Linear regression and gradient descent

CSI 4106 - Fall 2025

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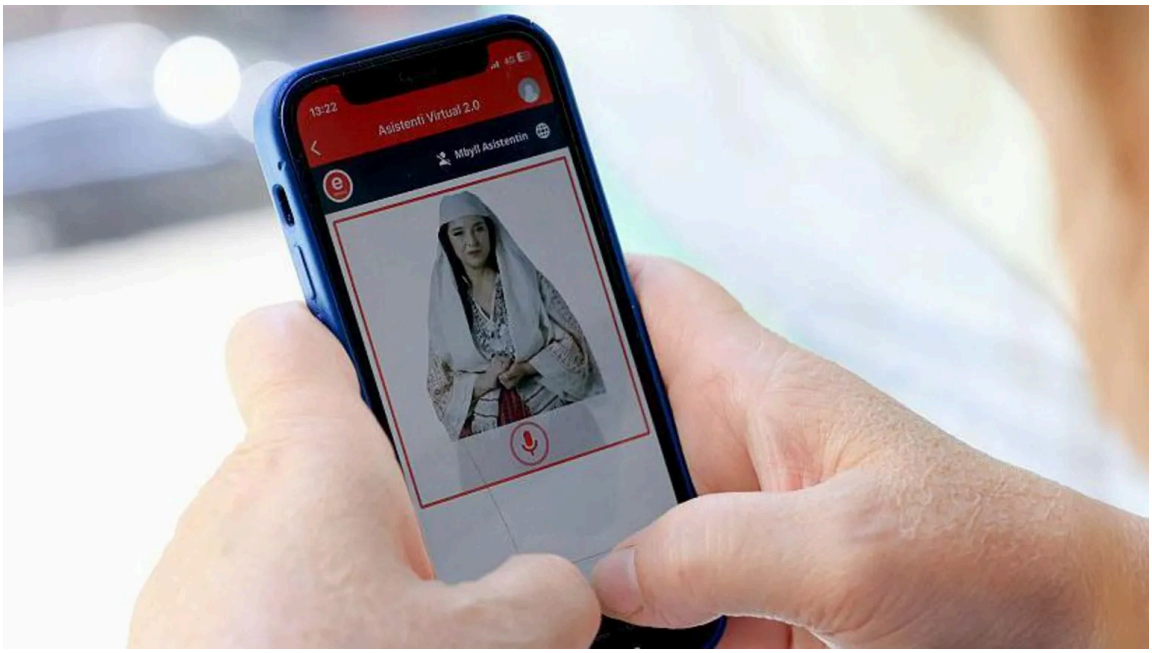
Version: Sep 16, 2025 17:58

Preamble

Message of the Day



World's first AI minister will eliminate corruption, says Albania's PM, by Guy Delauney, BBC, 2025-09-12.

Albania has appointed an **AI minister**, Diella, to the role of minister for public procurement. While the appointment is symbolic due to constitutional requirements, Diella aims to **eliminate corruption** in public tenders by leveraging AI for faster, more efficient, and accountable processes. The initiative has received mixed reactions, with some viewing it as a publicity stunt while others see potential for improving transparency and trust in public procurement.

Learning Objectives

- **Differentiate** regression tasks from classification tasks.

- **Articulate** the training methodology for linear regression models.
- **Interpret** the function of optimization algorithms in addressing linear regression.
- **Detail** the significance of partial derivatives within the *gradient descent algorithm*.
- **Contrast** the **batch**, **stochastic**, and **mini-batch** gradient descent methods.

In the previous lecture, we examined two distinct learning algorithms: k-nearest neighbors (KNN) and decision trees, each employing unique methods for model training and representation. KNN does not involve explicit learning; instead, the data itself constitutes the model. Conversely, decision trees utilize a greedy algorithm that begins with an empty tree and the full training dataset. The algorithm incrementally adds decision nodes, partitioning the parent dataset into subsets to achieve greater homogeneity (or purity) within each resulting classification compared to the parent node. This recursive process terminates when a node's data satisfies predefined stopping criteria, such as achieving a single class, reaching a minimum purity level, or attaining a maximum tree depth. Once the decision tree is constructed, the original data is no longer needed. This lecture aimed to demonstrate that supervised learning models can be represented in various ways, with each "learning" algorithm tailored to its specific model.

