

Gradient Descent

Many problems in Machine Learning are framed as *optimization* problems

- Find the choice of parameters Θ
- That minimizes a Loss function

The best (optimal) Θ is the one that minimizes the Average (across training examples) Loss

$$\Theta^* = \underset{\Theta}{\operatorname{argmin}} \mathcal{L}_{\Theta}$$

Many Classical ML problems are designed such that Θ^* has a closed-form solution

- Maximum likelihood estimates for Linear Regression

Closed form solutions, however, may only be feasible for Loss function of restricted form.

When a closed form solution is not possible, we may find Θ^* via a search process known as Gradient Descent.

The search process produces a sequence

$$\Theta_{(0)}^*, \Theta_{(1)}^*, \dots$$

of increasingly accurate estimates of the optimal Θ^* .

In the Deep Learning part of the course, virtually all Loss functions will require this form of solution.

Note

We previewed this method in the sub-module on [Gradient Boosting \(Ensembles.ipynb#Example:-Boosting-for-a-Regression-task\)](#).

Loss functions, review

- $\hat{\mathbf{y}}^{(i)} = h(\mathbf{x}^{(i)}; \Theta)$, the prediction for example $\mathbf{x}^{(i)}$ with target label $\mathbf{y}^{(i)}$
- Per-example loss

$$\mathcal{L}_{\Theta}^{(i)} = L(h(\mathbf{x}^{(i)}; \Theta), \mathbf{y}^{(i)}) = L(\hat{\mathbf{y}}^{(i)}, \mathbf{y})$$

- The Loss for the entire training set is simply the average (across examples) of the Loss for the example

$$\mathcal{L}_{\Theta} = \frac{1}{m} \sum_{i=1}^m \mathcal{L}_{\Theta}^{(i)}$$

Two common forms of L are Mean Squared Error (for Regression) and Cross Entropy Loss (for classification).

Optimization

How do we find the Θ^* that minimizes \mathcal{L} ?

$$\Theta^* = \underset{\Theta}{\operatorname{argmin}} \mathcal{L}_{\Theta}$$

One way is via a search-like procedure known as Gradient Descent:

We start with

- an initial guess for Θ^* for Θ^*
$$\Theta_{(0)}^* = \Theta_{(0)}$$
- and update the guess repeatedly

The update $\Theta_{(t)}$ on step t

- updates $\Theta_{(t)}^*$
- to
$$\Theta_{(t+1)}^* = \Theta_{(t)}^* + \Theta_{(t)}$$

The updates are guided by the objective of

- *decreasing* the loss \mathcal{L}_{Θ}

We achieve this objective at step t in two steps

First,

- Compute the loss \mathcal{L}_{Θ} using the current estimate $\Theta_{(t)}^*$:
 - averaging the per-example loss across the m across training examples
$$\langle \mathbf{X}, \mathbf{y} \rangle = [\mathbf{x}^{(i)}, \mathbf{y}^{(i)} | 1 \leq i \leq m]$$

Second, we compute the update $\Theta_{(t)}$ as

- the negative of the derivative of the loss with respect to Θ
 - evaluated at the current estimate of Θ^*

$$\Theta_{(t)} = -1 * \frac{\partial}{\partial \Theta} \mathcal{L}_{\Theta} \Big|_{\Theta = \Theta_{(t-1)}^*}$$

Why the negative ?

Since the derivative

- points in the direction of *increasing* loss
- and we want to decrease the loss
- the update is in the opposite direction (negative)

The update for Θ^* is

$$\begin{aligned}\Theta_{(t)}^* &= \Theta_{(t-1)}^* + \alpha * \Theta_{(t)} \\ &= \Theta_{(t-1)}^* - \alpha * \frac{\partial}{\partial \Theta} \mathcal{L}_{\Theta} \Big|_{\Theta = \Theta_{(t-1)}^*}\end{aligned}$$

Note

Θ is a vector

- of length n

as is the gradient

So the derivative should properly be replaced with the gradient ∇_{Θ}

$$\Theta_{(t)}^* = \Theta_{(t-1)}^* - \alpha * \nabla_{\Theta} \mathcal{L}_{\Theta} \Big|_{\Theta = \Theta_{(t-1)}^*}$$

Since the update decreases the Loss, this technique is called *Gradient Descent*.

Here is some illustrative code we will use to demonstrate the process.


```
In [5]: def f(x):
        return x**2

def deriv(f, x_0):
    h = 0.000000001          #step-size
    return (f(x_0 +h) - f(x_0))/h

def tangent(f, x_0, x=None):
    y_0 = f(x_0)
    slope = deriv(f, x_0)

    if x is not None:
        r = 2
        xmin, xmax = np.min(x), np.max(x)
        xlo, xhi = max(x_0 -r, xmin), min(x_0 +r, xmax)
    else:
        r = 2
        xlo, xhi = x_0 -r, x_0 + r

    xline = np.linspace(xlo, xhi, 10)
    yline = y_0 + slope*( xline - x_0)

    return xline, yline

def plot_tangent(f, x_s, x, ax, show_tangent=True):
    # Plot function
    _ = ax.plot(x, f(x))

    # Plot tangent point x_s
    y_s = f(x_s)
    ax.scatter(x_s, y_s, color='r', s=90)

    # Plot tangent line
    if show_tangent:
        xtang, ytang = tangent(f, x_s, x)
```

```
ax.plot(xtang, ytang, 'g--')
```

```
return ax
```

```
In [6]: def plot_step(f, x_s, x, show_tangent=True, visible=True):
        fig, ax = plt.subplots(1, 1, figsize=(12,6))

        y_s = f(x_s)

        # Plot the function, the point, and optionally: the tangent line
        _ = plot_tangent(f, x_s, x, ax, show_tangent=show_tangent)

        _ = ax.set_xlabel("$\Theta$", fontsize=16)
        _ = ax.set_ylabel("$L$", fontsize=16, rotation=0)

        if not visible:
            plt.close(fig)

        return fig, ax
```

```

In [7]: def plot_gradient_descent(max_steps=4, alphas=[ 0.1, 0.4, 0.7, 1.0 ]):

    fig, axs = plt.subplots(len(alphas), max_steps, figsize=(20,min(12, 6 * len
(alphas))))
    axs = axs.reshape( (len(alphas), max_steps) ) # Take care of special case w
here len(alpha) == 1

    for a_idx, alpha in enumerate(alphas):
        x_s = x_0

        for step in range(0,max_steps):
            ax = axs[a_idx, step]
            _ = ax.set_xlabel(" $\Theta$ ", fontsize=16)
            _ = ax.set_ylabel(" $L$ ", fontsize=16, rotation=0)
            _ = ax.set_title('$\\alpha$={a:3.2f}'.format(a=alpha))
            y_s = f(x_s)

            # Obtain tangent line at x0
            _ = plot_tangent(f, x_s, x, ax)

            # Update x_s
            slope = deriv(f, x_s)
            x_s = x_s + alpha * (- slope)

    _ = fig.tight_layout()

    plt.close(fig)
    return fig, axs

