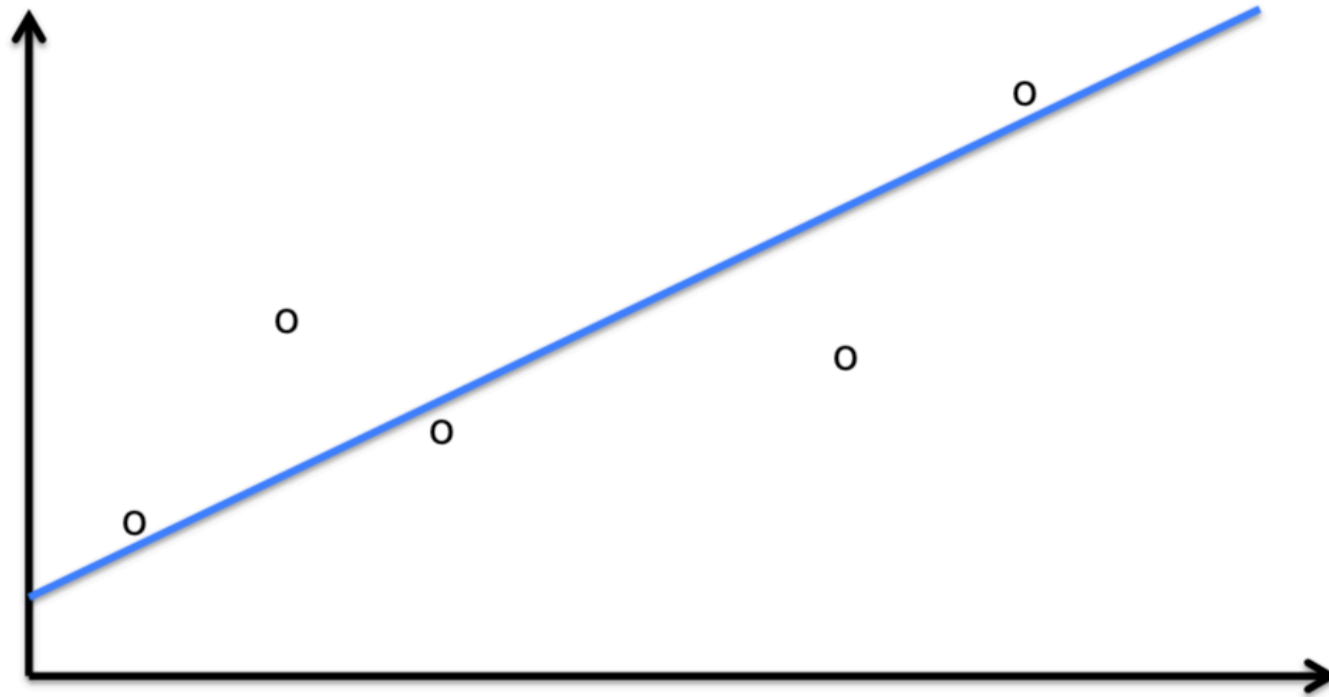
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Linear regression

Given some data $\{(x,y)\dots\}$, with $x, y \in \mathbb{R}$,
find a function $f(x) = w_1x + w_0$ such that $f(x) = y$.



Squared Loss

We want to find a weight vector \mathbf{w} which minimizes the loss (error) on the training data $\{(x_1, y_1) \dots (x_N, y_N)\}$

$$\begin{aligned} L(\mathbf{w}) &= \sum_{i=1}^N L_2(f_{\mathbf{w}}(x_i), y_i) \\ &= \sum_{i=1}^N (y_i - f_{\mathbf{w}}(x_i))^2 \end{aligned}$$

We need to minimize the loss on the training data: $\mathbf{w} = \operatorname{argmin}_{\mathbf{w}} \operatorname{Loss}(f_{\mathbf{w}})$

We need to set partial derivatives of $\operatorname{Loss}(f_{\mathbf{w}})$ with respect to w_1 , w_0 to zero.