In today's lecture, we will explore a training algorithm that is applicable to a diverse range of models, including neural networks.

Linear Regression

Rationale

Linear regression is introduced to conveniently present a well-known training algorithm, **gradient descent**. Additionally, it serves as a foundation for introducing **logistic regression**–a classification algorithm—which further facilitates discussions on **artificial neural networks**.

- Linear Regression
  - Gradient Descent
  - Logistic Regression
    - Neural Networks

From 2 to **2 trillion** parameters!

The training algorithms for machine learning models can vary significantly depending on the model (e.g., decision trees, SVMs, etc.). In order to fit our schedule, we will concentrate on this specific sequence.

The concept of linear regression can be traced back to the early work of Sir Francis Galton in the late 19th century. Galton introduced the idea of "regression" in his 1886

paper, which focused on the relationship between the heights of parents and their children. He observed that children's heights tended to regress towards the average, which led to the term "regression."

However, the mathematical formulation of linear regression is closely associated with the work of Karl Pearson, who in the early 20th century extended Galton's ideas to create the method of least squares for fitting a linear model. The method itself, though, was developed earlier in 1805 by Adrien-Marie Legendre and independently by Carl Friedrich Gauss for astronomical data analysis.

See: Stanton (2001).

Supervised Learning - Regression

- The **training data** is a collection of **labelled** examples.
  - $\{(x_i, y_i)\}_{i=1}^{N}$
    - Each x_i is a **feature vector** with D dimensions.
    - $x_i^{(j)}$ is the value of the **feature** j of the example i, for $j \in 1 \dots D$ and $i \in 1 \dots N$.
  - The **label** y_i is a **real number**.
- **Problem**: Given the data set as input, create a **model** that can be used to predict the value of y for an unseen x.

Can you think of examples of regression tasks?

1. **House Price Prediction**:
   - **Application**: Estimating the market value of residential properties based on features such as location, size, number of bedrooms, age, and amenities.
2. **Stock Market Forecasting**:
   - **Application**: Predicting future prices of stocks or indices based on historical data, financial indicators, and economic variables.
3. **Weather Prediction**:
   - **Application**: Estimating future temperatures, rainfall, and other weather conditions using historical weather data and atmospheric variables.
4. **Sales Forecasting**:
   - **Application**: Predicting future sales volumes for products or services by analyzing past sales data, market trends, and seasonal patterns.
5. **Energy Consumption Prediction**:
   - **Application**: Forecasting future energy usage for households, industries, or cities based on historical consumption data, weather conditions, and economic factors.
6. **Medical Cost Estimation**:

- **Application**: Predicting healthcare costs for patients based on their medical history, demographic information, and treatment plans.

7. **Traffic Flow Prediction**:
   - **Application**: Estimating future traffic volumes and congestion levels on roads and highways using historical traffic data and real-time sensor inputs.
8. **Customer Lifetime Value (CLV) Estimation**:
   - **Application**: Predicting the total revenue a business can expect from a customer over the duration of their relationship, based on purchasing behavior and demographic data.
9. **Economic Indicators Forecasting**:
   - **Application**: Predicting key economic indicators such as GDP growth, unemployment rates, and inflation using historical economic data and market trends.
10. **Demand Forecasting**:
    - **Application**: Estimating future demand for products or services in various industries like retail, manufacturing, and logistics to optimize inventory and supply chain management.
11. **Real Estate Valuation**:
    - **Application**: Assessing the market value of commercial properties like office buildings, malls, and industrial spaces based on location, size, and market conditions.
12. **Insurance Risk Assessment**:
    - **Application**: Predicting the risk associated with insuring individuals or properties, which helps in determining premium rates, based on historical claims data, and demographic factors.
13. **Ad Click-Through Rate (CTR) Prediction**:
    - **Application**: Estimating the likelihood that a user will click on an online advertisement based on user behavior, ad characteristics, and contextual factors.
14. **Loan Default Prediction**:
    - **Application**: Predicting the probability of a borrower defaulting on a loan based on credit history, income, loan amount, and other financial indicators.

Focusing on applications possibly running on a mobile device.

