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

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

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

$$\Theta^*_{(0)}, \Theta^*_{(1)}, \ldots$$

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)](Ensembles.ipynb#Example:-Boosting-for-a-Regression-task)

Loss functions, review

- $\hat{\mathbf{y}}^{(i)} = h(\mathbf{x}^{(\mathbf{i})}; \Theta)$, the prediction for example $\mathbf{x}^{(\mathbf{i})}$ with target label $\mathbf{y}^{(\mathbf{i})}$
- Per-example loss
$$\mathcal{L}_{\Theta}^{(\mathbf{i})} = L(\ h(\mathbf{x}^{(\mathbf{i})}; \Theta), \mathbf{y}^{(\mathbf{i})}\ ) = L(\hat{\mathbf{y}}^{(\mathbf{i})}, \mathbf{y})$$
- The Loss for the entire training set is simply the average (across examples) of the Loss for the example
$$\mathcal{L}_{\Theta} = \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}_{\Theta}^{(\mathbf{i})}$$

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 $\Theta^*_{(0)}$ 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 $\mathcal{L}_\Theta$

We achieve this objective at step t in two steps

First,

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

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

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

Note

Θ is a vector

- of length n

as is the gradient

So the derivative should properly be replaced with the gradient ∇_Θ

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

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.

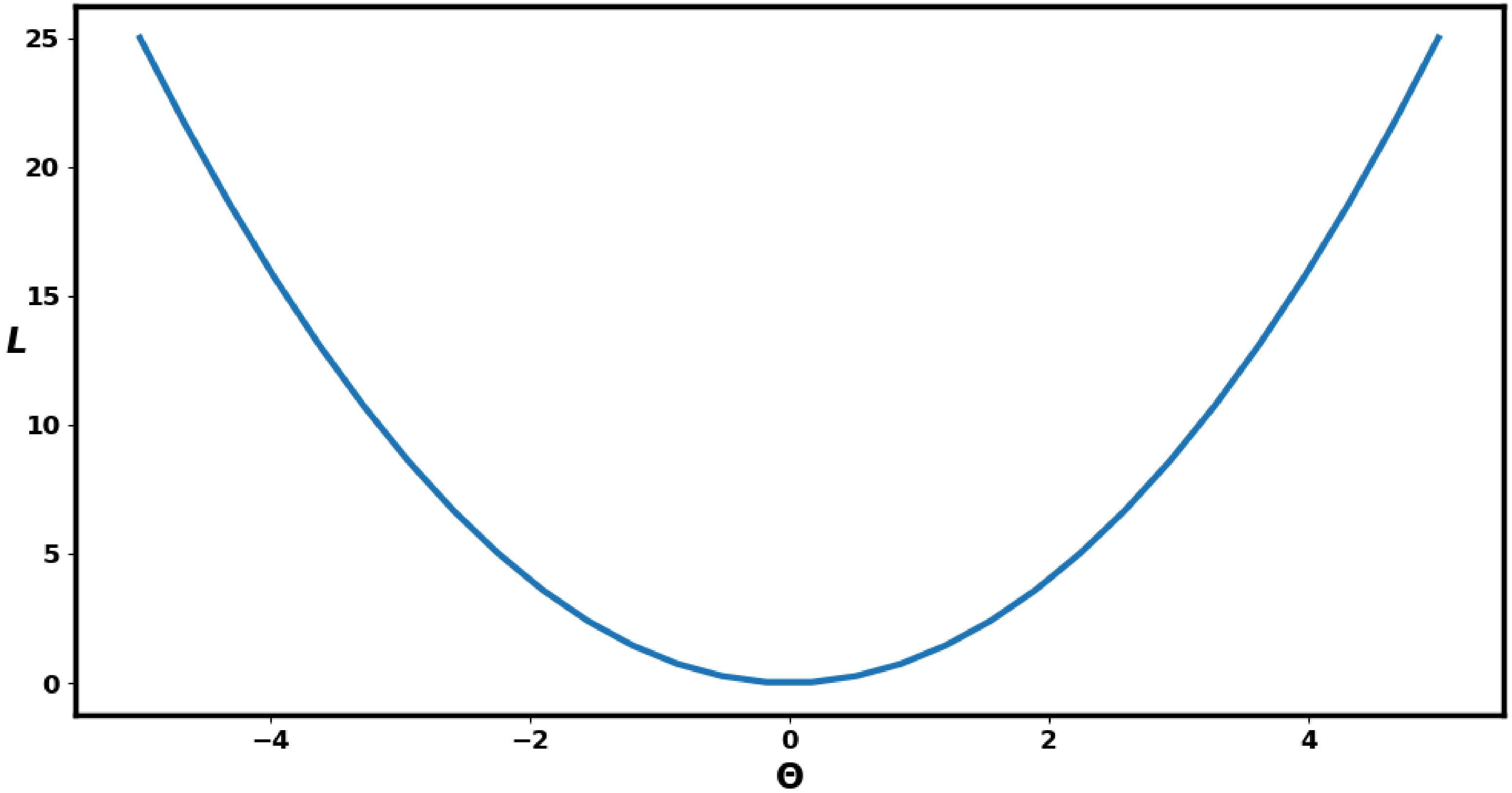
In this simple example: Θ is a vector of length 1.