```



```
In [8]: alpha = 0.4  
x = np.linspace(-5, +5, 30)
```

Gradient Descent: Overview

We illustrate the process with an example

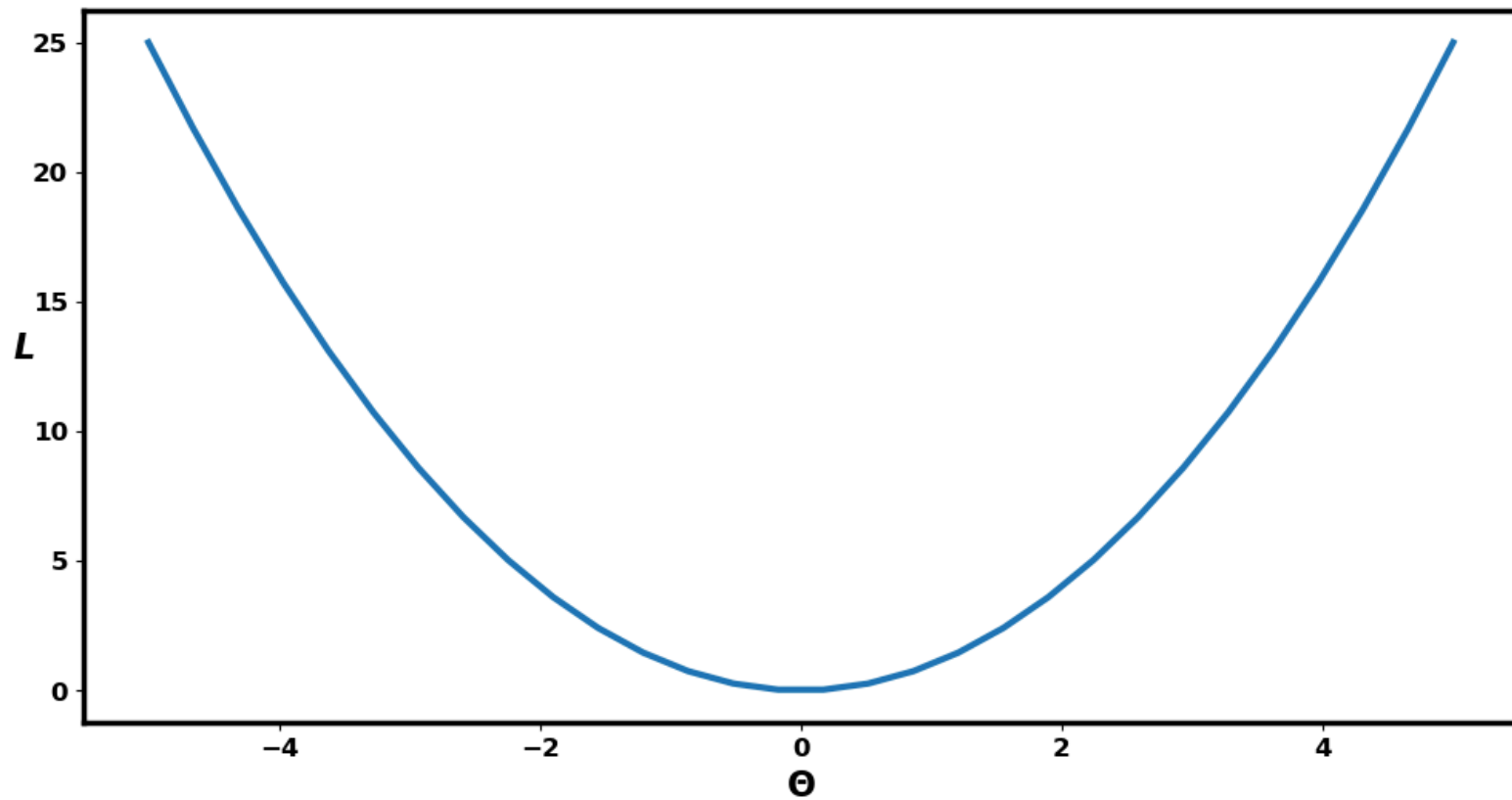
Let's plot a simple loss function as an illustration.

In this simple example: Θ is a vector of length 1.

```
In [9]: fig, ax = plt.subplots(1,1, figsize=(12,6))
        _ = ax.plot(x, f(x), linewidth=3)
        _ = ax.set_xlabel("$\Theta$", fontsize=16)
        _ = ax.set_ylabel("$L$", fontsize=16, rotation=0)
        plt.close(fig)
```

In [10]: fig

Out[10]:



Let's start off with a guess for Θ

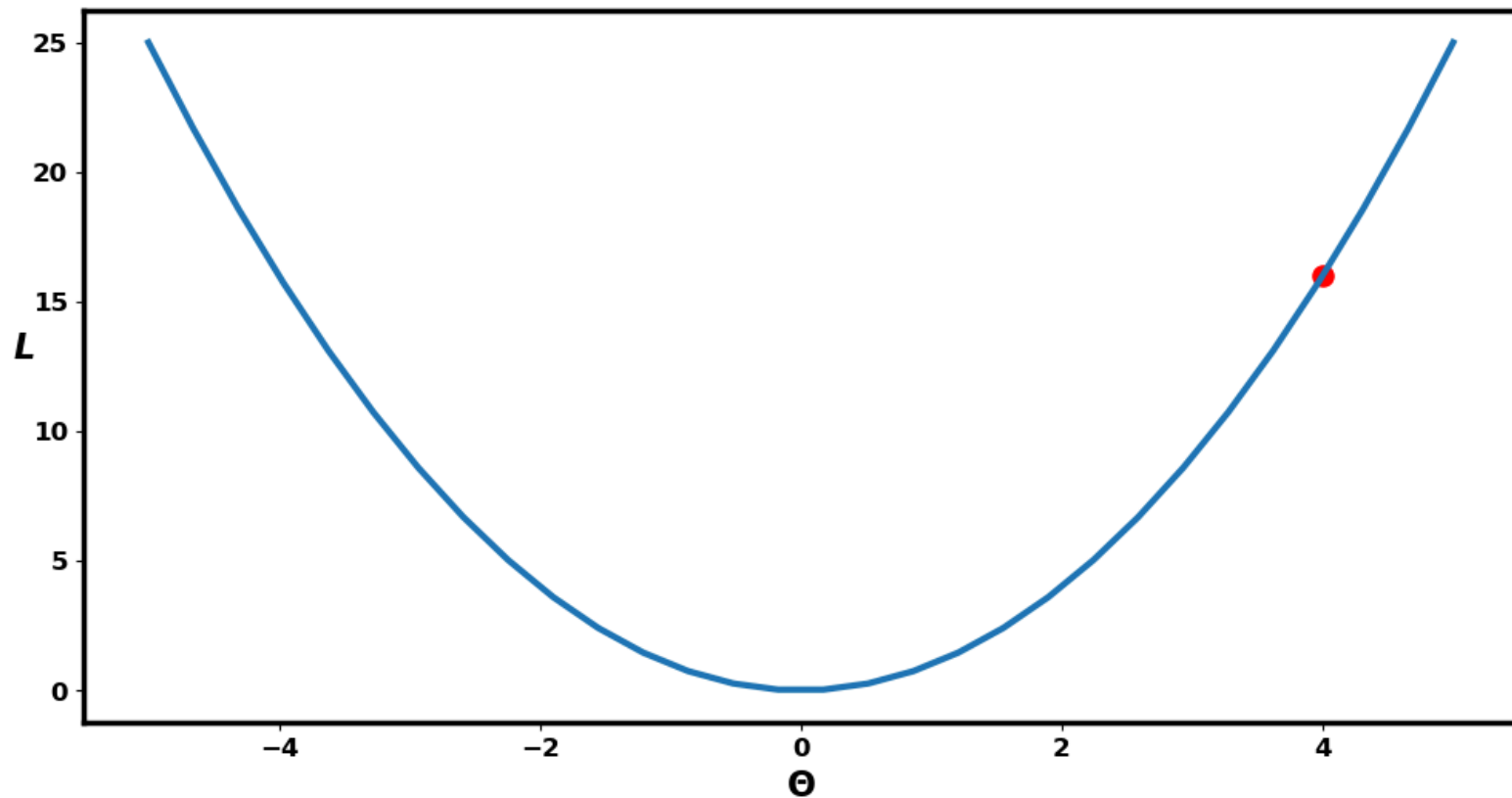
- we drop the superscript "*"

```
In [11]: x_0 = 4  
         x_s = x_0
```

```
In [12]: fig, ax = plot_step(f, x_s, x, show_tangent=False, visible=False)
```