1. **Battery Life Prediction**:
   - **Application**: Estimating remaining battery life based on usage patterns, running applications, and device settings.
2. **Health and Fitness Tracking**:
   - **Application**: Predicting calorie burn, heart rate, or sleep quality based on user activity, biometrics, and historical health data.
3. **Personal Finance Management**:

- **Application**: Forecasting future expenses or savings based on spending habits, income patterns, and budget goals.

4. **Weather Forecasting**:
   - **Application**: Providing personalized weather forecasts based on current location and historical weather data.
5. **Traffic and Commute Time Estimation**:
   - **Application**: Predicting travel times and suggesting optimal routes based on historical traffic data, real-time conditions, and user behavior.
6. **Image and Video Quality Enhancement**:
   - **Application**: Adjusting image or video quality settings (e.g., brightness, contrast) based on lighting conditions and user preferences.
7. **Fitness Goal Achievement**:
   - **Application**: Estimating the time needed to achieve fitness goals such as weight loss or muscle gain based on user activity and dietary input.
8. **Mobile Device Performance Optimization**:
   - **Application**: Predicting the optimal settings for device performance and battery life based on usage patterns and app activity.

Old Faithful Eruptions

In [1]:
```
import pandas as pd

WOLFRAM_CSV = "https://raw.githubusercontent.com/turcotte/csi4106-f25/refs/h
df = pd.read_csv(WOLFRAM_CSV)

# Renaming the columns
df = df.rename(columns={"Duration": "eruptions", "WaitingTime": "waiting"})
print(df.shape)
df.head(6)
```

```
(272, 2)
```

Attribution: Wolfram Research, “Sample Data: Old Faithful Eruptions” from the Wolfram Data Repository (2016) doi: 10.24097/wolfram.50727.data

The dataset used in this presentation was sourced from the Wolfram Research Data Repository, with its initial publication detailed in Azzalini and Bowman (1990).

Old Faithful Geyser

https://youtu.be/Qxf3xzirBrs

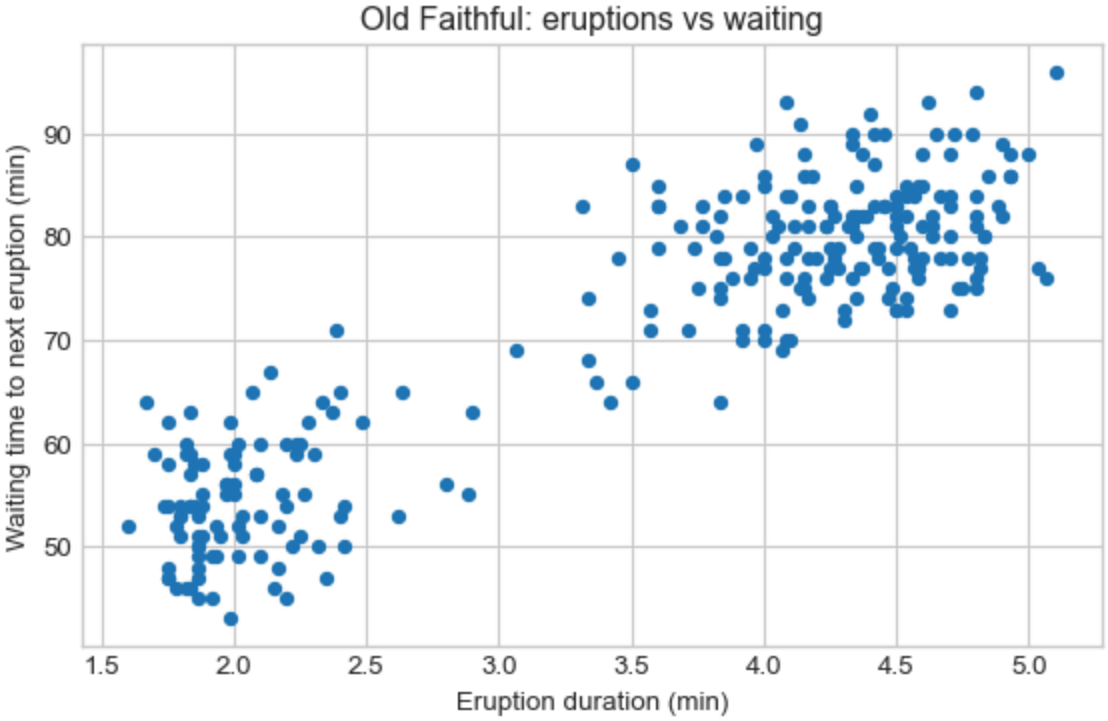
Attribution: Yellowstone National Park Trips

Old Faithful, situated in Yellowstone National Park, is renowned as the world’s most famous geyser. It can reach eruption heights of up to 140 feet. Notably, its eruption

intervals range between 60 and 110 minutes, contingent upon the duration of the preceding eruption.