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]:

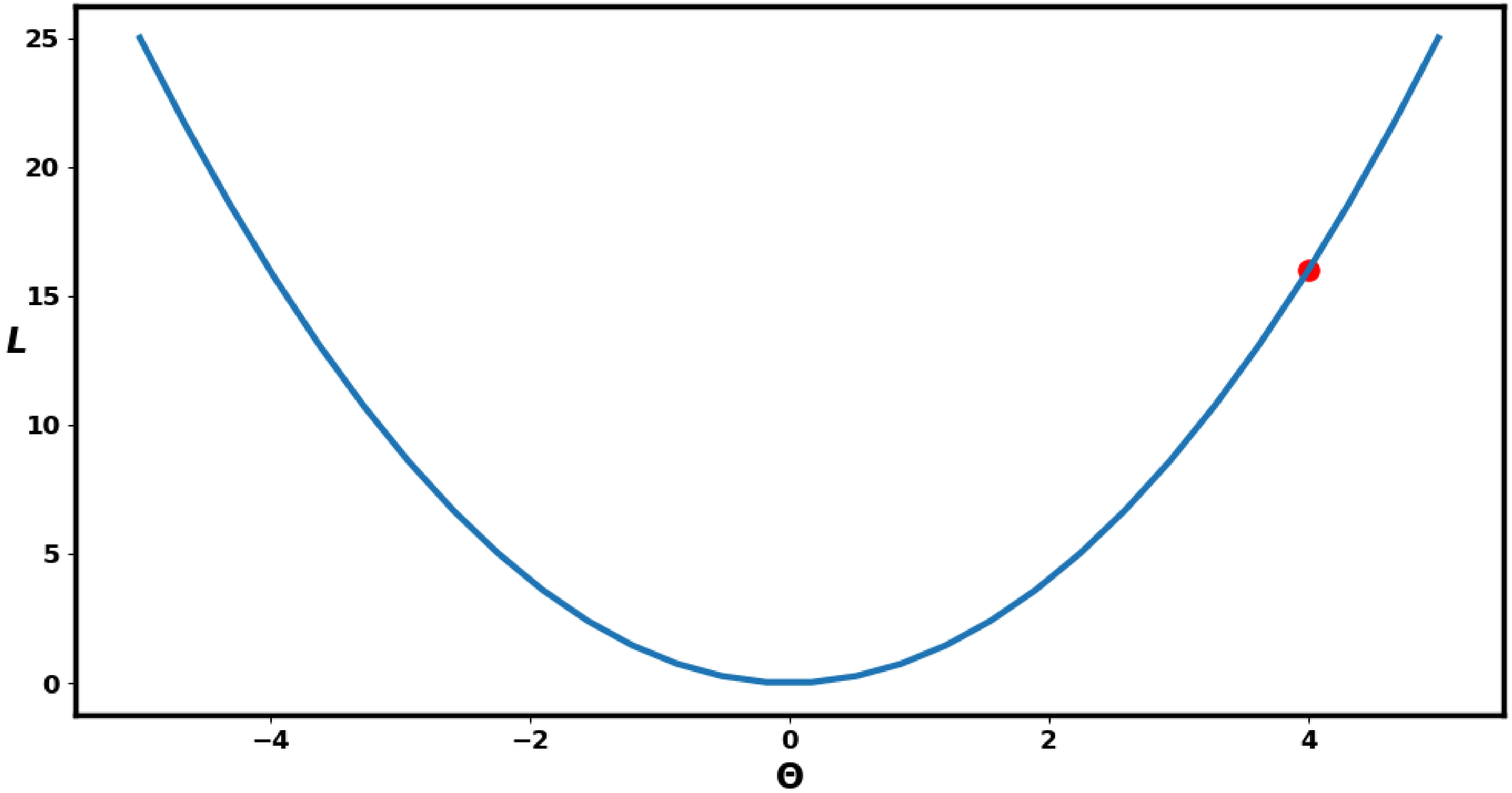
```
x_0 = 4
x_s = x_0
```

In [12]:

```
fig, ax = plot_step(f, x_s, x, show_tangent=False, visible=False)
```

