Optimization and Gradient Descent

INFO-4604, Applied Machine Learning

University of Colorado Boulder

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Prediction Functions

Remember: a **prediction function** is the function that predicts what the output should be, given the input.

Prediction Functions

Linear regression:

$$f(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + b$$

Linear classification (perceptron):

$$f(\mathbf{x}) = \begin{cases} 1, & \mathbf{w}^T\mathbf{x} + b \geq 0 \\ -1, & \mathbf{w}^T\mathbf{x} + b < 0 \end{cases}$$

Need to *learn* what **w** should be!

Learning Parameters

Goal is to learn to minimize error

- Ideally: true error
- Instead: training error

The **loss function** gives the training error when using parameters **w**, denoted L(**w**).

- Also called **cost function**
- More general: **objective function**
  (in general objective could be to minimize or maximize; with loss/cost functions, we want to minimize)

Learning Parameters

Goal is to minimize loss function.

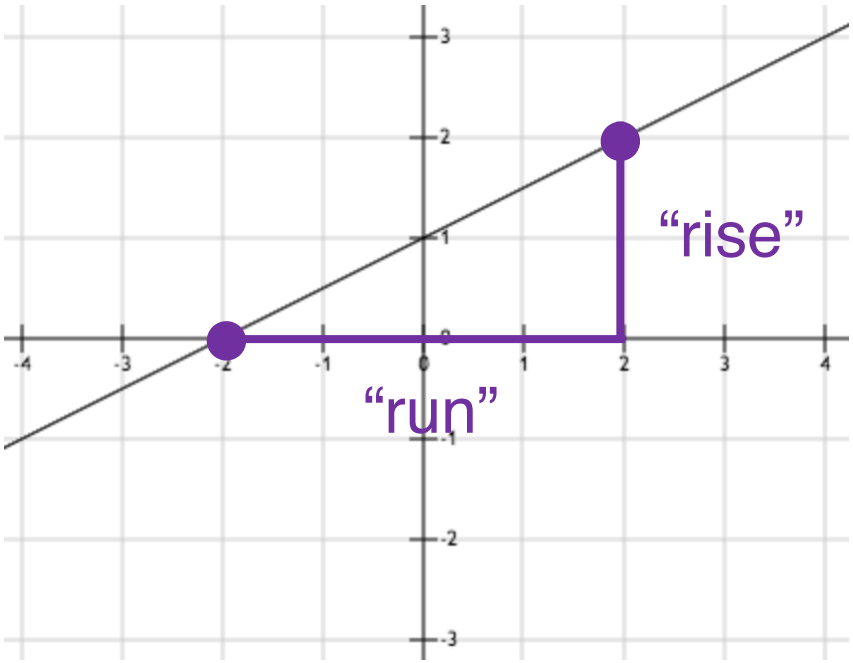
How do we minimize a function?

Let’s review some math.

Rate of Change

The slope of a line is also called the **rate of change** of the line.

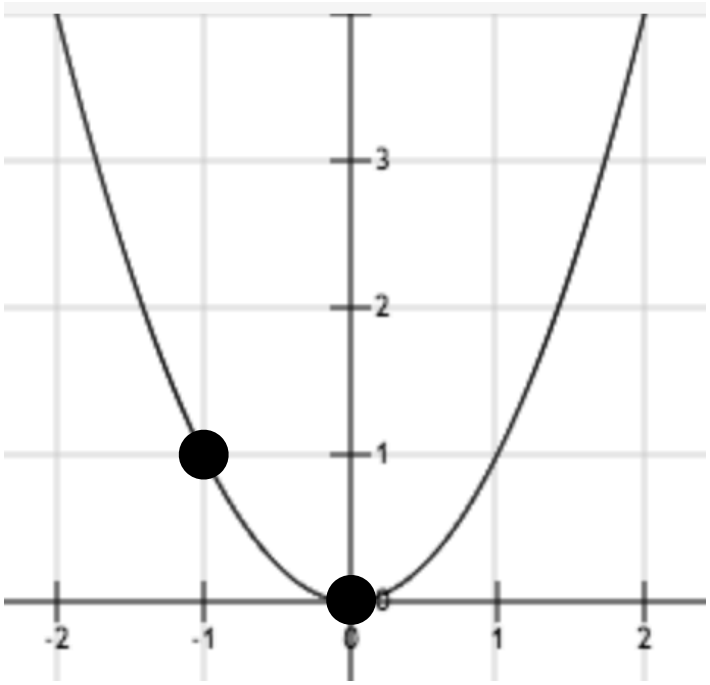
$y = \frac{1}{2}x + 1$



Rate of Change

For nonlinear functions, the “rise over run” formula gives you the average rate of change between two points

$f(x) = x^2$

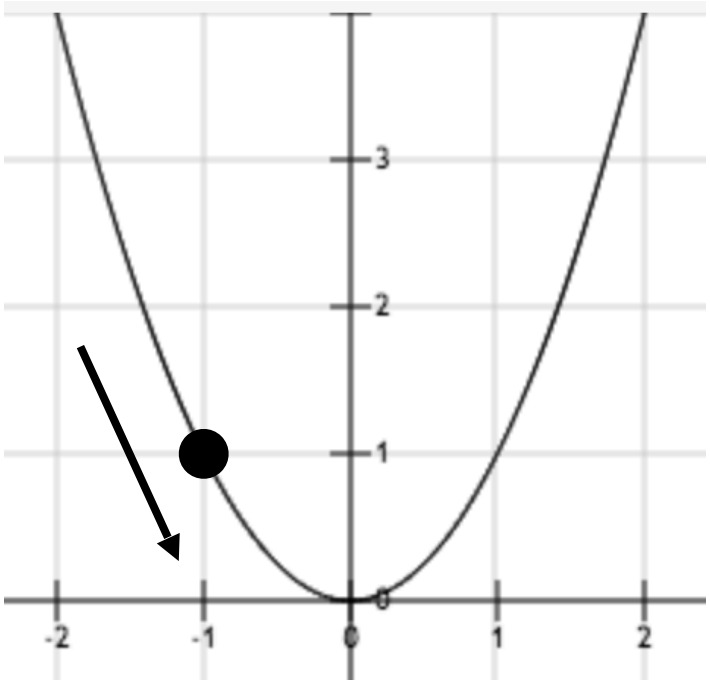


Average slope from x=-1 to x=0 is:
-1

Rate of Change

There is also a concept of rate of change at individual points (rather than two points)