Quick Visualization

In [2]:
```
import matplotlib.pyplot as plt

plt.figure(figsize=(6,4))
plt.scatter(df["eruptions"], df["waiting"], s=20)
plt.xlabel("Eruption duration (min)")
plt.ylabel("Waiting time to next eruption (min)")
plt.title("Old Faithful: eruptions vs waiting")
plt.tight_layout()
plt.show()
```



The duration of the current eruption appears to have a linear relationship with the subsequent wait time: shorter eruption durations tend to precede shorter wait times, while longer eruption durations are associated with longer wait times.

Problem

- Predict the **waiting time until the next eruption (min)**, y, based on the **duration of the current eruption (min)**, x.

Selecting a problem characterized by a single attribute allows us to better focus our discussion and enhance the clarity of visualization.

---

https://youtu.be/qxo8p8PtFeA?si=Buy1DF-T1qPsVE2S

Linear Regression

A **linear model** assumes that the value of the **label**, $\hat{y}_i$, can be expressed as a **linear combination** of the feature values, $x_i^{(j)}$:

$$\hat{y}_i = \theta_0 + \theta_1 x_i^{(1)} + \theta_2 x_i^{(2)} + \ldots + \theta_D x_i^{(D)}$$

. . .

Here, θ_j is the jth parameter of the (linear) **model**, with θ_0 being the **bias** term/parameter, and $\theta_1 \ldots \theta_D$ being the **feature weights**.

In my presentations, I use $\hat{y}_i$ and $h(x_i)$ synonymously.

In statistical contexts, the notation $\hat{y}_i$ is employed to denote the estimator of the true value y_i. This represents the predicted or estimated outcome based on a given model.

Conversely, in machine learning, the notation $h(x_i)$ is used, where h represents the hypothesis function or model applied to the input data x_i. The hypothesis function h is derived from a predefined hypothesis space, which encompasses the set of all possible models that can be used to map input data to predicted outcomes.

The parameter θ_0 is called the **bias term** (also "intercept") because:

- It **shifts the prediction independently of the inputs**.
- Geometrically, it moves the regression hyperplane up or down (or left/right in classification), so the model is not forced to pass through the origin.
- In machine learning terms, it acts like a **constant offset**, compensating for systematic effects not explained by the features.

So it's called "bias" because it introduces a fixed baseline to which the contributions of the other parameters are added.

In a machine learning model, the **parameters** are the **weights** and the **biases**.

Definition

Problem: find values for all the model parameters so that the model **"best fits"** the training data.