In [13]: fig

Out[13]:



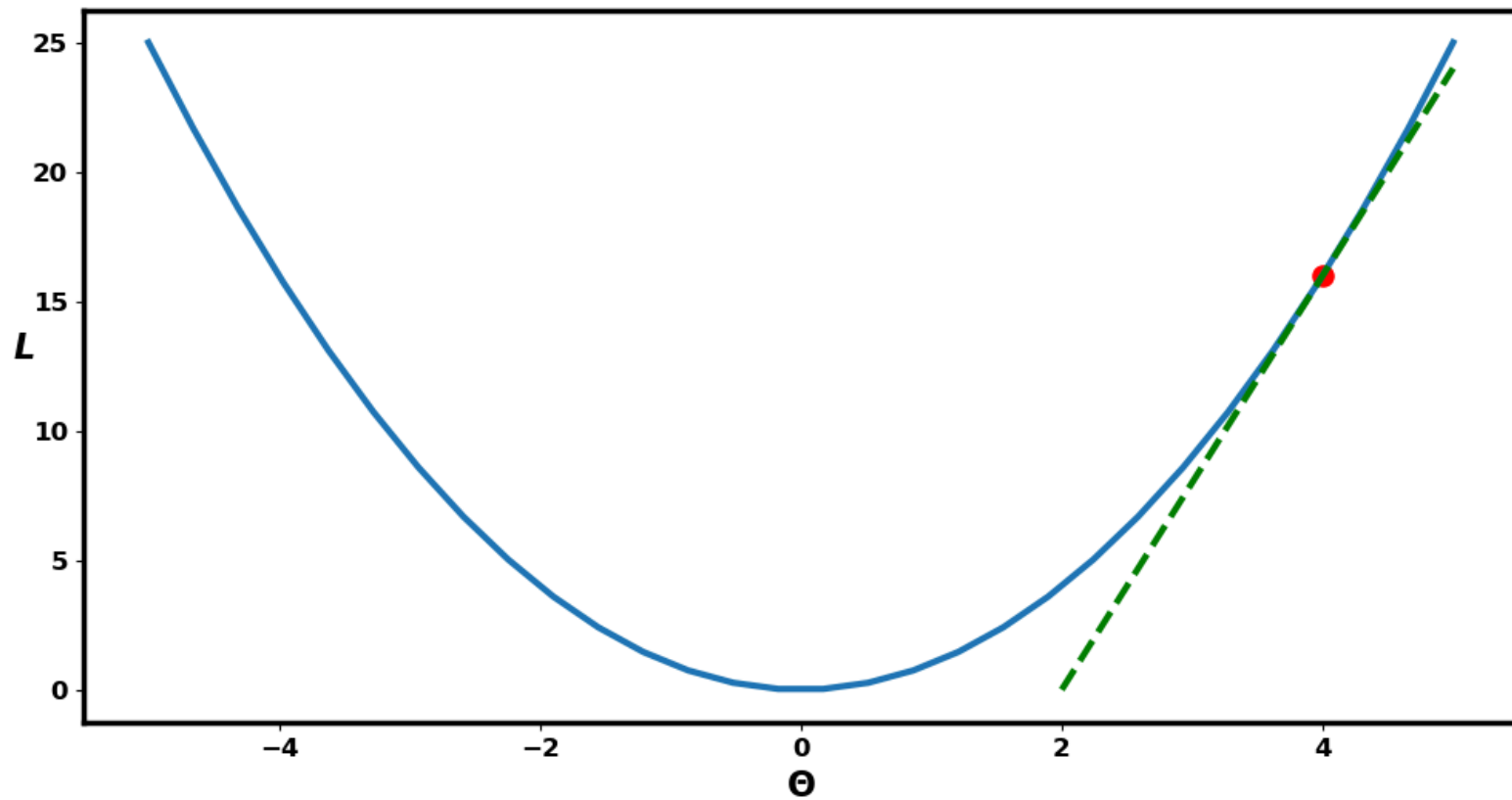
Clearly not at a minimum.