In [13]:
```
fig
```

Out[13]:



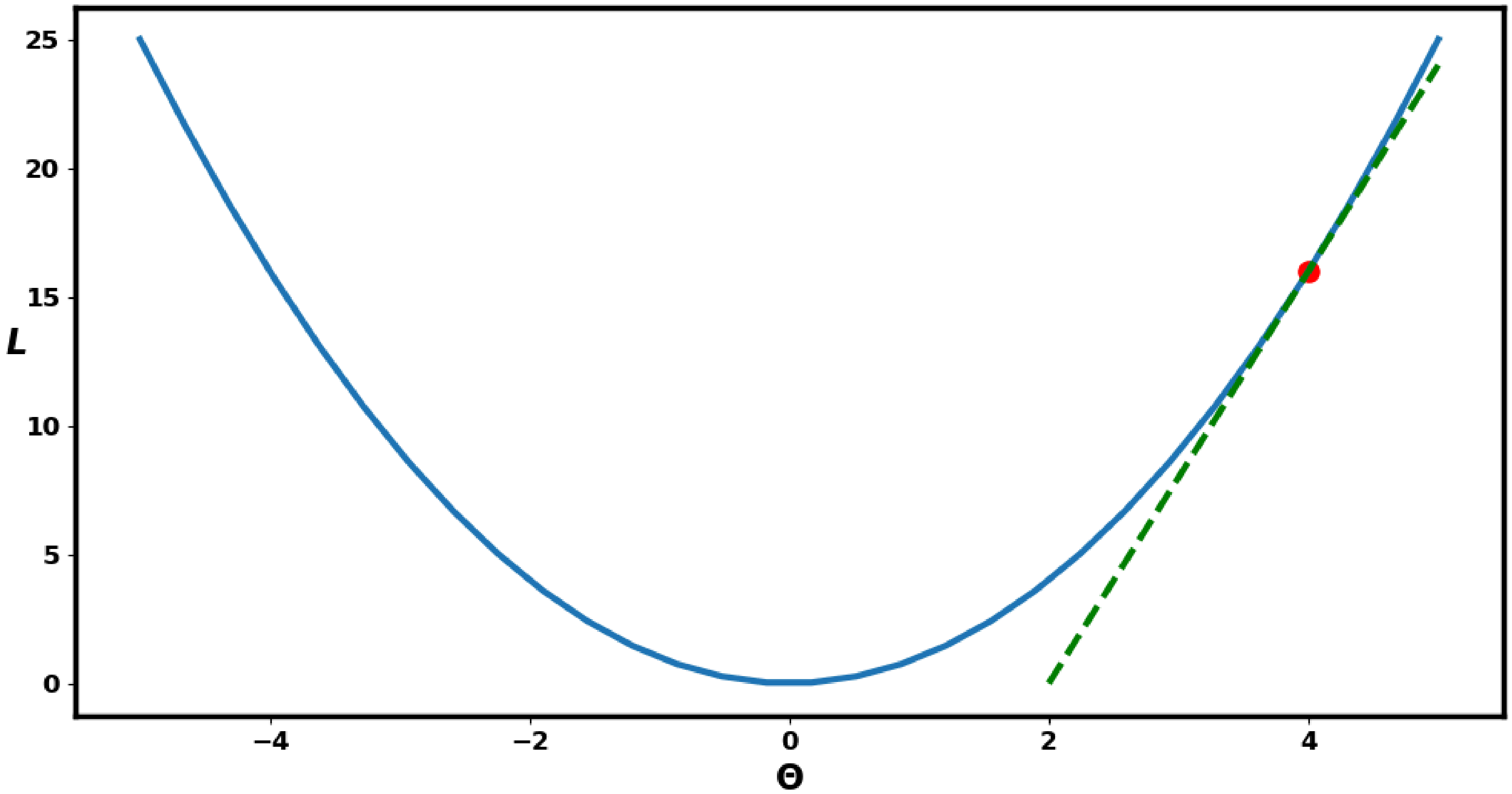
Clearly not at a minimum.