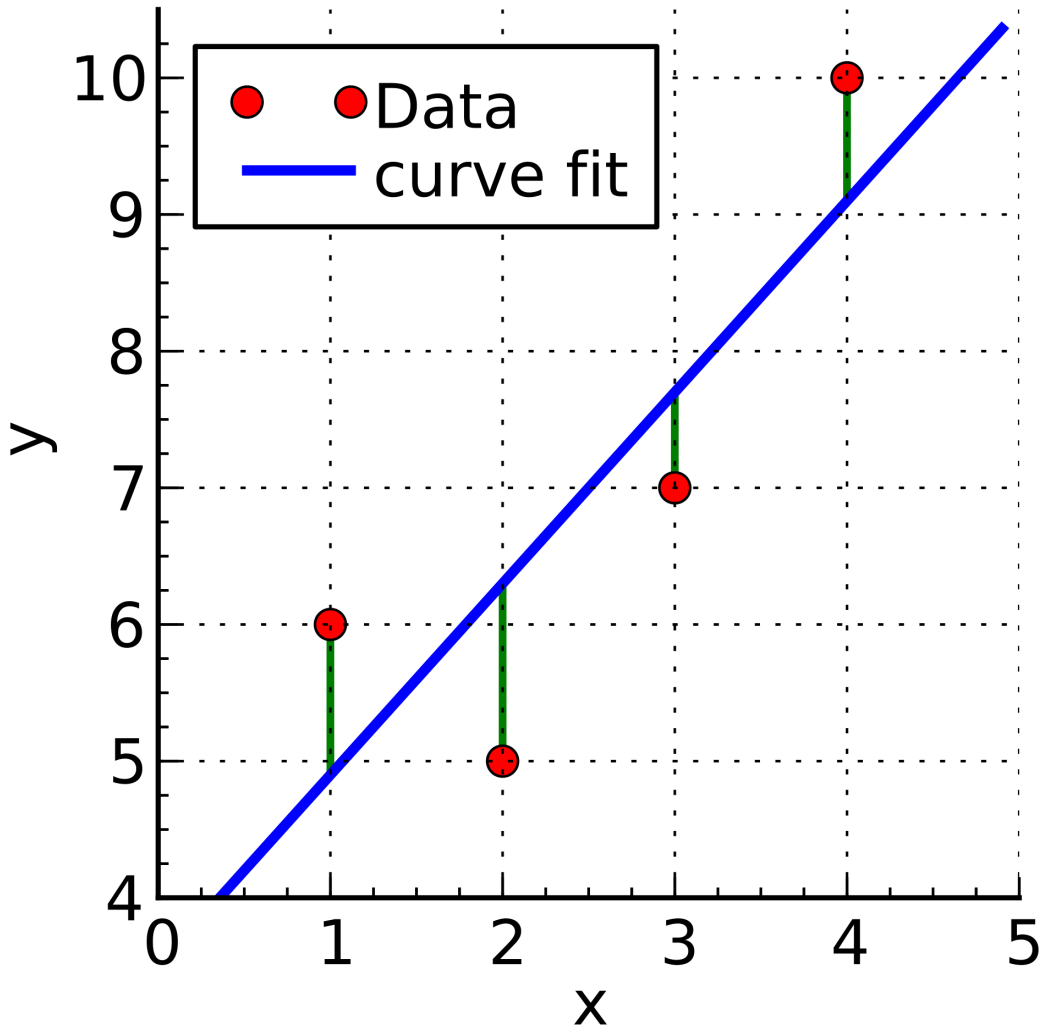
. . .

- The **Root Mean Square Error** is a common performance measure for regression problems.

$$\sqrt{\frac{1}{N}\sum_{1}^{N}[h(x_i) - y_i]^2}$$

In practical implementation, algorithms typically optimize the mean squared error (MSE) due to its mathematical tractability and the fact that it converges to the same parameter estimates as other error measures. While our current focus is on using MSE, the algorithm can be adapted to work with a range of objective functions.

Minimizing RMSE



Attribution: Krishnavedala, CC BY-SA 3.0, via Wikimedia Commons

Learning

In [3]:
```
from sklearn.linear_model import SGDRegressor
from sklearn.model_selection import train_test_split
```

```python
from sklearn.metrics import mean_squared_error, r2_score

# Prepare data
X = df[["eruptions"]].values  # shape (n_samples, 1)
y = df["waiting"].values      # shape (n_samples,)

X_train, X_test, y_train, y_test = train_test_split(
    X, y, test_size=0.2, random_state=42
)

# Fit via SGDRegressor — linear model via gradient descent
sgd = SGDRegressor(
    loss="squared_error",
    penalty=None,
    learning_rate="constant",
    eta0=0.01,
    max_iter=2000,
    tol=None,
    random_state=42
)

sgd.fit(X_train, y_train)

print("Learned parameters:")
print(f"  intercept = {sgd.intercept_[0]:.3f}")
print(f"  slope     = {sgd.coef_[0]:.3f}")

y_pred = sgd.predict(X_test)
print(f"Test MSE = {mean_squared_error(y_test, y_pred):.2f}")
print(f"Test R²  = {r2_score(y_test, y_pred):.3f}")
```