Compute the gradient of \mathcal{L}_Θ at initial guess x_s

```
In [14]: x_s = x_0  
fig, ax = plot_step(f, x_s, x, visible=False)
```

In [15]: fig

Out[15]:



Let's modify our guess by moving in proportion (α) to the negative of the gradient:

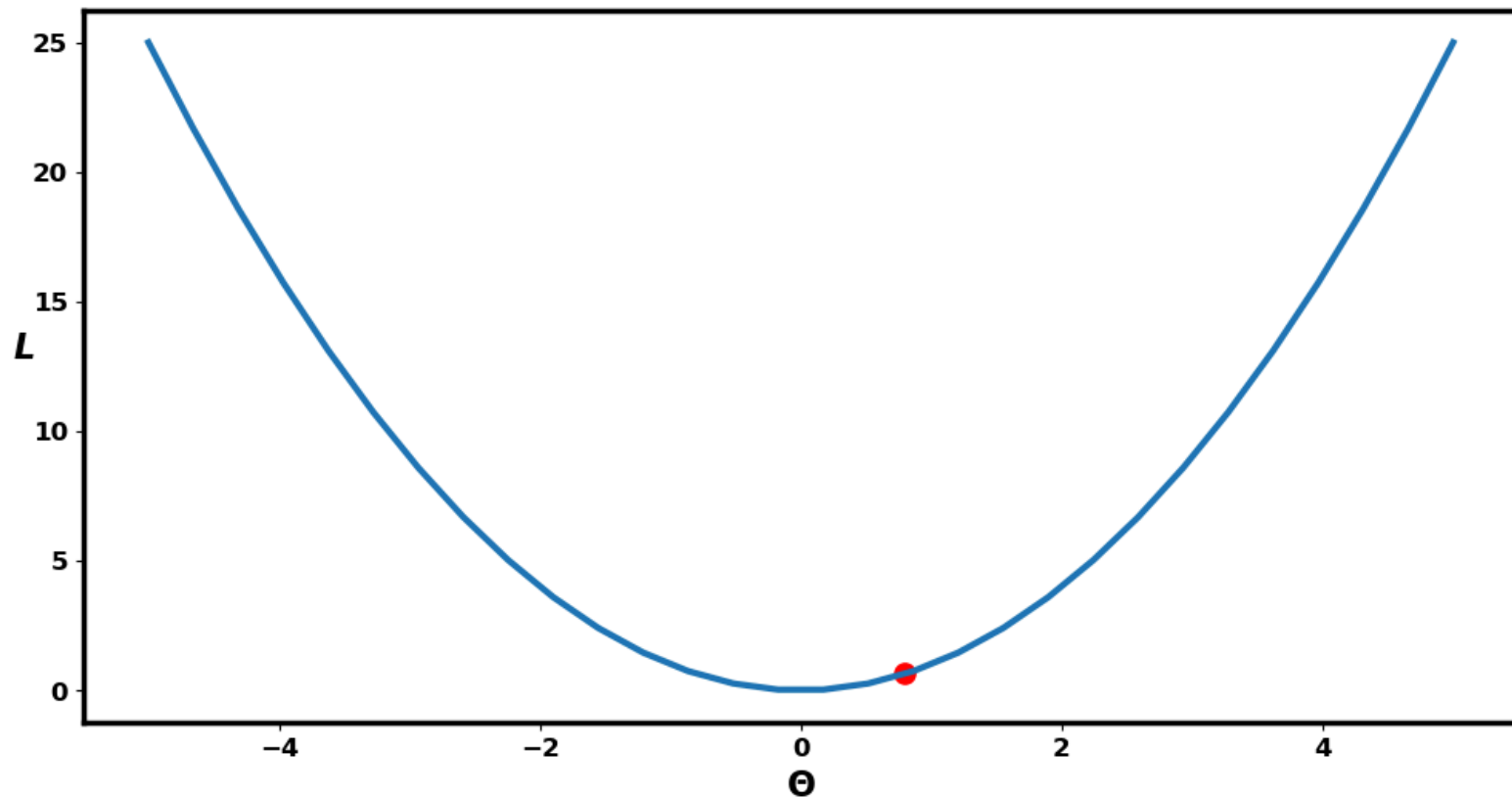
$$\Theta := \Theta - \alpha * \nabla_{\Theta} \mathcal{L}_{\Theta}$$

```
In [16]: # Update x_s  
slope = deriv(f, x_s)  
x_s = x_s + alpha * (- slope)
```

```
In [17]: fig, ax = plot_step(f, x_s, x, show_tangent=False, visible=False)
```

In [18]: fig

Out[18]:



By following the gradient as we did: we wind up at a new Θ where \mathcal{L}_{Θ} is reduced compared to that at the original guess.

Taking the gradient of the \mathcal{L} at the new point, we continue the iterative process.


```
In [19]: if CREATE_MOVIE:  
         _= gdh.create_gif2(x, f, x_0, out="images/gd.gif", alpha=alpha)
```

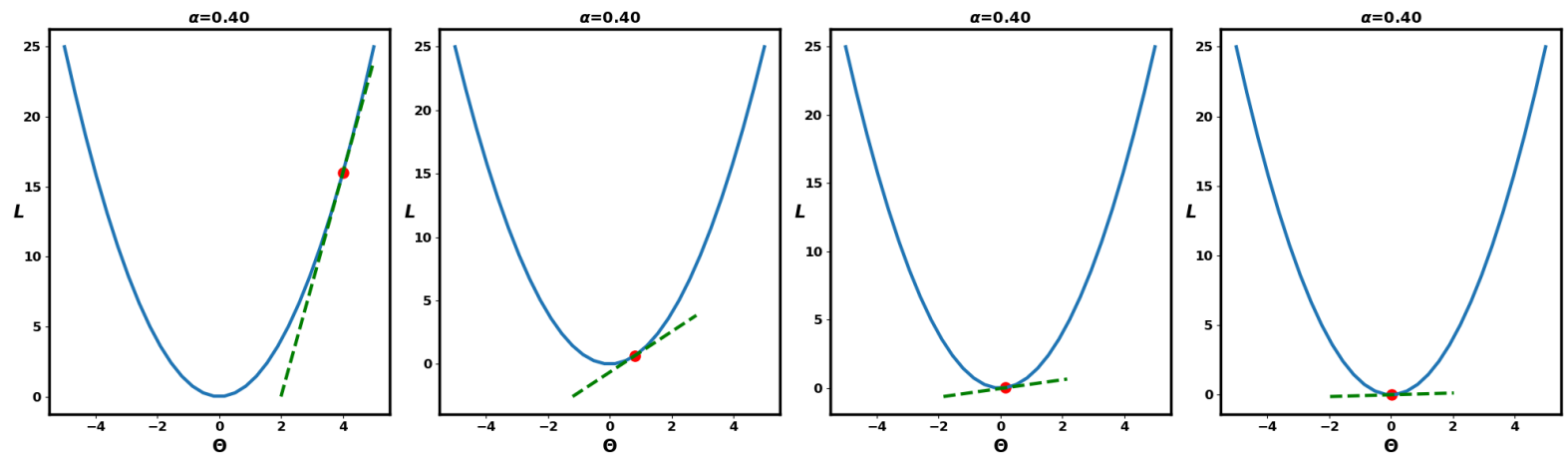
```
In [20]: _= gdh.display_gif("images/gd.gif")
```

```
In [21]: fig, axs = plot_gradient_descent(alphas= [ alpha ])
```

Below we visualize the progress of the iterative procedure as frames from the movie.

In [22]: fig

Out[22]:



Gradients: vector derivatives

We illustrated the use of Gradient Descent to find the minimum of a function of a single variable.

The same procedure works when the function is of higher dimension.