Compute the gradient of $\mathcal{L}_\Theta$ 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)
```

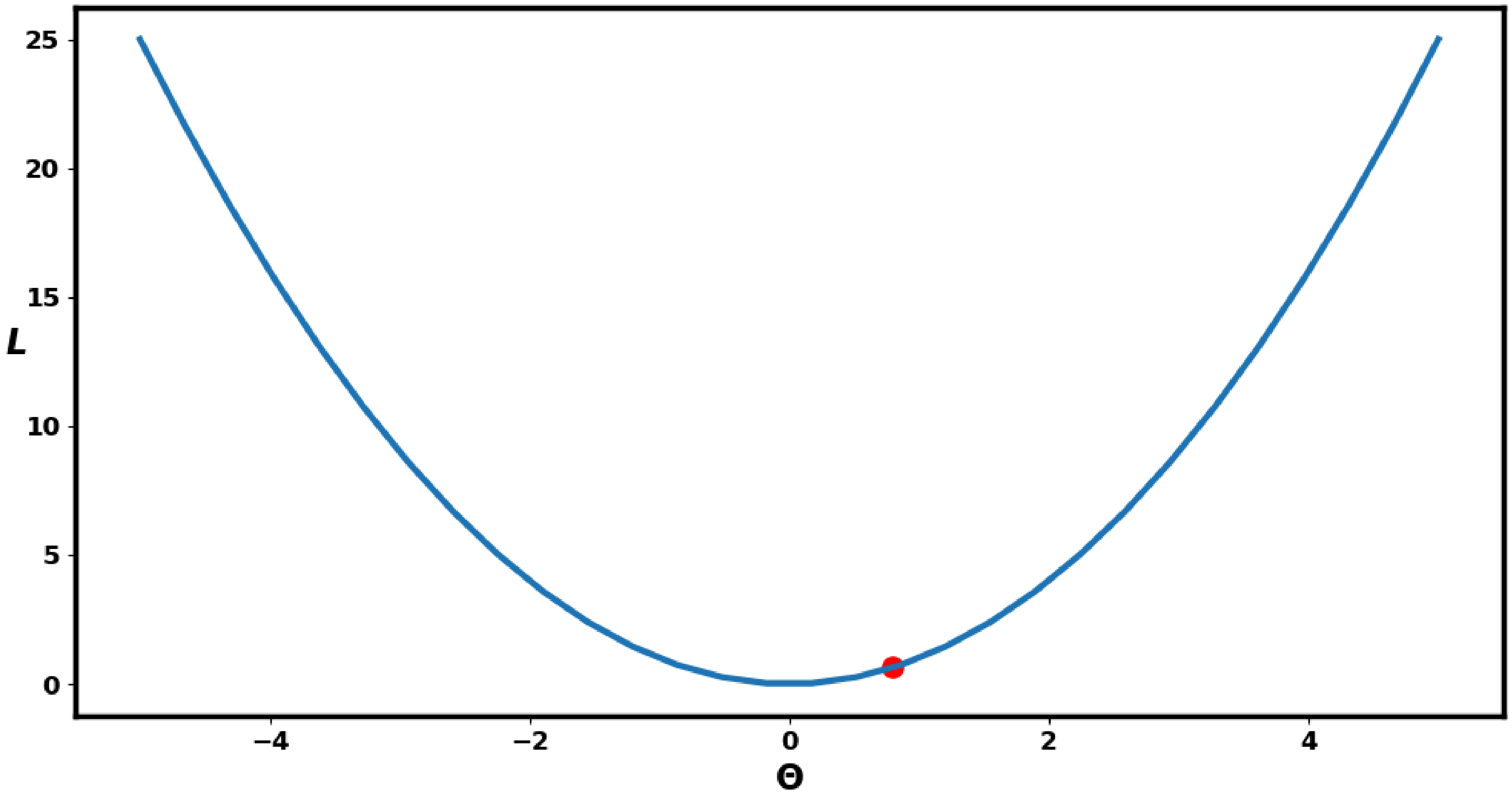
In [17]:

```
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 $\mathcal{L}_\Theta$ is reduced compared ot 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")
```

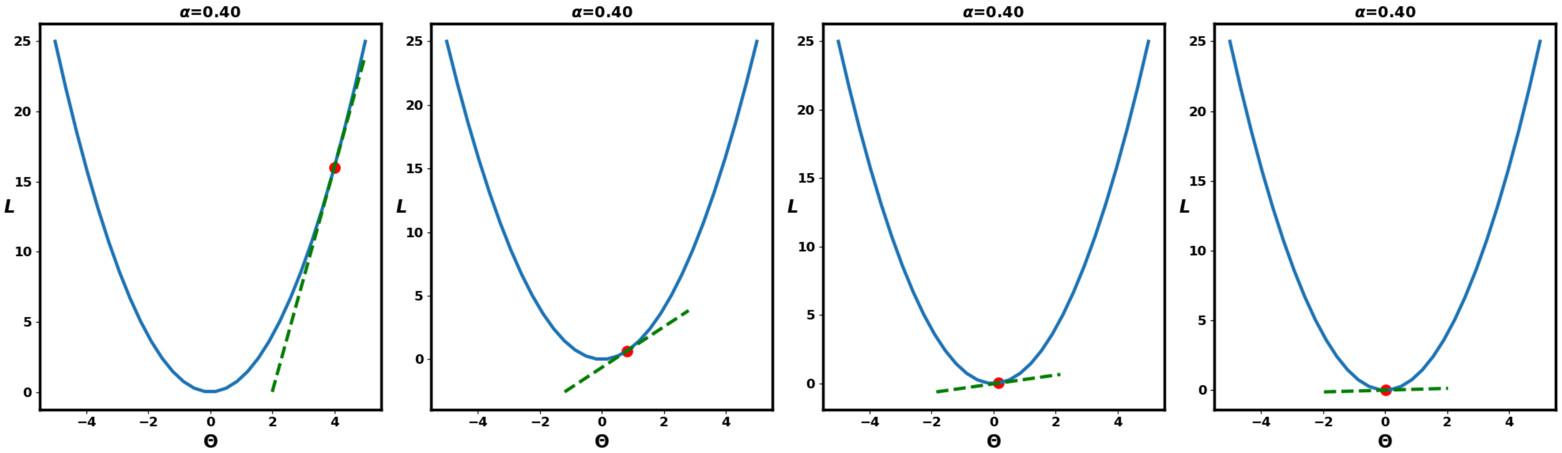
In [21]:

```
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 $\mathbf{x}^{(\mathbf{i})}$ (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

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

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

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

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

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

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

Thus we can update our estimate of vector Θ

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

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.

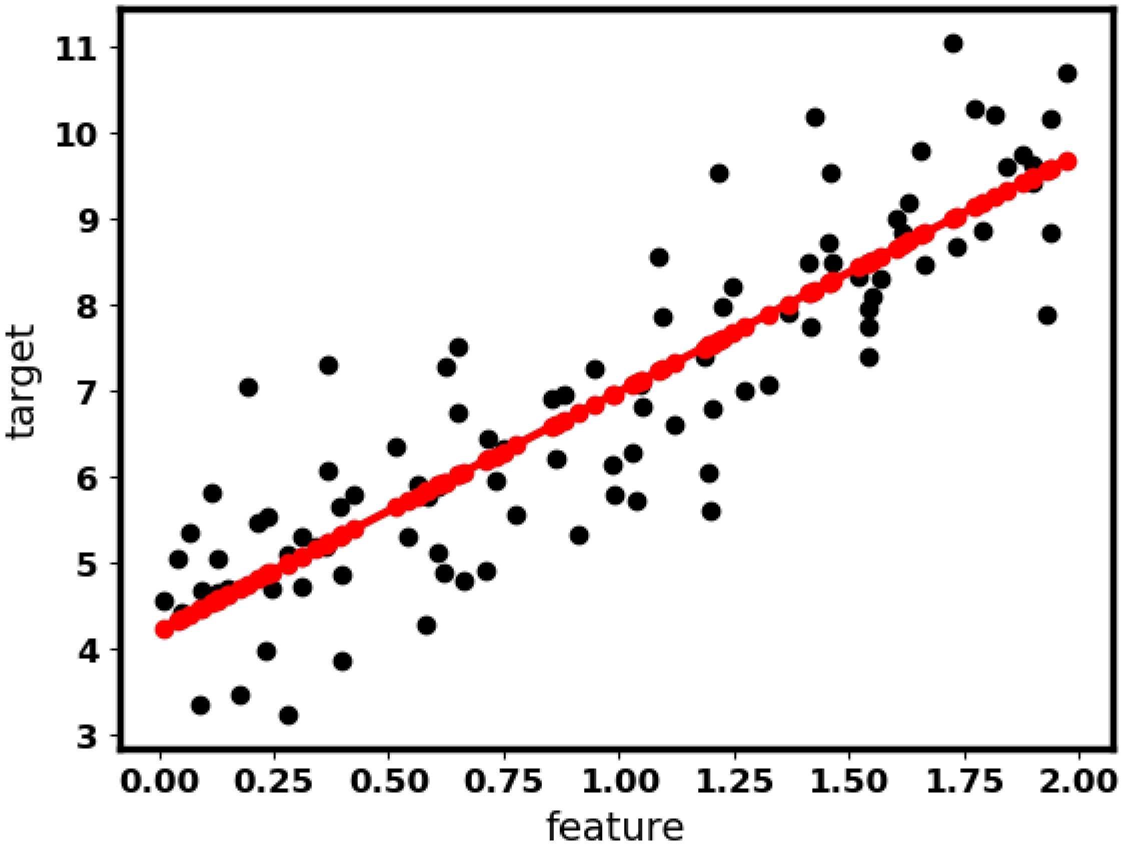
Let's illustrate Batch Gradient Descent on an example.