$f(x) = x^2$

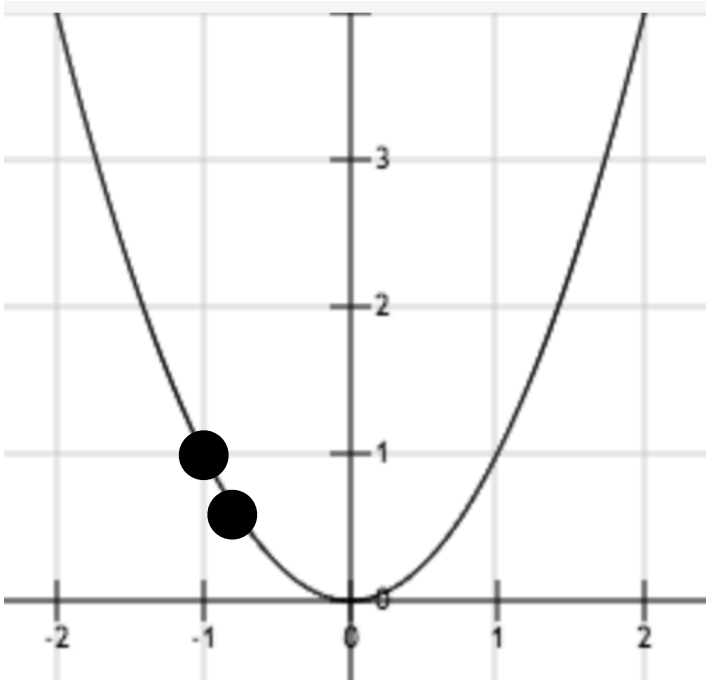


Slope at x=-1 is:
-2

Rate of Change

The slope at a point is called the **derivative** at that point

$f(x) = x^2$



Intuition:
Measure the slope between two points that are really close together

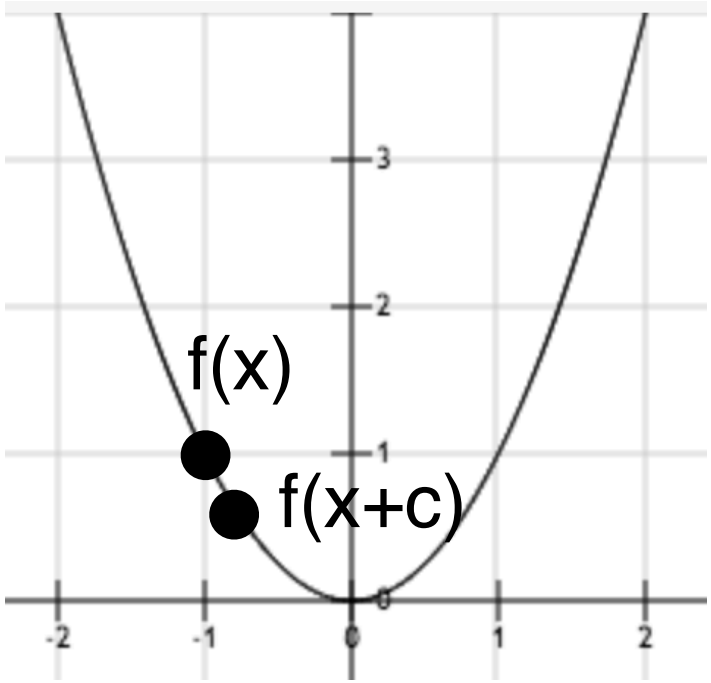
Rate of Change

The slope at a point is called the **derivative** at that point

Intuition: Measure the slope between two points that are really close together

$$\frac{f(x + c) - f(x)}{c}$$

Limit as *c* goes to zero



Maxima and Minima

Whenever there is a peak in the data, this is a **maximum**

The **global** maximum is the highest peak in the entire data set, or the largest f(x) value the function can output

A **local** maximum is any peak, when the rate of change switches from positive to negative

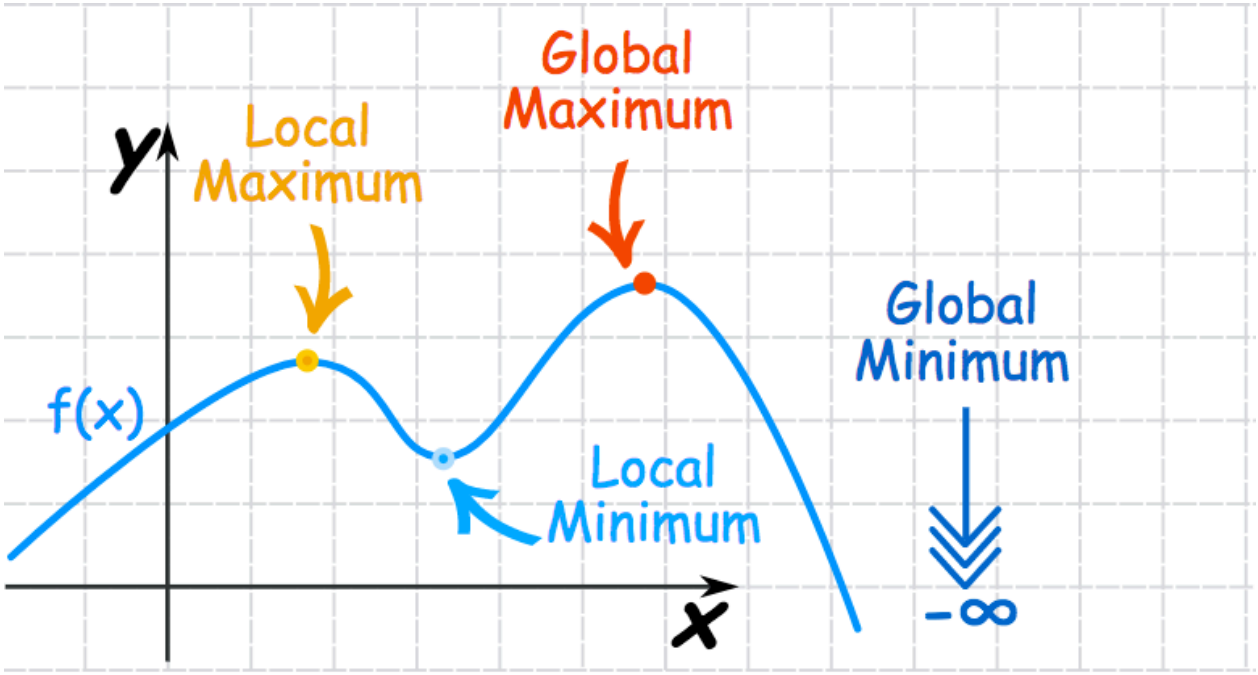
Maxima and Minima

Whenever there is a trough in the data, this is a **minimum**

The **global** minimum is the lowest trough in the entire data set, or the smallest f(x) value the function can output

A **local** minimum is any trough, when the rate of change switches from negative to positive

Maxima and Minima



From: https://www.mathsisfun.com/algebra/functions-maxima-minima.html

All global maxima and minima are also local maxima and minima

Derivatives

The derivative of $f(x) = x^2$ is $2x$

Other ways of writing this:

$f'(x) = 2x$

$d/dx\ [x^2] = 2x$

$df/dx = 2x$

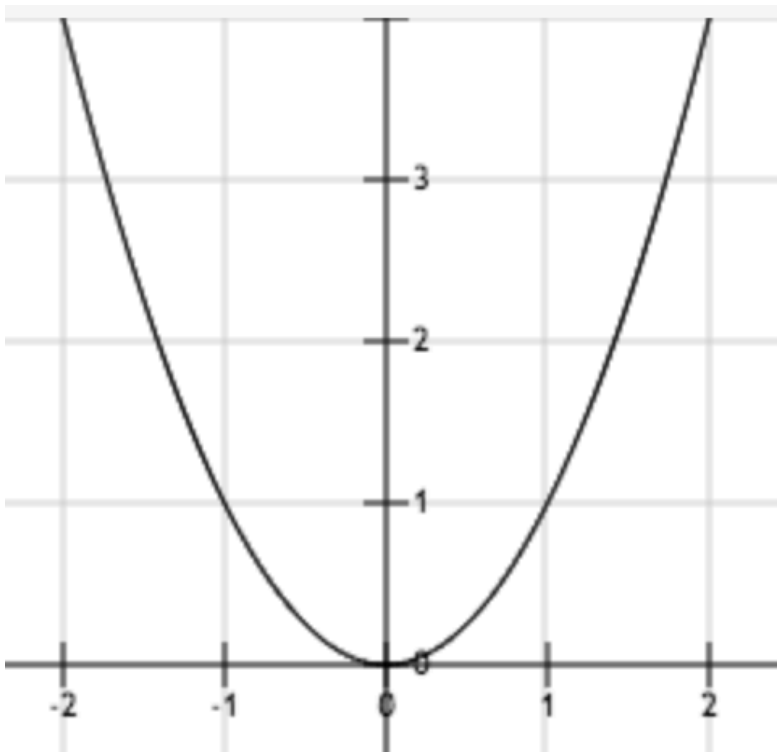
The derivative is also a function! It depends on the value of x.