Let's illustrate with the MSE Loss often used in Linear Regression, when $\mathbf{x}^{(i)}$ (and hence Θ) is of dimension n .

$$\mathbf{y} = \Theta^T \cdot \mathbf{x}$$

With $(n + 1)$ features (including the constant)

- Θ is a vector of length $(n + 1)$
- $\frac{\partial}{\partial \Theta} \mathcal{L}_{\Theta} = \nabla_{\Theta} \mathcal{L}_{\Theta}$, is a vector of length $(n + 1)$

$$\nabla_{\Theta} \mathcal{L}_{\Theta} = \begin{pmatrix} \frac{\partial}{\partial \Theta_0} \mathcal{L}_{\Theta} \\ \frac{\partial}{\partial \Theta_1} \mathcal{L}_{\Theta} \\ \vdots \\ \frac{\partial}{\partial \Theta_n} \mathcal{L}_{\Theta} \end{pmatrix}$$

Using MSE Loss as the Loss function

$$\mathcal{L}_{\Theta} = \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}, \Theta) = \frac{1}{m} \sum_{i=1}^m (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)})^2$$

$$\nabla_{\Theta} \mathcal{L}_{\Theta} = \begin{pmatrix} \frac{\partial}{\partial \Theta_0} \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}, \Theta) \\ \frac{\partial}{\partial \Theta_1} \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}, \Theta) \\ \vdots \\ \frac{\partial}{\partial \Theta_n} \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}, \Theta) \end{pmatrix}$$

Whereas in our code

- We computed derivatives *numerically*
- We will compute them below *analytically*, using calculus

Analytic (closed form) derivatives are much faster to compute.

- During the Deep Learning part of the course, we will see how to *automatically* obtain analytic derivatives

$$\begin{aligned}
\frac{\partial}{\partial \Theta_j} \text{MSE}(\mathbf{y}, \hat{\mathbf{y}}, \Theta) &= \frac{1}{m} \sum_{i=1}^m \frac{\partial}{\partial \Theta_j} (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)})^2 && \text{definition} \\
&= \frac{1}{m} \sum_{i=1}^m 2 * (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)}) \frac{\partial}{\partial \Theta_j} (-\hat{\mathbf{y}}^{(i)}) && \text{chain rule} \\
&= -\frac{1}{m} \sum_{i=1}^m 2 * (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)}) \frac{\partial}{\partial \Theta_j} (\Theta * \mathbf{x}^{(i)}) && \hat{\mathbf{y}}^{(i)} = \Theta^T \cdot \mathbf{x}^{(i)} \\
&= -\frac{1}{m} \sum_{i=1}^m 2 * (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)}) \mathbf{x}_j^{(i)} \\
&= -\frac{2}{m} \sum_{i=1}^m (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)}) \mathbf{x}_j^{(i)}
\end{aligned}$$

Thus the gradient for Linear Regression can be written in matrix form as

$$\nabla_{\theta} \text{MSE}(X, \theta) = -\frac{2}{m} \mathbf{X}^T (\Theta^T \mathbf{X} - \mathbf{y}) \quad \text{since } \hat{\mathbf{y}} = \Theta^T \mathbf{x}$$

Thus we can update our estimate of vector Θ

$$\Theta := \Theta - \alpha * \nabla_{\Theta} \text{MSE}(X, \theta)$$

This will be particularly useful when working with NumPy as the gradient calculation is a vector operation that is implemented so as to be fast.

Gradient Descent versus MLE

For Linear Regression, there is a closed form solution for finding the optimal Θ .

We will demonstrate that the Gradient Descent search comes arbitrarily close.

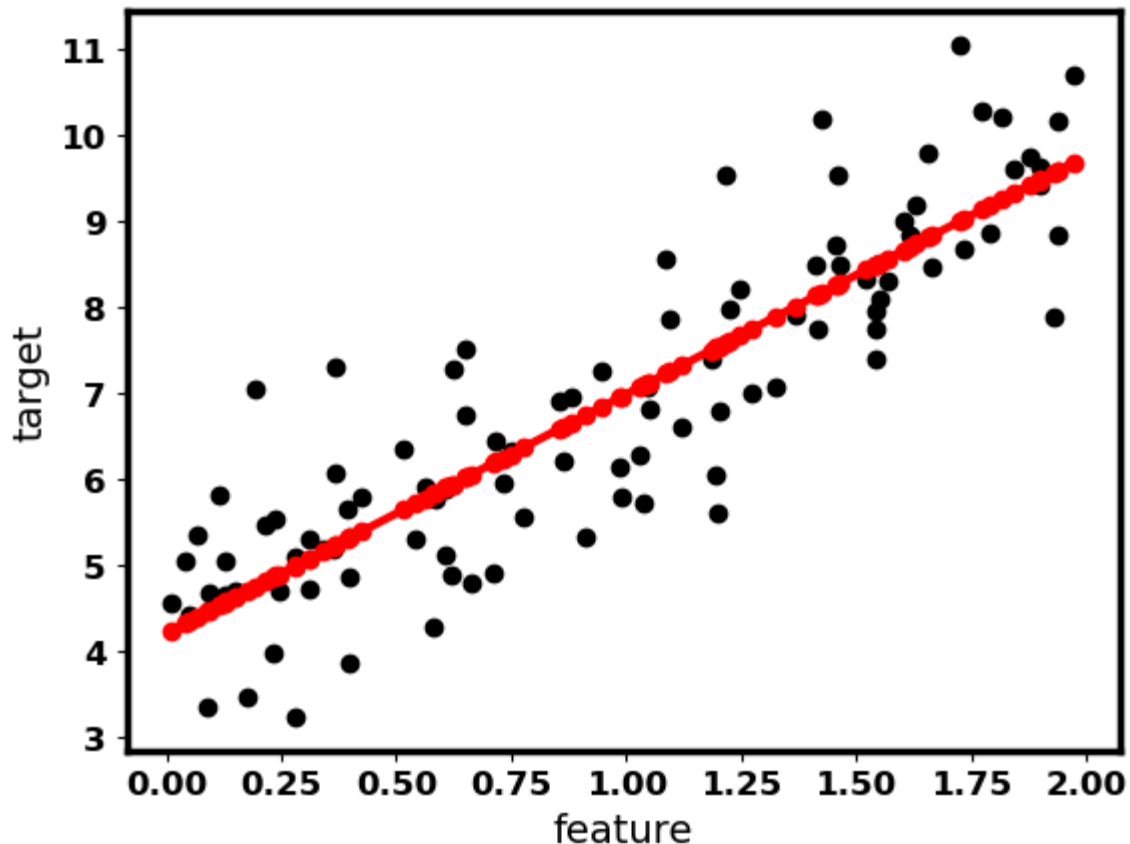
Let's illustrate Batch Gradient Descent on an example.