There is a closed form solution for linear regression

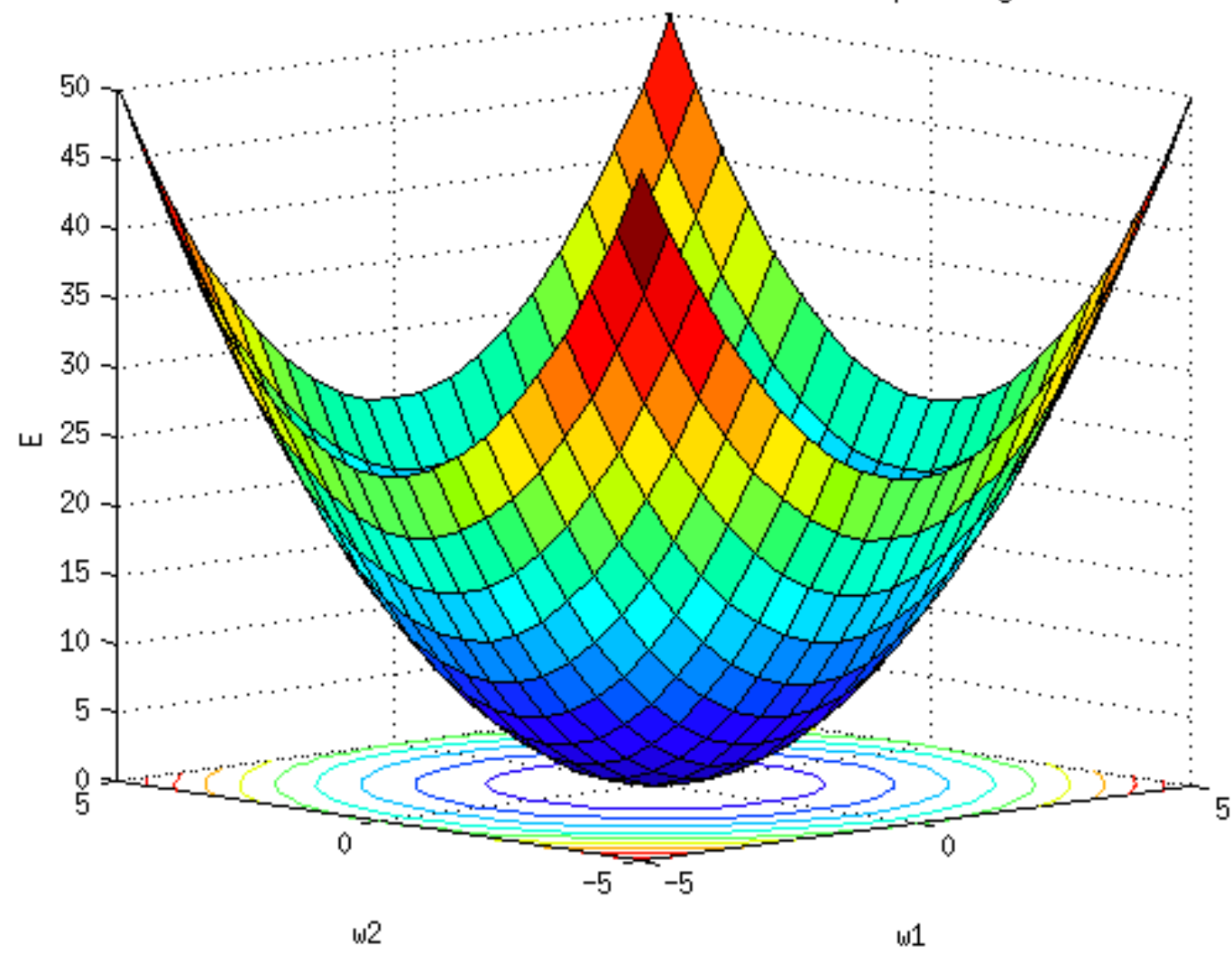
Gradient Descent

In general, we won't be able to find a closed-form solution, so we need an iterative (local search) algorithm.