- The rate of change is different at different points

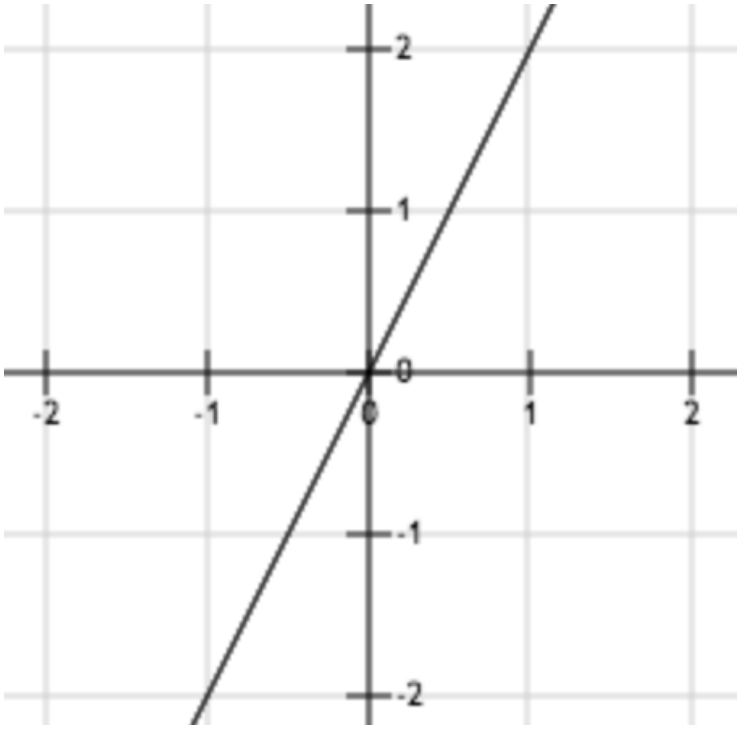
Derivatives

The derivative of $f(x) = x^2$ is $2x$

f(x)



f’(x)



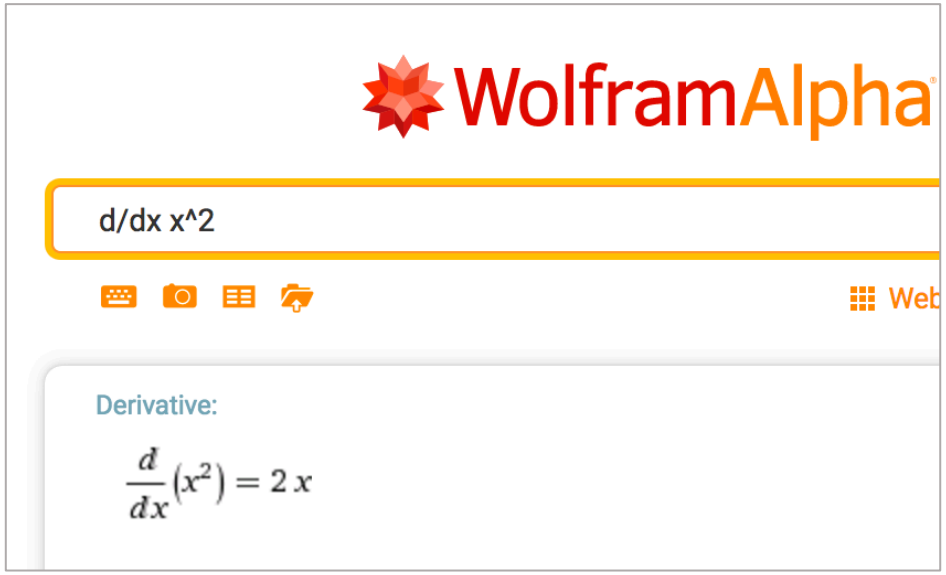
Derivatives

How to calculate a derivative?

- Not going to do it in this class.

Some software can do it for you.

- Wolfram Alpha



Derivatives

What if a function has multiple arguments?

Ex: $f(x_1, x_2) = 3x_1 + 5x_2$

$df/dx_1 = 3 + 5x_2$ The derivative "with respect to" x_1

$df/dx_2 = 3x_1 + 5$ The derivative "with respect to" x_2

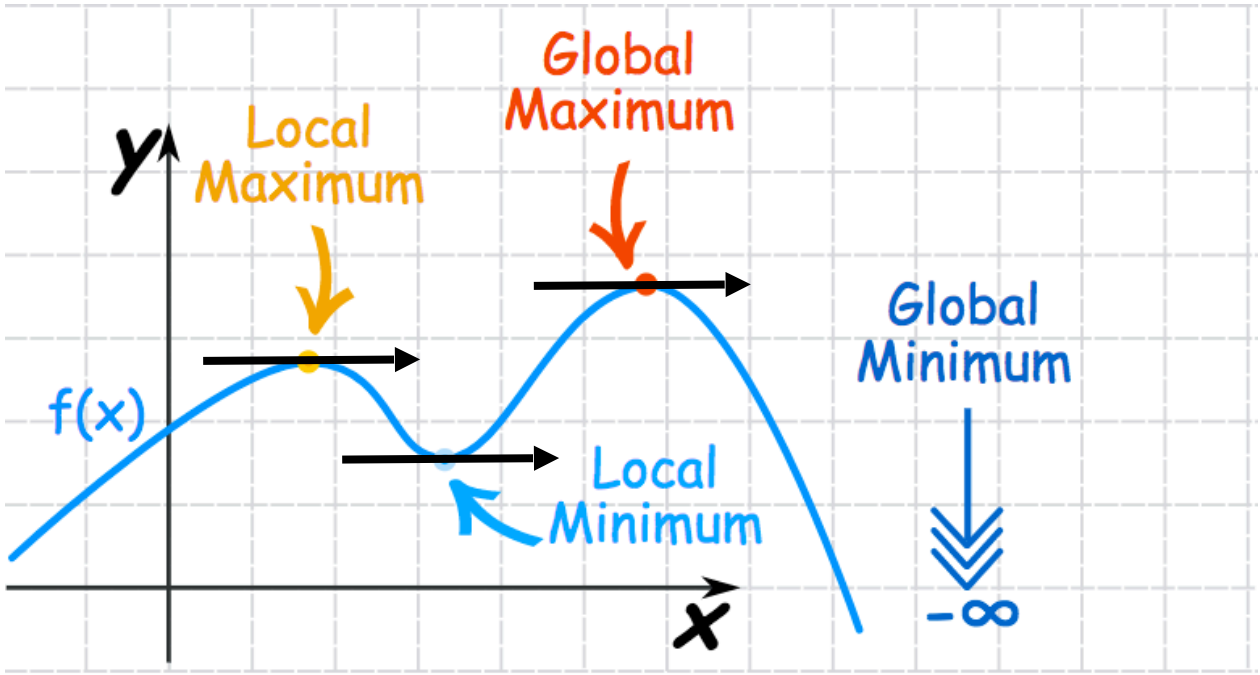
These two functions are called **partial derivatives**.

The vector of all partial derivatives for a function f is called the **gradient** of the function:

$$\nabla f(x_1, x_2) = < df/dx_1 , df/dx_2 >$$

Finding Minima

The derivative is *zero* at any local maximum or minimum.



Finding Minima

The derivative is *zero* at any local maximum or minimum.

One way to find a minimum: set f'(x)=0 and solve for x.

$f(x) = x^2$

$f'(x) = 2x$

$f'(x) = 0$ when $x = 0$, so minimum at $x = 0$

Finding Minima

The derivative is *zero* at any local maximum or minimum.

One way to find a minimum: set f’(x)=0 and solve for x.

- For most functions, there isn’t a way to solve this.
- Instead: algorithmically search different values of x until you find one that results in a gradient near 0.

Finding Minima

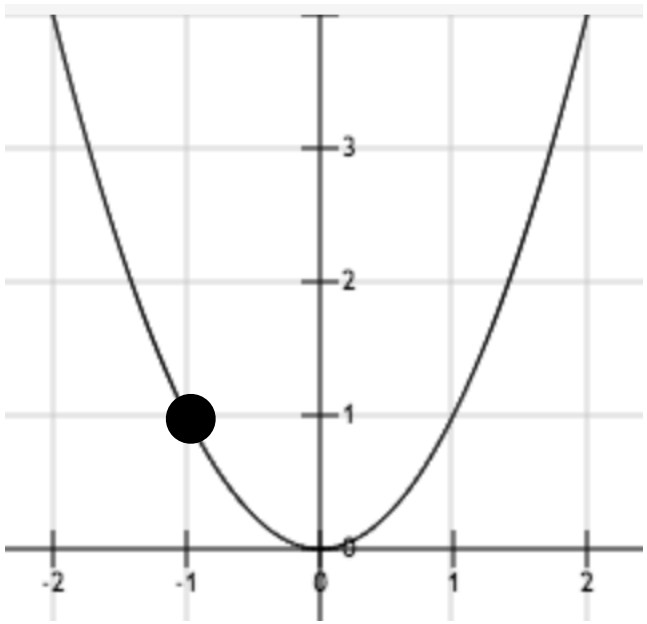
If the derivative is positive, the function is **increasing.**

- Don't move in that direction, because you'll be moving away from a trough.