First, we use sklearn's `LinearRegression` as a baseline against which we will compare the Θ obtained from Gradient Descent.

```
In [23]: X_lr, y_lr = gdh.gen_lr_data()
clf_lr = gdh.fit_lr(X_lr,y_lr)
fig, ax = gdh.plot_lr(X_lr, y_lr, clf_lr)

theta_lr = (clf_lr.intercept_, clf_lr.coef_)

# Insert the intercept into the array of parameters
theta_lr = np.append( np.array([clf_lr.intercept_]), clf_lr.coef_)
```



Now let's perform Batch Gradient Descent and compare the Θ 's

```
In [24]: gd_theta = gdh.batchGradientDescent_lr(X_lr, y_lr)
         theta_lr - gd_theta
```

```
Out[24]: array([ 7.99360578e-15, -8.43769499e-15])
```


The Θ 's are equal up to 15 decimal points.

Aside

We can also find the optimal Θ by directly minimizing a user-defined Loss

- exactly the same as MSE in this case
- using a non-SGD optimizer (from `scipy`)

```
In [25]: theta_minimize_loss = gdh.minimize_loss_lr(X_lr, y_lr)
         theta_lr - theta_minimize_loss
```

```
Out[25]: array([-1.24766748e-08,  1.33493256e-08])
```

The Θ 's are equal up to 15 decimal points.

Let's look at the code for Batch Gradient Descent and examine the details

```
alpha = 0.1 n_iterations = 1000 m = 100 theta = np.random.randn(2,1)
for iteration in range(n_iterations):
    gradients = 2/m * X_b.T.dot(X_b.dot(theta) - y)
    theta = theta - alpha * gradients
```

- We use the closed form, analytic expression for the gradient
- We update

$$\Theta = \Theta - \alpha * \text{gradient}$$

Notice that the "step size" ($\alpha * \text{gradient}$)

- Is "big" when the gradient is large
- Is "small" when the gradient is small (close to optimal)

Since the Θ 's computed by Gradient Descent and Linear Regression are the same, it's no surprise that the predictions are too.

- As demonstrated in the following code

```
In [26]: X_new = np.array([[0], [2]])
gd_y_pred = gdh.predict(X_new, theta_lr)
clf_y_pred = clf_lr.predict(X_new)

gd_y_pred == clf_y_pred
```

```
Out[26]: array([[ True, False],
               [False,  True]])
```

Gradient Descent in depth

There are many subtleties to Gradient Descent.

As Gradient Descent will be a *key tool* in the Deep Learning part of the course, we briefly explore a few issues below.

How big should α be ?

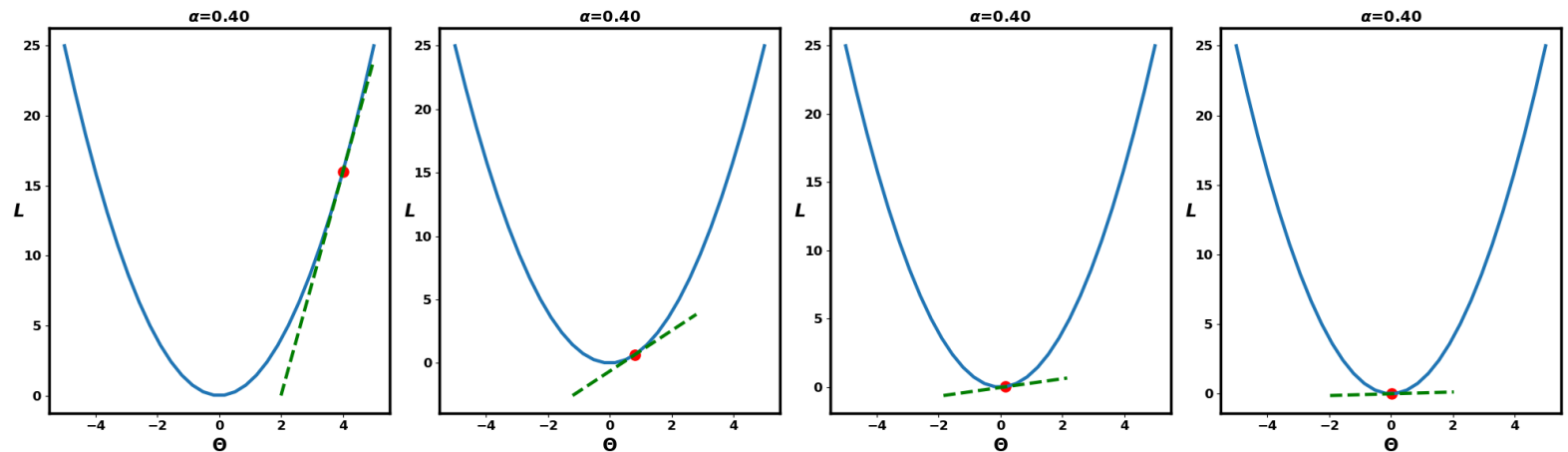
The "step size" we take along the direction of the gradient is α .

Does the choice of α matter ?

Here are 4 steps with $\alpha = 0.40$

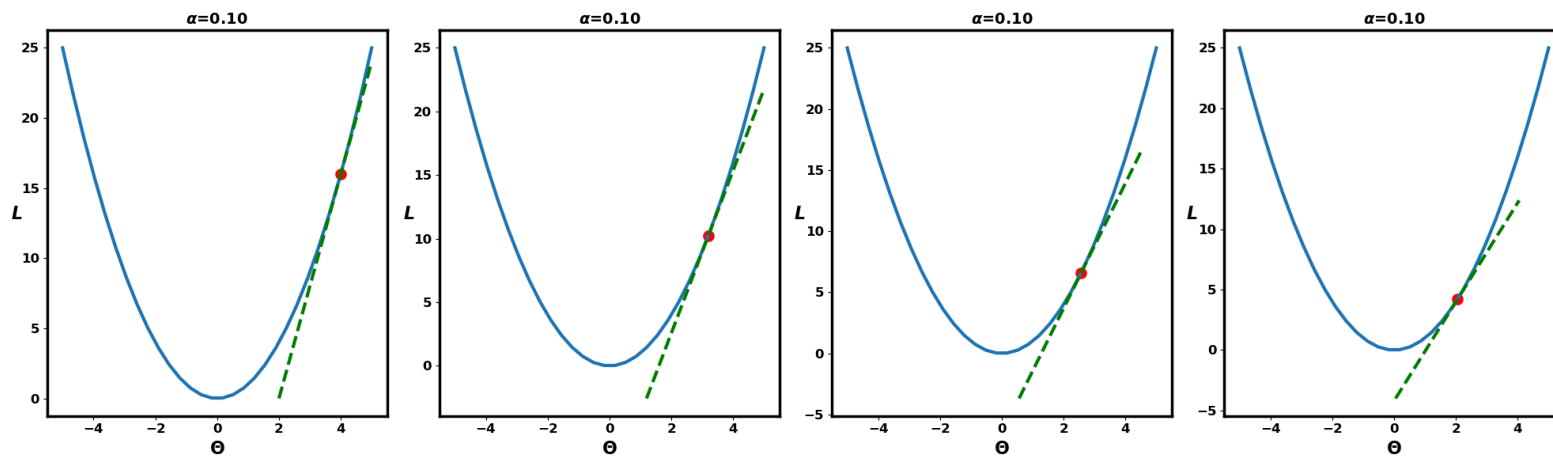
```
In [27]: fig, axs = plot_gradient_descent(alphas= [ alpha ])
fig
```