We will start with an initial weight vector \mathbf{w} , and update each element iteratively in the direction of its gradient:

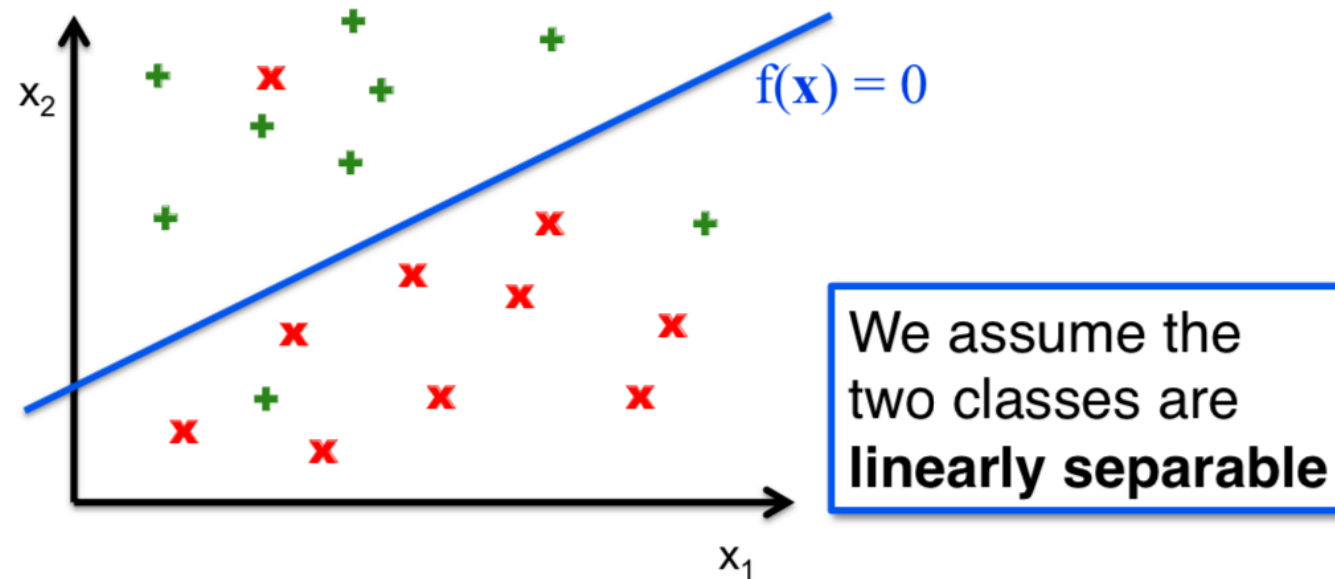
$$w_i := w_i - \alpha \frac{d}{dw_i} \text{Loss}(\mathbf{w})$$

Error Surface of a Linear Neuron with Two Input Weights



Can we use linear 'surfaces' to do classification?

The input $\mathbf{x} = (x_1, \dots, x_d) \in \mathbb{R}^d$ is real-valued vector,
We want to learn $f(\mathbf{x})$.