If the derivative is negative, the function is **decreasing.**

- Keep going, since you're getting closer to a trough

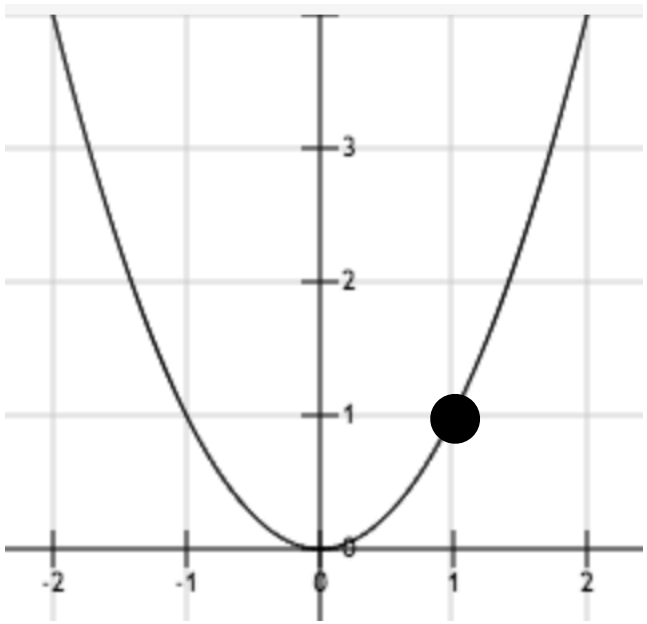
Finding Minima



f’(-1) = -2
At x=-1, the function is decreasing as x gets larger. This is what we want, so let’s make x larger.
Increase x by the size of the gradient:

-1 + 2 = 1

Finding Minima



f’(-1) = -2
At x=-1, the function is decreasing as x gets larger. This is what we want, so let’s make x larger.
Increase x by the size of the gradient:

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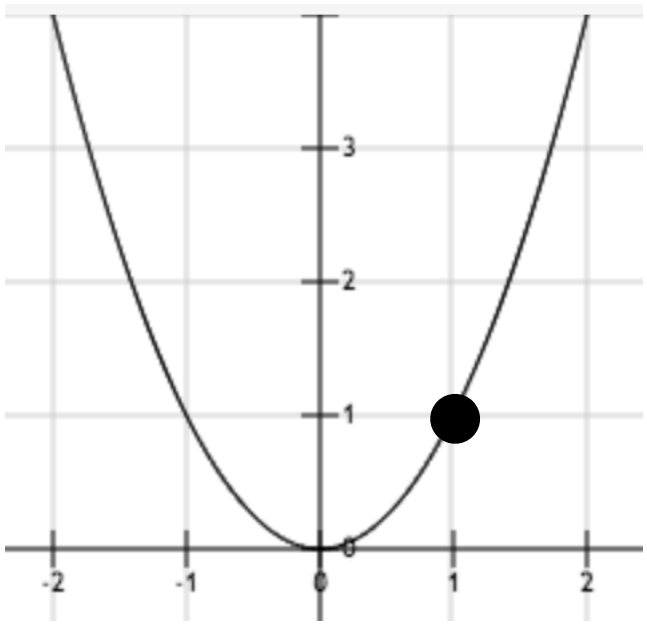
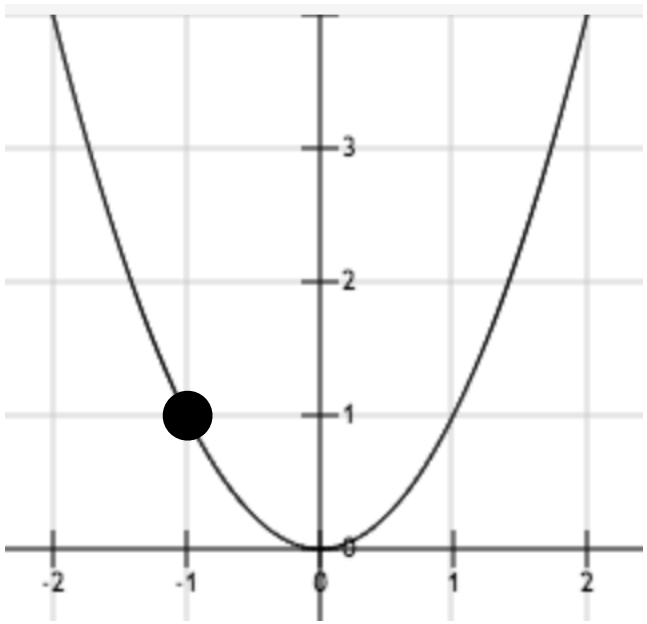
Finding Minima



f’(1) = 2
At x=1, the function is increasing as x gets larger. This is not what we want, so let’s make x smaller. Decrease x by the size of the gradient:

1 - 2 = -1

Finding Minima



f’(1) = 2
At x=1, the function is increasing as x gets larger. This is not what we want, so let’s make x smaller. Decrease x by the size of the gradient:

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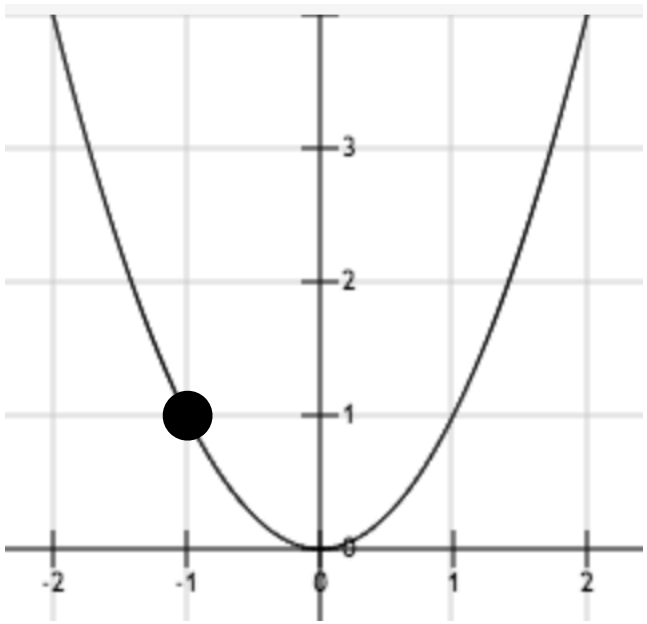
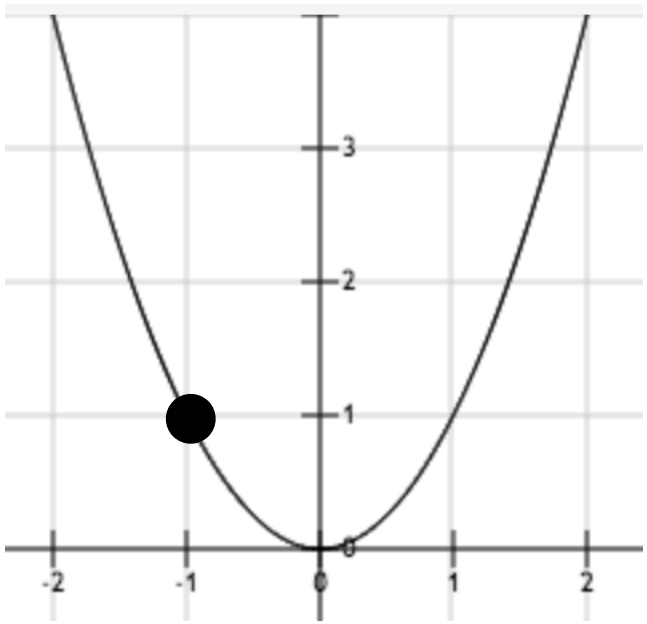
Finding Minima



We will keep jumping between the same two points this way.

We can fix this be using a learning rate or step size.