Out[27]:



```
In [28]: fig, axs = plot_gradient_descent(alphas= [ 0.1 ])
fig
```

Out[28]:

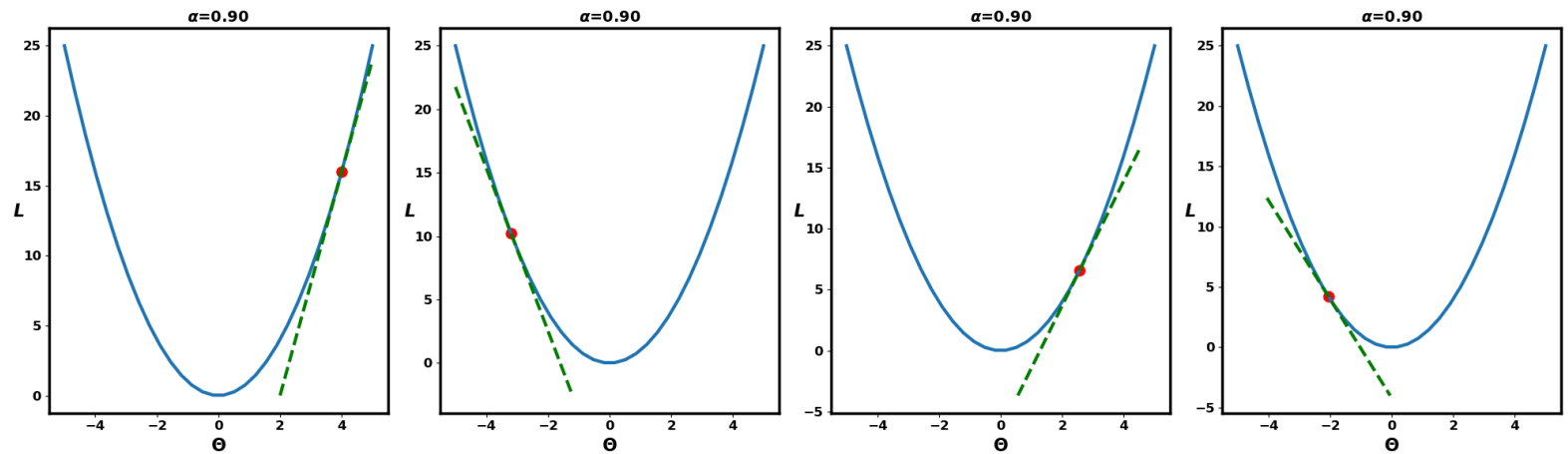


Convergence toward the optimal is much slower.

What if we used a larger $\alpha = 0.9$?

```
In [29]: fig, axs = plot_gradient_descent(alphas= [ 0.9 ])
fig
```

Out[29]:



You can see that we over-shoot the optimal repeatedly.

This may be problematic

- For more complex loss functions: we may "skip" over a local optimum

An adaptive learning rate schedule may be the solution:

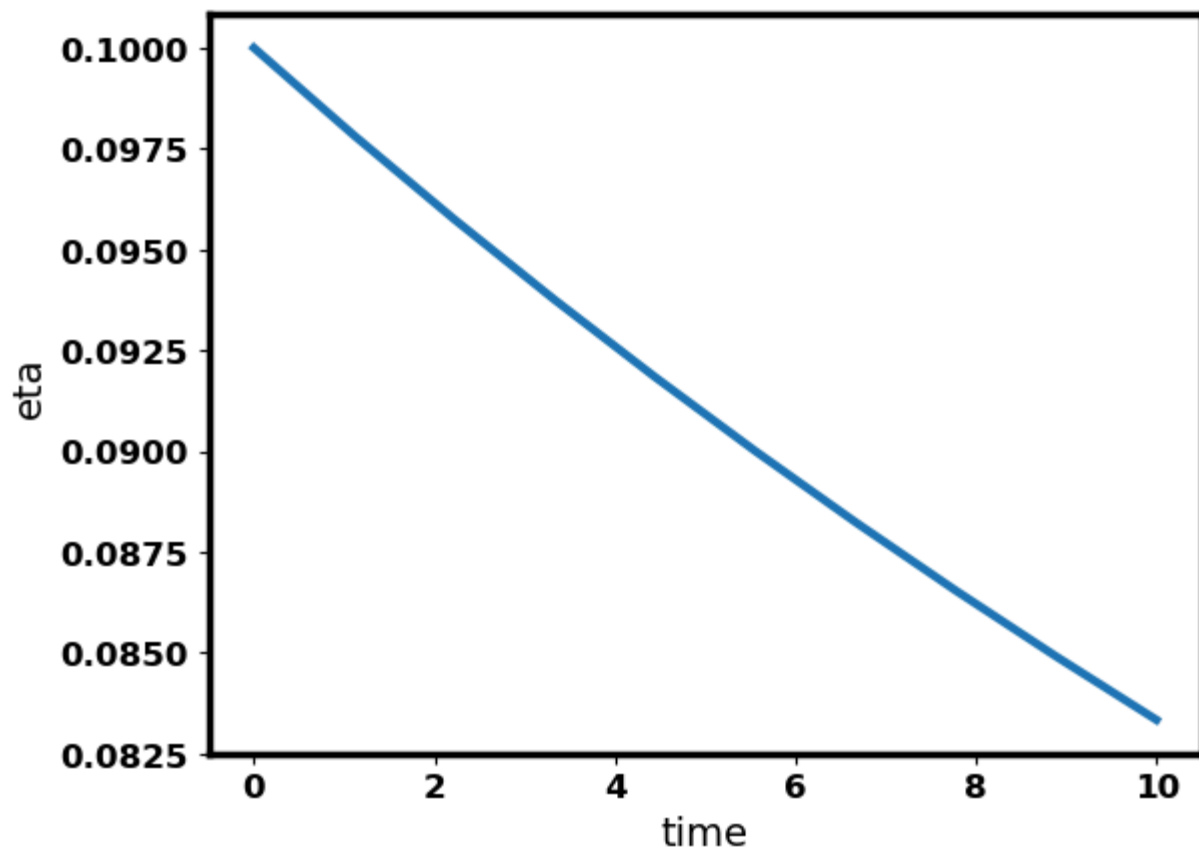
- Take big steps at first
- Take smaller steps toward end

```
In [30]: t0, t1 = 5, 50 # learning schedule hyperparameters
```

```
def learning_schedule(t):  
    return t0 / (t + t1)
```

```
t = np.linspace(0, 10, 10)
```

```
fig = plt.figure()  
ax = fig.add_subplot(1,1,1)  
_ = ax.plot(t, learning_schedule(t))  
_ = ax.set_xlabel("time")  
_ = ax.set_ylabel("eta")
```



We will revisit Learning Rate schedules in the Deep Learning part of the course.