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" ($\alpha * \mathbf{gradient}$)

- 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 ?

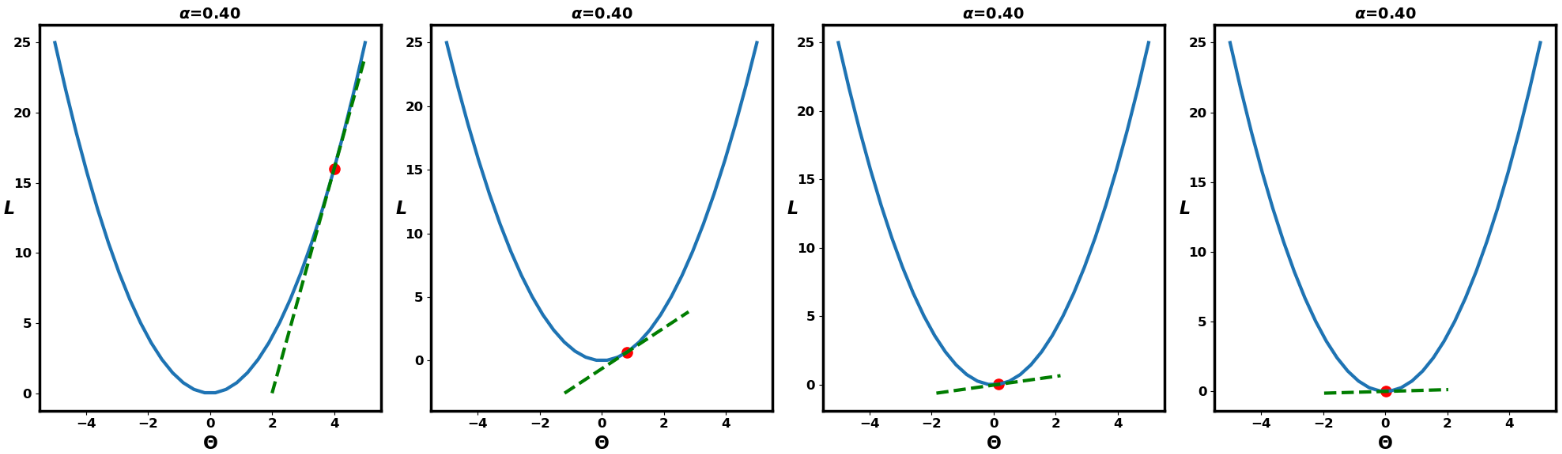
The "step size" we take along the direction of the gradient is α.

Does the choice of α matter ?