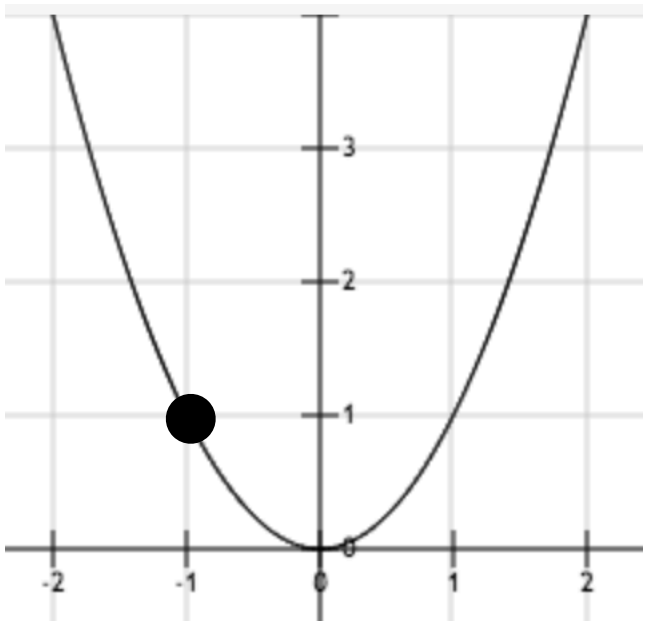
Finding Minima



$f'(-1) = -2$

$x \mathrel{+}= 2\eta =$

Finding Minima

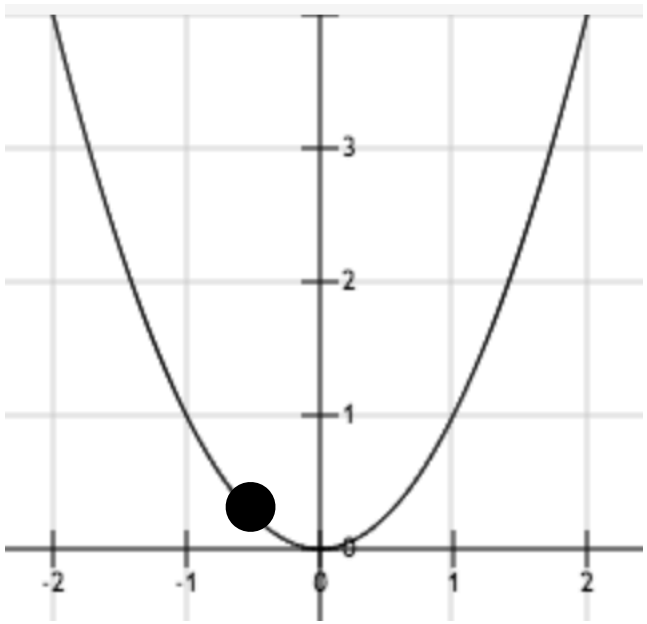


$f'(-1) = -2$

$x \mathrel{+}= 2\eta =$

Let's use $\eta = 0.25$.

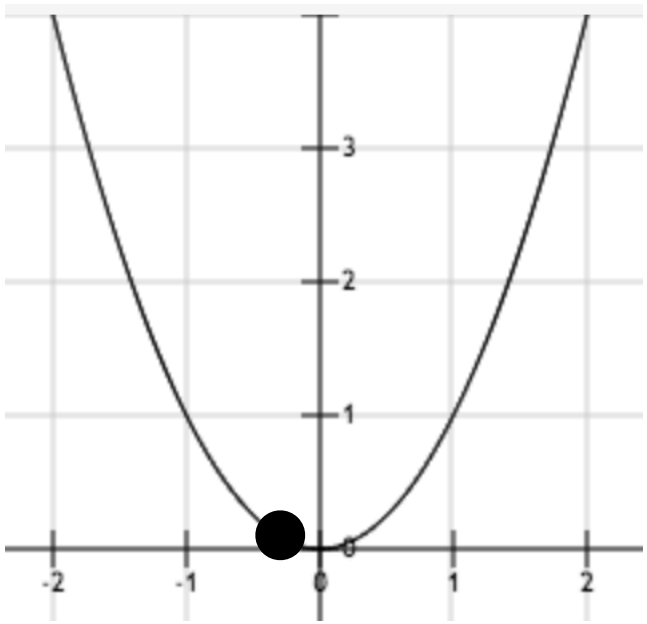
Finding Minima



f’(-1) = -2

x = -1 + 2(.25) = -0.5

Finding Minima



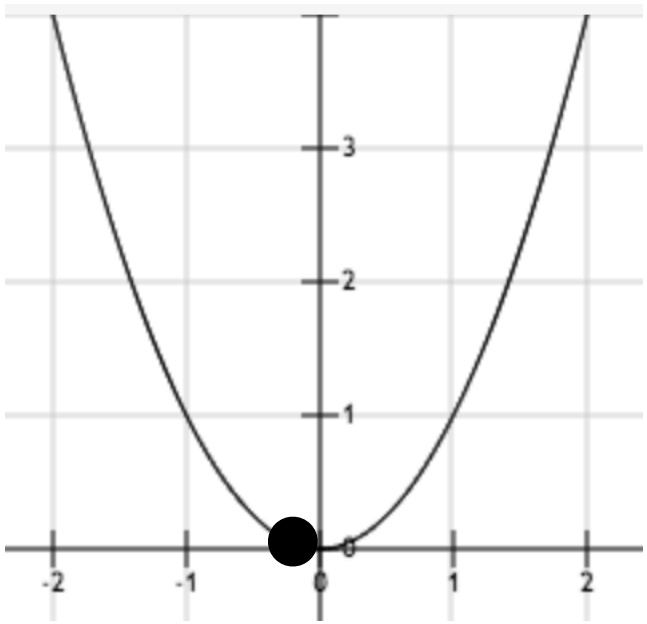
f’(-1) = -2

x = -1 + 2(.25) = -0.5

f’(-0.5) = -1

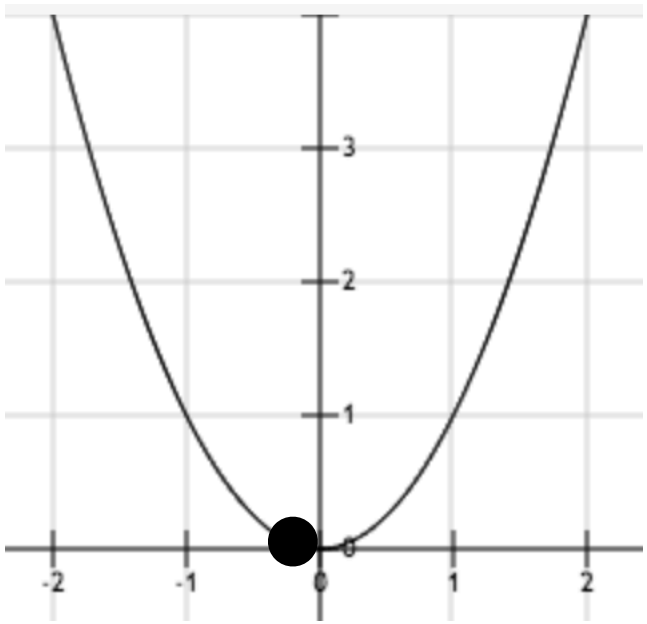
x = -0.5 + 1(.25) = -0.25

Finding Minima



f’(-1) = -2
x = -1 + 2(.25) = -0.5
f’(-0.5) = -1
x = -0.5 + 1(.25) = -0.25
f’(-0.25) = -0.5
x = -0.25 + 0.5(.25) = -0.125

Finding Minima



f’(-1) = -2
x = -1 + 2(.25) = -0.5
f’(-0.5) = -1
x = -0.5 + 1(.25) = -0.25
f’(-0.25) = -0.5
x = -0.25 + 0.5(.25) = -0.125

Eventually we’ll reach x=0.

Gradient Descent

1. Initialize the parameters $\mathbf{w}$ to some guess (usually all zeros, or random values)
2. Update the parameters:
   $$\mathbf{w} = \mathbf{w} - \eta \nabla L(\mathbf{w})$$
3. Update the learning rate η (How? Later…)
4. Repeat steps 2-3 until $\nabla L(\mathbf{w})$ is close to zero.

Gradient Descent

Gradient descent is guaranteed to eventually find a *local* minimum if:

- the learning rate is decreased appropriately;
- a finite local minimum exists (i.e., the function doesn't keep decreasing forever).

Gradient Ascent

What if we want to find a local *maximum*?

Same idea, but the update rule moves the parameters in the opposite direction:

$$\mathbf{w} = \mathbf{w} + \eta \nabla L(\mathbf{w})$$

Learning Rate

In order to guarantee that the algorithm will converge, the learning rate should decrease over time. Here is a general formula.