Mini batch Gradient Descent

The Average Loss function in Classical Machine Learning has the form

$$\mathcal{L}_{\Theta} = \frac{1}{m} \sum_{i=1}^m \mathcal{L}_{\Theta}^{(i)}$$

That is, it is composed of m sub-expressions where m is the number of training examples.

- Each subexpression requires a computation and a derivative

Thus, for large sets of training examples, Gradient Descent can be expensive.

It may be possible to *approximate* \mathcal{L}_Θ using fewer than m expressions.

- Choose a *random subset* (of size $m' \leq m$) of examples: $I = \{i_1, \dots, i_{m'}\}$
- Approximate \mathcal{L}_Θ on I

$$\mathcal{L}_\Theta \approx \frac{1}{|I|} \sum_{i \in I} \mathcal{L}_\Theta^{(i)}$$

This means it is possible to update Θ after evaluating only $m' \leq m$ expressions.

Whereas Gradient Descent computes an exact \mathcal{L}_{Θ} to perform a single update of Θ :

Mini batch Gradient Descent

- Takes $b = m/m'$ smaller steps, each updating Θ
- Each small step using an approximation of \mathcal{L}_{Θ} based on $m' \leq m$ examples

It does this by

- Choosing batch size m'
- Partitioning the set of example indices $\{i | 1 \leq i \leq m\}$
 - into b batches of size m'
 - Batch $i' : b_{(i')}$ is one partition consisting of m' example indices
 - Each small step uses a single batch to approximate \mathcal{L}_{Θ} and update Θ

The collection of b small steps (comprising all examples) is called an *epoch*

So one epoch of Mini batch Gradient Descent performs b updates.

When batch size $m' = m$, we have our original algorithm known as *Batch Gradient Descent*.

How does one choose $m' \leq m$?

- Want m' large enough so approximations aren't too noisy
 - Don't want losses of the mini-batches of each epoch to be too different
- Often determined by *external* considerations
 - GPU memory (preview of Deep Learning)

Initializing Θ

As we will see in the Deep Learning part of the course

- Initial Θ is *not a trivial* choice

Consider a Loss function like the Hinge Loss

- Our initial choice of Θ could leave us in a *flat* area of the Loss function
- No derivative, but maybe not optimal
- No way to escape !

When to stop

Deciding when to stop the iterative process is another choice to be made

- Stop when decrease in \mathcal{L}_Θ is "too small"

Improvements to Gradient Descent

[Simon Ruder survey \(https://arxiv.org/abs/1609.04747\)](https://arxiv.org/abs/1609.04747)

[Gradient Descent Cheatsheet \(https://towardsdatascience.com/10-gradient-descent-optimisation-algorithms-86989510b5e9\)](https://towardsdatascience.com/10-gradient-descent-optimisation-algorithms-86989510b5e9)

The update step

$$\Theta = \Theta - \alpha * \frac{\partial \mathcal{L}_{\Theta}}{\partial \Theta}$$

where α is the learning rate.

The improvements to Gradient Descent modify

- α , the learning rate
- $\frac{\partial \mathcal{L}_{\Theta}}{\partial \Theta}$ the gradient

In order to be able to flexibly change the definition of both the gradient and the learning rate at each time step t , we will re-write the update step at time t as

$$\Theta_{(t)} = \Theta_{(t-1)} - \alpha' * V_{(t)}$$

$V_{(t)}$ will be our modified gradient and α' our modified learning rate.

Momentum: modify the gradient

In vanilla Gradient Descent, the gradients at time $(t - 1)$ and time t are completely independent.

This has the potential for gradients to rapidly change direction (recall, they are a vector).

To smooth out jumps we could compute a modified gradient $V_{(t)}$ as:

$$V_{(t)} = \beta_V * V_{(t-1)} + (1 - \beta_V) * \frac{\partial \mathcal{L}_\Theta}{\partial \Theta}$$

(Initialize $V_0 = 0$)

That is, the modified gradient is a weighted combination of the previous gradient and the new gradient.

Typically $\beta_V \approx 0.9$ so the old gradient dominates.

$V_{(t)}$ is the exponentially weighted moving average of the gradient.

Hence, there is "momentum" in the gradients in that they can't jump suddenly.

RMSprop: Modify the learning rate

Let

$$S_{(t)} = \beta_S * S_{(t-1)} + (1 - \beta_S) * \left(\frac{\partial \mathcal{L}_\Theta}{\partial \Theta} \right)^2$$

That is, $S_{(t)}$ is the exponentially weighted *variance* of the gradient.

(Initialize $S_0 = 0$)

Rather than using a learning rate of α , the RMSprop algorithm uses

$$\alpha' = \frac{1}{\sqrt{S_{(t)} + \epsilon}} * \alpha$$

The intuition is that if the gradient with respect to Θ_j is noisy (i.e., large variance) we want to damp updates in that component.

This also has the advantage that

- A rarely updated element Θ_i , having a low variance,
- Will have a relatively larger update when it is encountered than a more frequently encountered feature.

Typically $\beta_S \approx 0.9$ so the old variance dominates.

Why the extra ϵ ? We've seen this before (e.g., $\log(x + \epsilon)$): it's to avoid mathematical issues of certain functions (inverse, log) when the argument is 0.

AdaM: Modify both the gradient and the learning rate

The AdaM (Adaptive Moment) algorithm modifies *both*

- The gradient
- The learning rate

via exponentially weighted moving averages of the gradient as well as its variance.

$$\begin{aligned}V_{(t)} &= \beta_V * V_{(t-1)} + (1 - \beta_V) \frac{\partial \mathcal{L}_\Theta}{\partial \Theta} \\S_{(t)} &= \beta_S * S_{(t-1)} + (1 - \beta_S) * \left(\frac{\partial \mathcal{L}}{\partial \Theta} \right)^2 \\ \alpha' &= \frac{1}{\sqrt{S_{(t)} + \epsilon}} * \alpha\end{aligned}$$

Bias correction

You will have observed that we initialized to 0 the moving averages for gradients ($V_0 = 0$) and the variance of the gradients ($S_0 = 0$).

So the values are "biased" towards 0 with the bias having greatest effect for small t (i.e., when the number of "actual" values is small).

We can correct for the bias by dividing by $(1 - \beta^t)$:

$$\begin{aligned}\hat{V} &= \frac{V_{(t)}}{1 - \beta_V^t} \\ \hat{S} &= \frac{S_{(t)}}{1 - \beta_S^t}\end{aligned}$$

```
In [31]: print("Done")
```

Done