Here are 4 steps with $\alpha = 0.40$

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

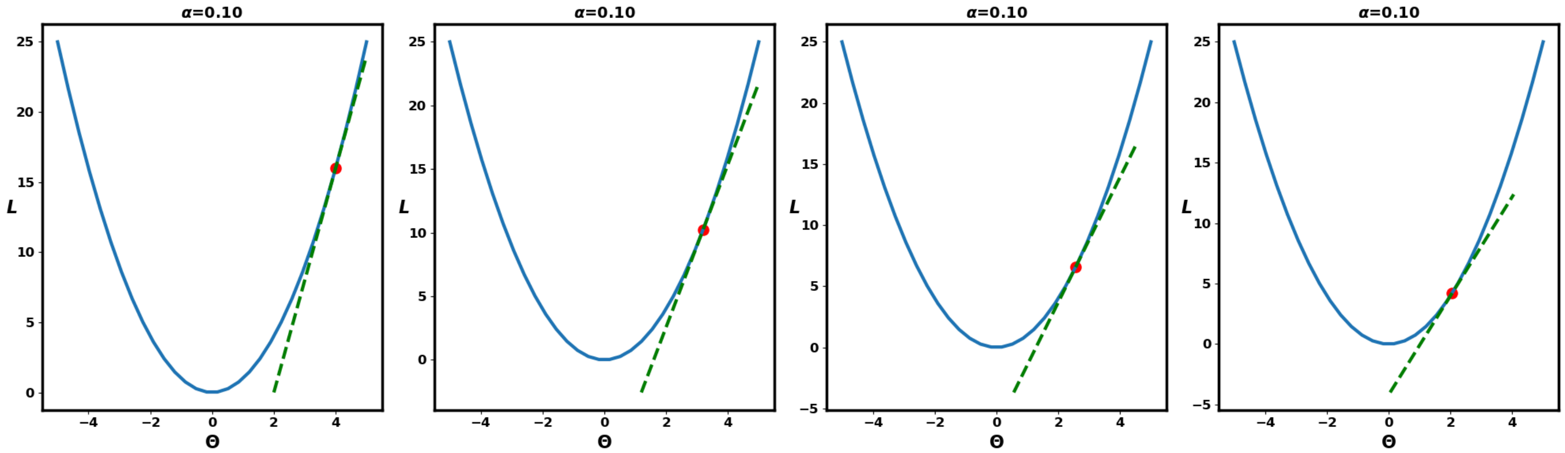
Out[27]:



In [28]:

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

Out[28]:

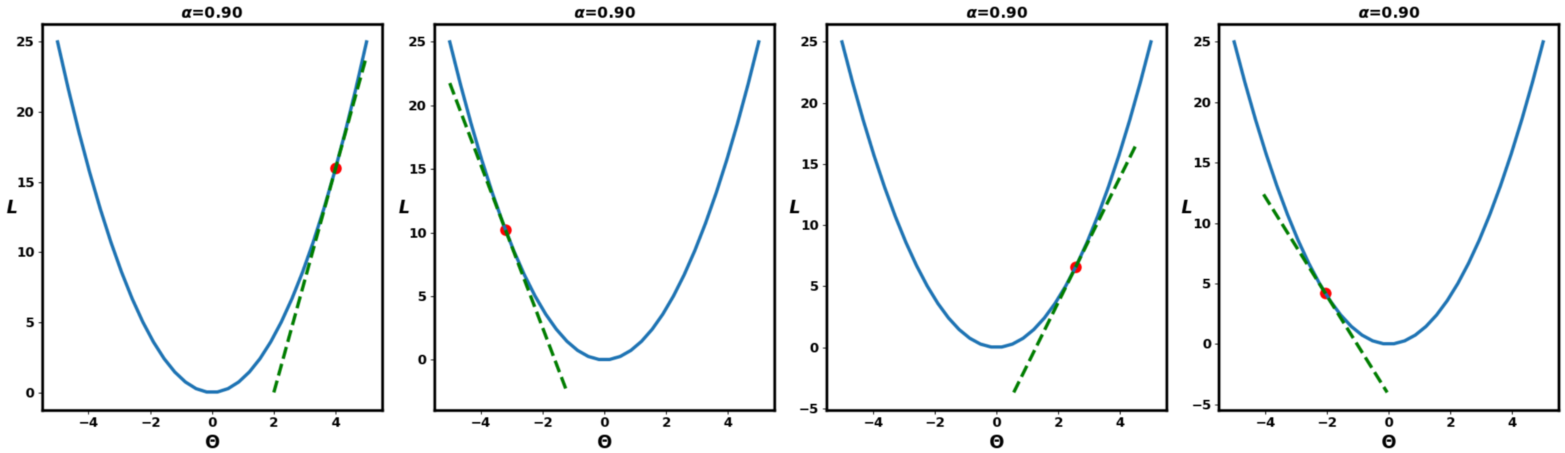


Convergence toward the optimal is much slower.