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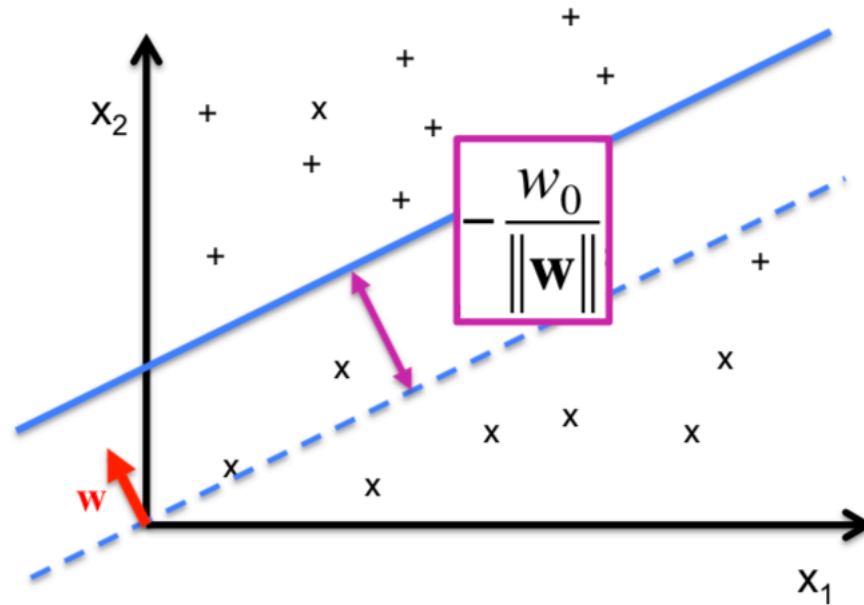
We assume the classes are linearly separable, so
we choose a **linear discriminant function**:

$$f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} + w_0$$

- $\mathbf{w} = (w_1, \dots, w_d) \in \mathbb{R}^d$ is a **weight vector**
- w_0 is a **bias term**
- $-w_0$ is also called a **threshold**: $-w_0 = \mathbf{w} \cdot \mathbf{x}$

The **weight vector \mathbf{w}** defines the **orientation** of the decision boundary.

The **bias term w_0** defines the perpendicular **distance** of the decision boundary to the origin.



Equivalently, redefine

$$\mathbf{x} = (1, x_1, \dots, x_d) \in \mathbb{R}^{d+1}$$

$$\mathbf{w} = (w_0, w_1, \dots, w_d) \in \mathbb{R}^{d+1}$$

$$f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x}$$

$$\text{Define } C_1 = 1 \quad C_2 = 0$$

Our classification hypothesis then becomes

$$h_{\mathbf{w}}(\mathbf{x}) = \begin{cases} 1 & \text{if } f(\mathbf{x}) = \mathbf{w} \cdot \mathbf{x} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Our classification hypothesis then becomes

$$h_{\mathbf{w}}(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w} \cdot \mathbf{x} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

We can also think of $h_{\mathbf{w}}(\mathbf{x})$ as a threshold function.

$$h_{\mathbf{w}}(\mathbf{x}) = \text{Threshold}(\mathbf{w} \cdot \mathbf{x}),$$

where $\text{Threshold}(\mathbf{z}) = \begin{cases} 1 & \text{if } \mathbf{z} \geq 0 \\ 0 & \text{otherwise} \end{cases}$

Learning the weights

We need to choose \mathbf{w} to minimize classification loss.

But we cannot compute this in closed form, because the gradient of \mathbf{w} is either 0 or undefined.

Iterative solution:

- Start with initial weight vector \mathbf{w} .
- For each example (\mathbf{x}, y) update weights \mathbf{w} until all items are correctly classified.

Observations

If we classify an item (\mathbf{x}, y) correctly,
we don't need to change \mathbf{w} .

If we classify an item (\mathbf{x}, y) incorrectly,
there are two cases:

- $y = 1$ (above the true decision boundary)
 $h_{\mathbf{w}}(\mathbf{x}) = 0$ (below the true decision boundary)
We need to move our decision boundary up!
- $y = 0$ (below the true decision boundary)
 $h_{\mathbf{w}}(\mathbf{x}) = 1$ (above the true decision boundary)
We need to move our decision boundary down!

Learning the weights

Evaluating $y - h_{\mathbf{w}}(\mathbf{x})$ will tell us what to do:

- $h_{\mathbf{w}}(\mathbf{x})$ is correct: $y - h_{\mathbf{w}}(\mathbf{x}) = 0$ (stay!)

- If $y = 1$, but we predict $h_{\mathbf{w}}(\mathbf{x}) = 0$

$$y - h_{\mathbf{w}}(\mathbf{x}) = 1 - 0 = 1$$

(move up!)