At iteration t:

$\eta_t = c_1 / (t^a + c_2)$,

where $0.5 < a < 2$

$c1 > 0$

$c2 \geq 0$

Stopping Criteria

For most functions, you probably won't get the gradient to be exactly equal to **0** in a reasonable amount of time.

Once the gradient is sufficiently close to **0**, stop trying to minimize further.

How do we measure how close a gradient is to **0**?

Distance

A special case is the distance between a point and zero (the *origin*).

$$d(\mathbf{p}, \mathbf{0}) = \sqrt{\sum_{i=1}^{k} (p_i)^2}$$

This is called the **Euclidean norm** of **p**

- A norm is a measure of a vector's length
- The Euclidean norm is also called the **L2 norm**

Distance

A special case is the distance between a point and zero (the *origin*).

$$d(\mathbf{p}, \mathbf{0}) = \sqrt{\sum_{i=1}^{k} (p_i)^2}$$

Also written: $\|\mathbf{p}\|$

Stopping Criteria

Stop when the norm of the gradient is below some threshold, θ:

$$||\nabla L(\mathbf{w})|| < \theta$$

Common values of θ are around .01, but if it is taking too long, you can make the threshold larger.

Gradient Descent

1. Initialize the parameters $\mathbf{w}$ to some guess (usually all zeros, or random values)
2. Update the parameters:
   $$\mathbf{w} = \mathbf{w} - \eta \nabla L(\mathbf{w})$$
   $$\eta = c_1 / (t^a + c_2)$$
3. Repeat step 2 until $\|\nabla L(\mathbf{w})\| < \theta$ or until the maximum number of iterations is reached.

End Sep 11th

Revisiting Perceptron

In perceptron, you increase the weights if they were an underestimate and decrease if they were an overestimate.

$$w_j \mathrel{+}= \eta\,(y_i - f(x_i))\,x_{ij}$$

This looks similar to the gradient descent rule.

- Is it? We'll come back to this.

Adaline

Similar algorithm to perceptron (but uncommon):

Predictions use the same function:

$$f(\mathbf{x}) = \begin{cases} 1, & \mathbf{w}^T\mathbf{x} \geq 0 \\ -1, & \mathbf{w}^T\mathbf{x} < 0 \end{cases}$$

(here the bias b is folded into the weight vector **w**)

Adaline

Perceptron minimizes the number of errors.

Adaline instead tries to make $\mathbf{w}^T\mathbf{x}$ close to the correct value (1 or -1, even though $\mathbf{w}^T\mathbf{x}$ can be any real number).

Loss function for Adaline:

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T\mathbf{x}_i)^2$$

This is called the **squared error**. (This is the same loss function used for linear regression.)

Adaline

What is the derivative of the loss?

$$L(\mathbf{w}) = \sum_{i=1}^{N} (y_i - \mathbf{w}^T \mathbf{x_i})^2$$

$$dL/dw_j = \sum_{i=1}^{N} -2\, x_{ij}\, (y_i - \mathbf{w}^T \mathbf{x_i})$$

Adaline

The gradient descent algorithm for Adaline updates each feature weight using the rule:

$$w_j \mathrel{+}= \eta \sum_{i=1}^{N} 2\, x_{ij} (y_i - \mathbf{w}^T \mathbf{x_i})$$

Two main differences from perceptron:

- $(y_i - \mathbf{w}^T \mathbf{x_i})$ is a real value, instead of a binary value (perceptron either correct or incorrect)
- The update is based on the entire training set, instead of one instance at a time.

Adaline

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Stochastic Gradient Descent

A variant of gradient descent makes updates using an approximate of the gradient that is only based on one instance at a time.

$L_i(\mathbf{w}) = (y_i - \mathbf{w}^T\mathbf{x_i})^2$

$dL_i/dw_j = -2\, x_{ij}\, (y_i - \mathbf{w}^T\mathbf{x_i})$

Stochastic Gradient Descent

General algorithm for SGD:

1. Iterate through the instances in a random order
   a) For each instance x_i, update the weights based on the gradient of the loss for that instance only:

      $$\mathbf{w} = \mathbf{w} - \eta \nabla L_i(\mathbf{w}; \mathbf{x_i})$$

The gradient for one instance's loss is an approximation to the true gradient

- stochastic = random
  The *expected* gradient is the true gradient

Adaline

The gradient descent algorithm for Adaline updates each feature weight using the rule:

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Two main differences from perceptron:

- $(y_i - \mathbf{w}^T \mathbf{x_i})$ is a real value, instead of a binary value (perceptron either correct or incorrect)
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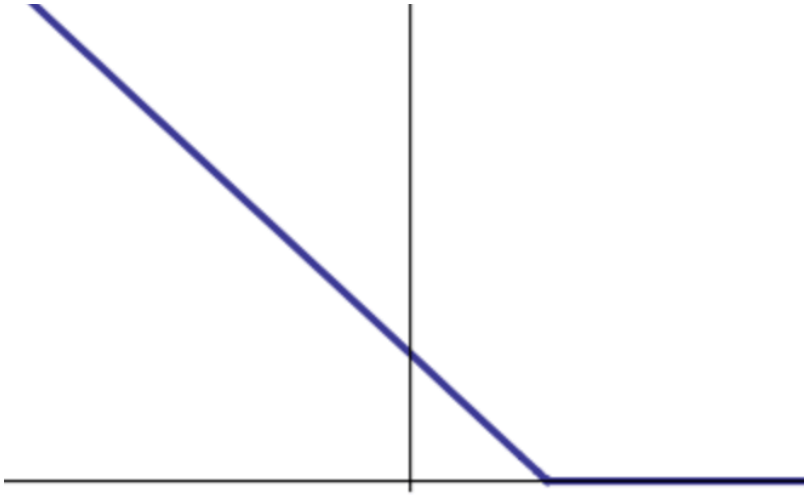
Revisiting Perceptron

Perceptron has a different loss function:

$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\,(\mathbf{w}^T\mathbf{x_i}) \geq 0 \\ -\,y_i\,(\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$



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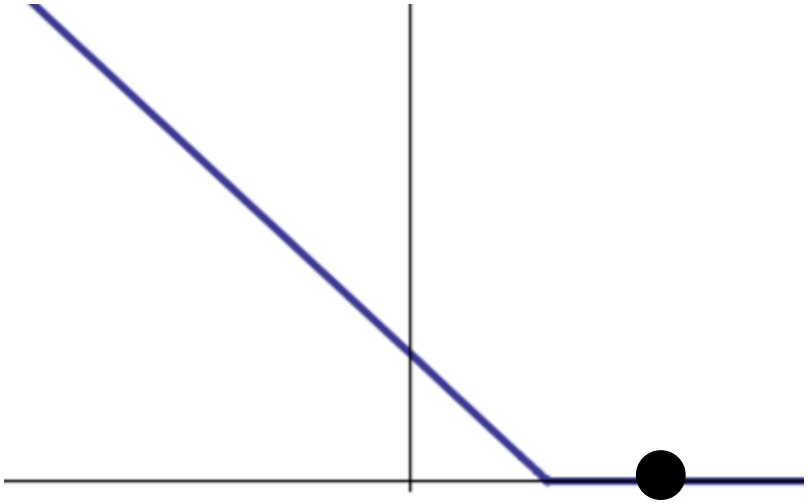

The derivative here is 0. No gradient descent updates if the prediction was correct.