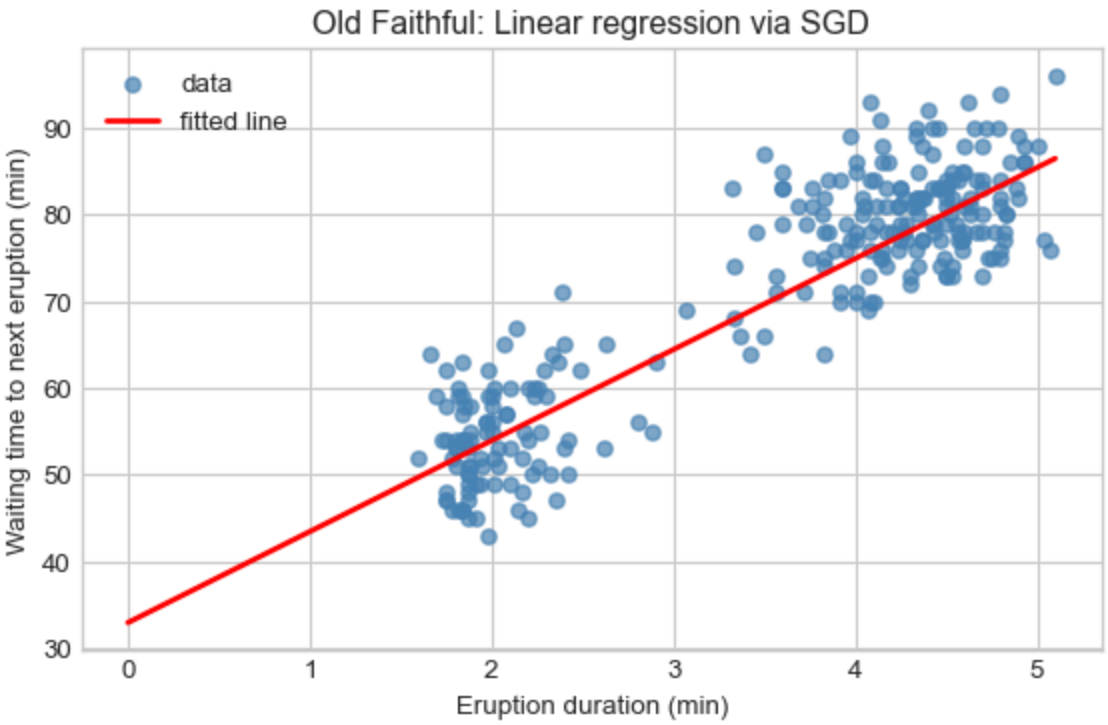
```
Learned parameters:
  intercept = 32.910
  slope     = 10.503
Test MSE = 43.02
Test R²  = 0.671
```

Visualization

In [4]:

```python
import numpy as np

# Scatter the data
plt.figure(figsize=(6,4))
plt.scatter(X, y, color="steelblue", s=30, alpha=0.7, label="data")

# Plot the fitted line
x_line = np.linspace(0, X.max(), 100).reshape(-1, 1)
y_line = sgd.predict(x_line)
plt.plot(x_line, y_line, color="red", linewidth=2, label="fitted line")

plt.xlabel("Eruption duration (min)")
plt.ylabel("Waiting time to next eruption (min)")
plt.title("Old Faithful: Linear regression via SGD")
plt.legend()
```

```
plt.tight_layout()
plt.show()
```



In the plot above, the line $x = 0$ is included to facilitate the visualization of the intercept, which is given by $\theta_0 = 32.910$.

Characteristics

A typical **learning algorithm** comprises the following components:

1. A **model**, often consisting of a set of **parameters** whose values will be **"learnt"**.
2. An **objective function**.
   - In the case of **regression**, this is often a **loss function**, a function that quantifies misclassification. The **Root Mean Square Error** is a common loss function for regression problems.

$$\sqrt{\frac{1}{N}\sum_{1}^{N}[h(x_i) - y_i]^2}$$

3. **Optimization** algorithm

Optimization

Until some termination criteria is met[1]:

- **Evaluate** the loss function, comparing $h(x_i)$ to y_i.

- **Make small changes to the parameters**, in a way that reduces the value of the loss function.

Remarks

- It is important to separate the **optimization algorithm** from the **problem** it addresses.
- For **linear regression**, an exact analytical solution exists, but it presents certain limitations.
- **Gradient descent** serves as a general algorithm applicable not only to linear regression, but also to logistic regression, deep learning, t-SNE (t-distributed Stochastic Neighbor Embedding), among various other problems.
- There exists a diverse range of optimization algorithms that **do not rely on gradient-based methods**.