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:

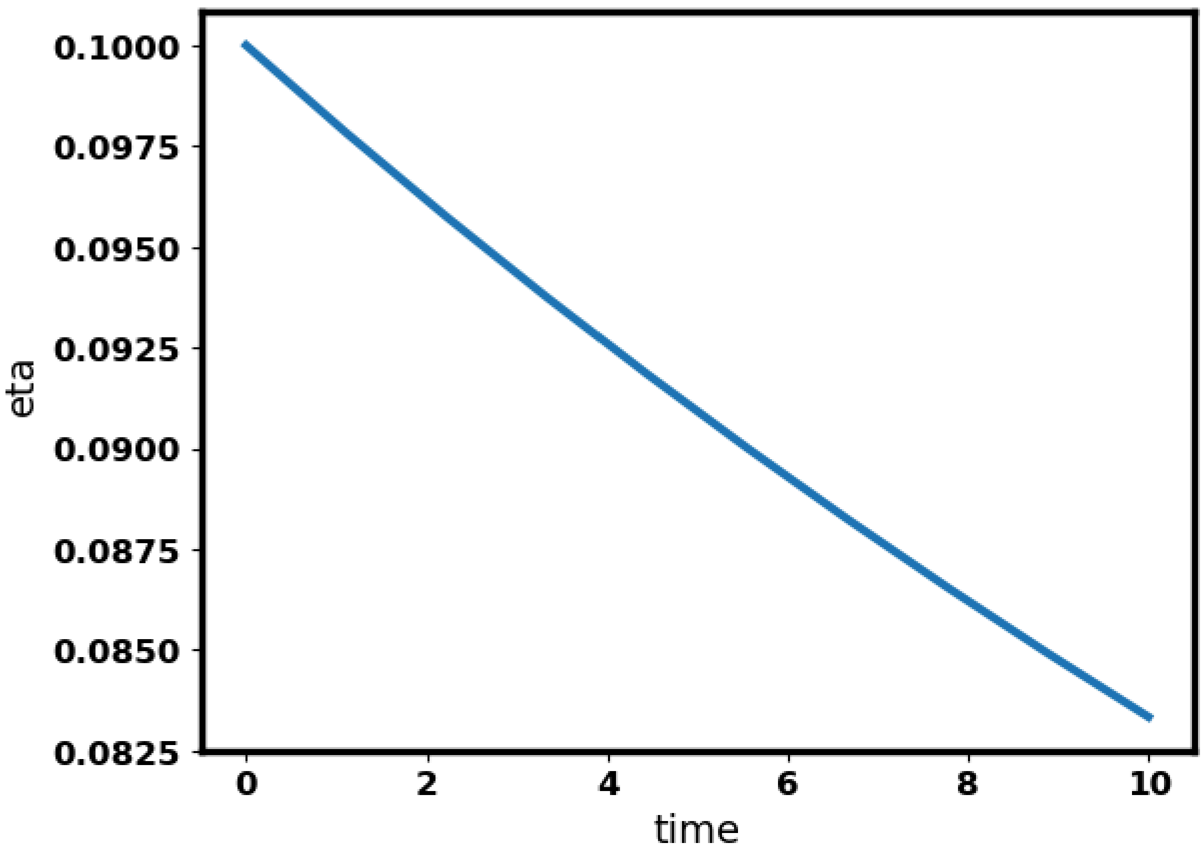
- Take big steps at first
- Take smaller steps toward end

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")
```


0.1000
0.0975
0.0950
0.0925
0.0900
0.0875
0.0850
0.0825
eta
0
2
4
6
8
10
time

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

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

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* $\mathcal{L}_\Theta$ using fewer than m expressions.

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

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

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

Whereas Gradient Descent computes an exact $\mathcal{L}_\Theta$ 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 $\mathcal{L}_\Theta$ based on $m' \leq m$ examples

It does this by

- Choosing batch size m'
- Partitioning the set of example indices $\{i | 1 \le i \le m\}$
    - 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 $\mathcal{L}_\Theta$ 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 $m' \le m$?

- 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 $\mathcal{L}_\Theta$ 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, e 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
```