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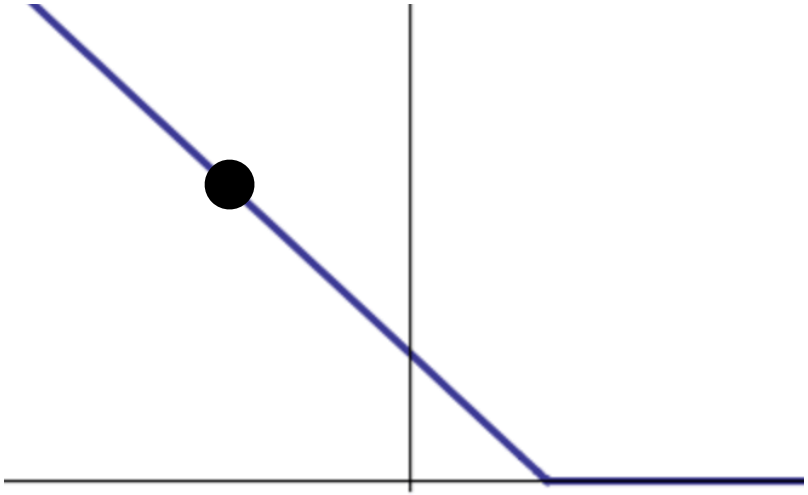
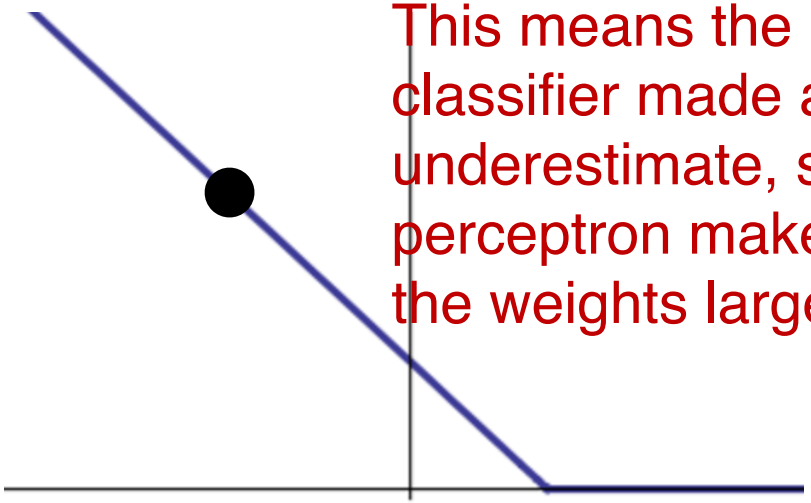


The derivative here is $-y_i x_{ij}$. If x_{ij} is positive, dL_i/w_j will be negative when y_i is positive, so the gradient descent update will be positive.

Revisiting Perceptron

Perceptron has a different loss function:

$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\,(\mathbf{w}^T\mathbf{x_i}) \geq 0 \\ -\,y_i\,(\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$



This means the classifier made an underestimate, so perceptron makes the weights larger.

The derivative here is $-y_i x_{ij}$. If x_{ij} is positive, dL_i/w_j will be negative when y_i is positive, so the gradient descent update will be positive.

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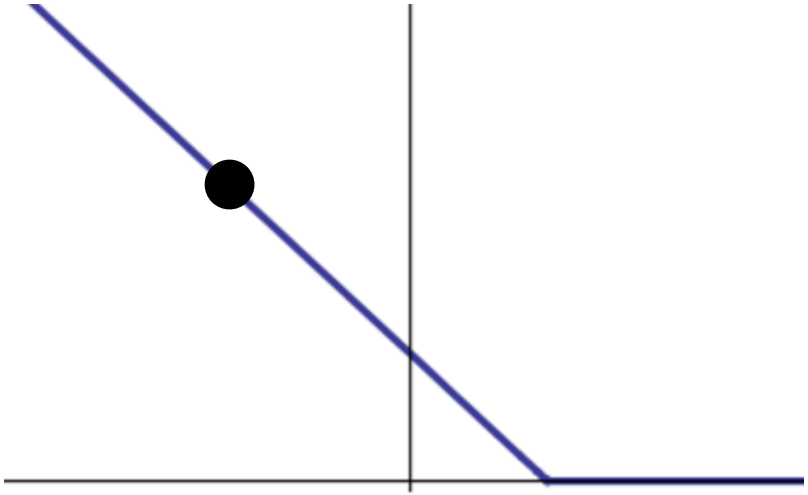
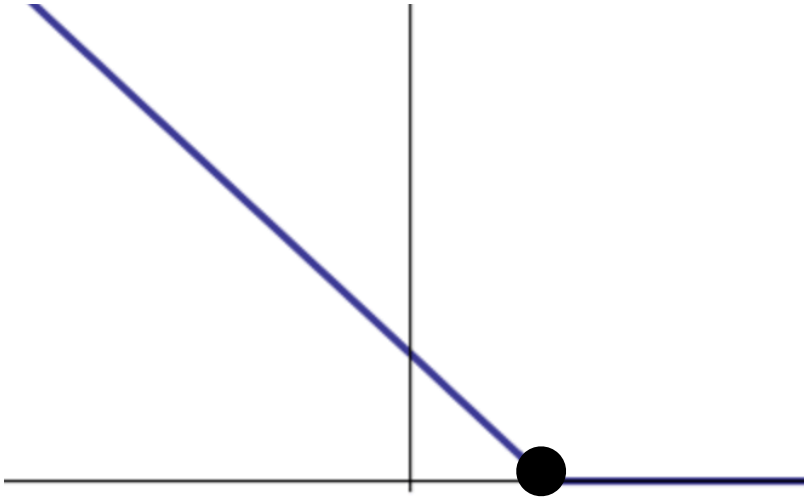


The derivative here is $-y_i x_{ij}$. If x_{ij} is positive, dL_i/w_j will be positive when y_i is negative, so the gradient descent update will be negative.

Revisiting Perceptron

Perceptron has a different loss function:

$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\,(\mathbf{w}^T\mathbf{x_i}) \geq 0 \\ -\,y_i\,(\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$

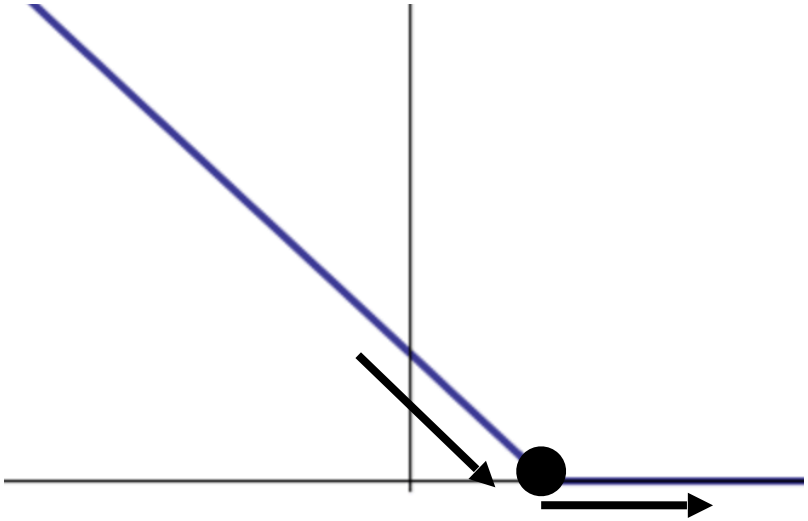


The derivative doesn't actually exist at this point (the function isn't smooth)

Revisiting Perceptron

Perceptron has a different loss function:

$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\ (\mathbf{w}^T\mathbf{x_i}) \geq 0 \\ -\ y_i\ (\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$



A **subgradient** is a generalization of the gradient for points that are not differentiable.

0 and $-y_i x_{ij}$ are both valid subgradients at this point.

Revisiting Perceptron

Perceptron has a different loss function:

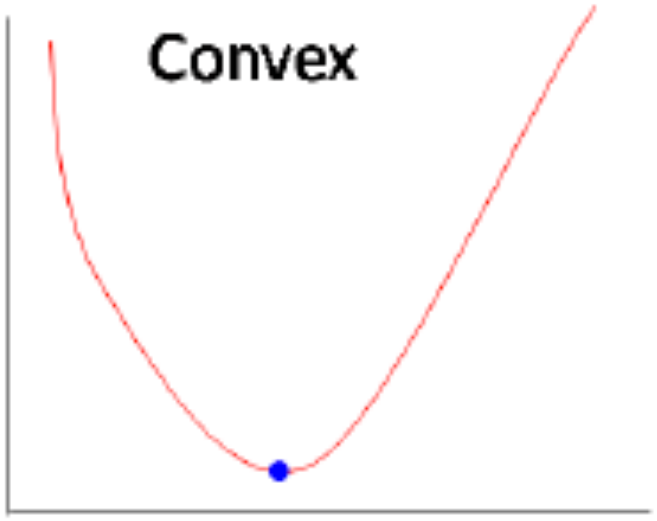
$$L_i(\mathbf{w}; \mathbf{x_i}) = \begin{cases} 0, & y_i\ (\mathbf{w}^T\mathbf{x_i}) \geq 0 \\ -\ y_i\ (\mathbf{w}^T\mathbf{x_i}), & \text{otherwise} \end{cases}$$