- If $y = 0$, but we predict $h_{\mathbf{w}}(\mathbf{x}) = 1$

$$y - h_{\mathbf{w}}(\mathbf{x}) = 0 - 1 = -1$$

(move down!)

Learning the weights (initial attempt)

Iterative solution:

- Start with initial weight vector \mathbf{w} .
- For each example (\mathbf{x}, y) update weights \mathbf{w} until all items are correctly classified.

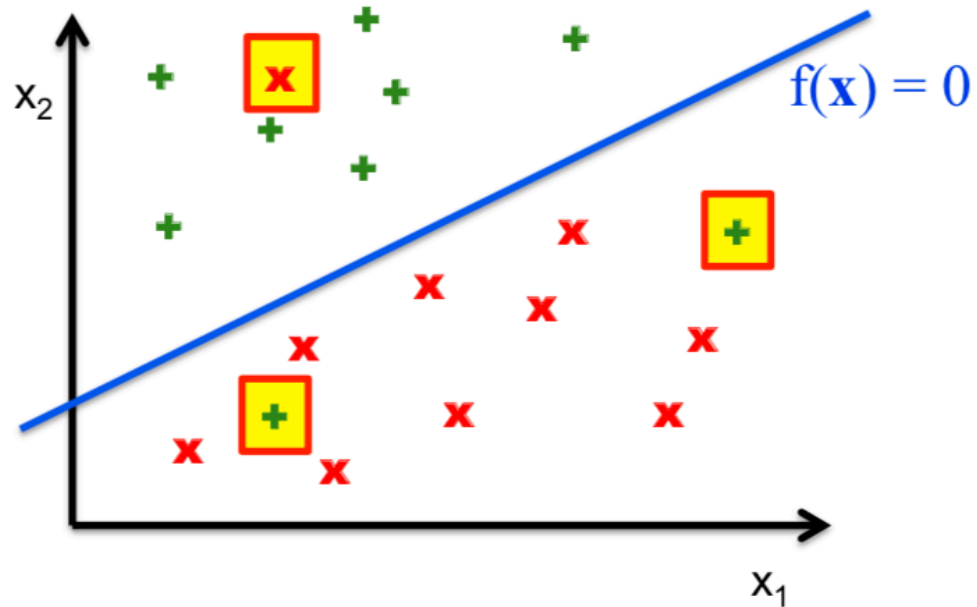
Update rule:

For each example (\mathbf{x}, y) update each weight w_i :

$$w_i := w_i + (y - h_{\mathbf{w}}(\mathbf{x}))x_i$$

There's a problem!

Real data is not perfectly separable.
There will be noise, and our features may not be sufficient.



Learning the weights

Observation:

When we've only seen a few examples, we want the weights to change a lot.

After we've seen a lot of examples, we want the weights to change less and less, because we can now classify most examples correctly.

Solution: We need a **learning rate** which decays over time.

Learning the weights (Perceptron algorithm)

Iterative solution:

- Start with initial weight vector \mathbf{w} .
- For each example (\mathbf{x}, y) update weights \mathbf{w} until \mathbf{w} has converged (does not change significantly anymore)

Perceptron update rule ('online'):

- For each example (\mathbf{x}, y) update each weight w_i :
$$w_i := w_i + \alpha (y - h_{\mathbf{w}}(\mathbf{x}))x_i$$
- α decays over time t ($t = \text{\#examples}$) e.g $\alpha = n/(n+t)$

Batch/Epoch Perceptron Learning

Choose a convergence criterion (#epochs, min $\|\Delta \mathbf{w}\|$, ...)

Choose a learning rate α , an initial \mathbf{w}

Repeat until convergence:

$$\Delta \mathbf{w} = \sum_{\mathbf{x}} \alpha \text{ err } \mathbf{x} \quad (\text{sum over training set holding } \mathbf{w})$$

$$\mathbf{w} \leftarrow \mathbf{w} + \Delta \mathbf{w} \quad (\text{update with accumulated changes})$$

Now it always converges, regardless of α (will influence the rate), and whether or not training points are linearly