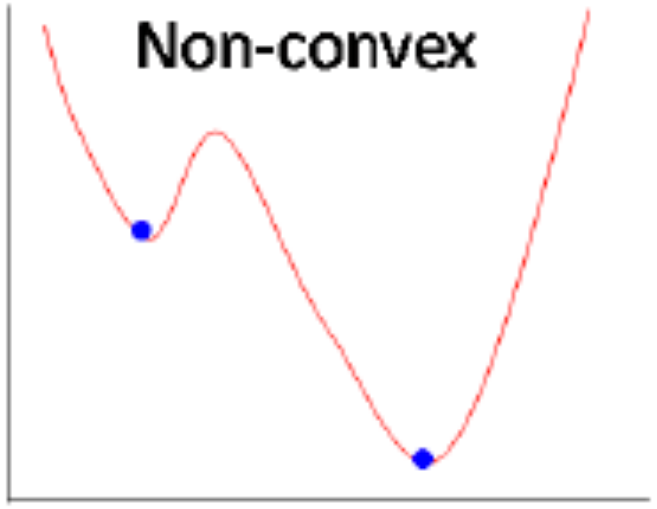
Perceptron is a stochastic gradient descent algorithm using this loss function (and using the subgradient instead of gradient)

Convexity

How do you know if you've found the global minimum, or just a local minimum?

A **convex** function has only one minimum:

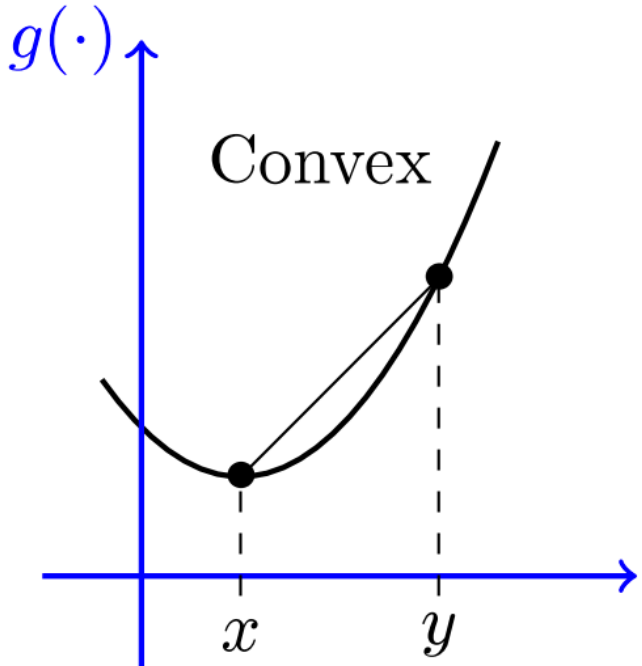




Convexity

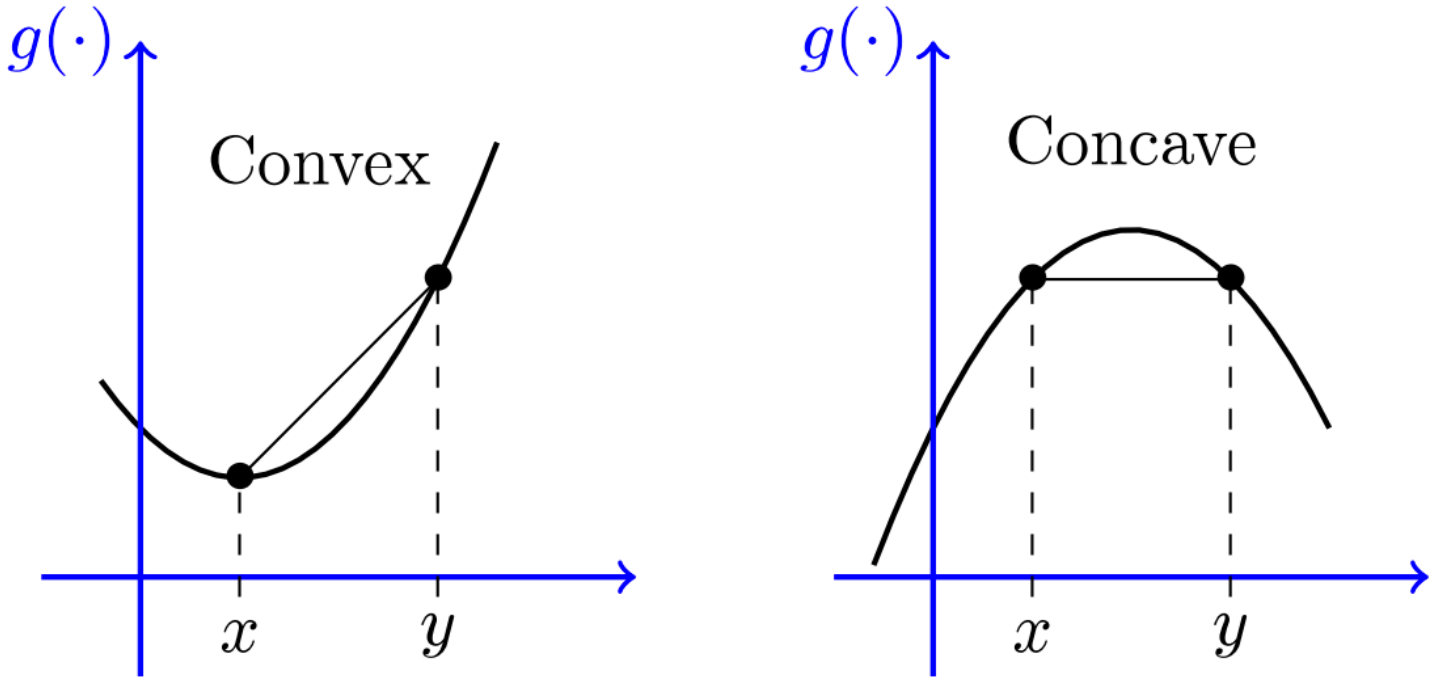
How do you know if you've found the global minimum, or just a local minimum?

A **convex** function has only one minimum:



Convexity

A **concave** function has only one maximum:

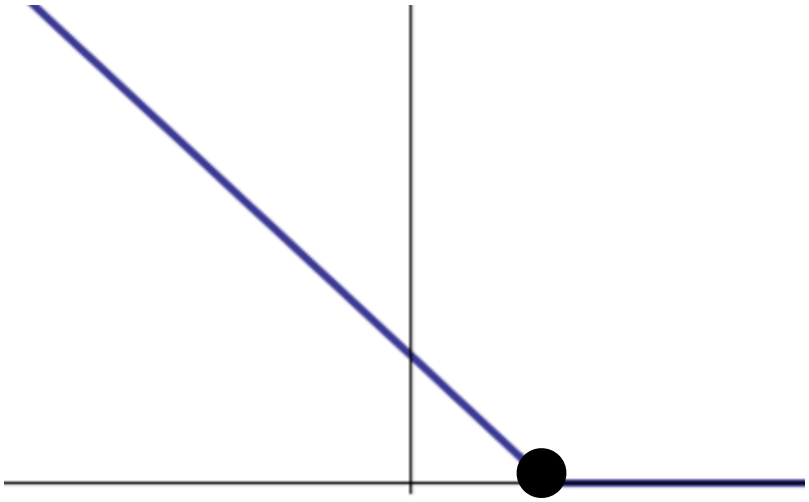


Sometimes people use “convex” to mean either convex or concave

Convexity

Squared error is a convex loss function, as is the perceptron loss.

Note: convexity means there is only one minimum value, but there may be multiple parameters that result in that minimum value.



Summary

Most machine learning algorithms are some combination of a loss function + an algorithm for finding a local minimum.

- Gradient descent is a common minimizer, but there are others.

With most of the common classification algorithms, there is only one global minimum, and gradient descent will find it.

- Most often: supervised functions are convex, unsupervised functions are non-convex.

Summary

1. Initialize the parameters $\mathbf{w}$ to some guess (usually all zeros, or random values)
2. Update the parameters:
   $$\mathbf{w} = \mathbf{w} - \eta \nabla L(\mathbf{w})$$
   $$\eta = c_1 / (t^a + c_2)$$
3. Repeat step 2 until $\|\nabla L(\mathbf{w})\| < \theta$ or until the maximum number of iterations is reached.