Optimization — single feature

- **Model** (hypothesis):

$$h(x_i; \theta) = \theta_0 + \theta_1 x_i^{(1)}$$

- **Loss/cost function**:

$$J(\theta_0, \theta_1) = \frac{1}{N} \sum_{i=1}^{N} [h(x_i; \theta) - y_i]^2$$

Goal: find θ_0, θ_1 that minimize J, by iteratively updating the parameters.

This screen is paramount for our presentation, and it is essential to grasp its content fully, as it often causes confusion.

In machine learning, an algorithm generates a model, denoted as h. This model is derived from the training data, represented by X. After the model is trained, it can be utilized to predict outcomes for new, unseen data points, denoted by x_{new}. Once trained, the model's parameters, θ, become fixed. The model functions by mapping each input x_i to a predicted output $\hat{y}_i$, $x_i \mapsto \hat{y}_i$.

The cost function is used to determine the optimal parameter values, θ, for the model h. On this screen, the loss is specified as the mean squared error. Our goal is to identify θ such that the model h minimizes its error on the training dataset X. The loss function maps the parameter pair (θ_0, θ_1) to a non-negative real number $\mathbb{R}_{\geq 0}$, $(\theta_0, \theta_1) \mapsto \mathbb{R}_{\geq 0}$, which aggregates errors across all data points.

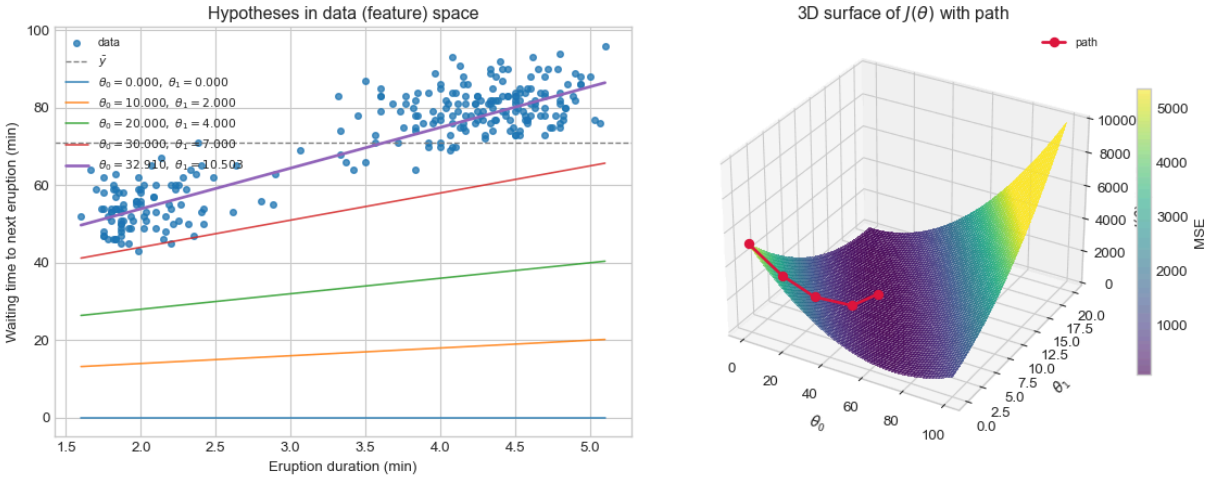
Gradient descent is a process that operates in the parameter space, where it adjusts θ to minimize the loss, rather than in the feature space of the data.

The notation $h(x_i; \theta)$ indicates that the value of the function h (of the model) depends on the input example x_i as well as the parameters θ. The semicolon is used to semantically differentiate these two sets of values. This convention comes from the field of statistics. In machine learning, we also use the notation $h_\theta(x_i)$, which can be considered more appropriate. In this context, we refer to an indexed family of functions, where θ specifically determines which function h_θ should be used. This notation is read as follows: "the function h, parameterized by θ, applied to the input x_i."

Hypothesis vs Parameter Space

[1] E.g. the value of the **loss function no longer decreases** or the **maximum number of iterations**.

In [5]:



In this example, we use the Old Faithful geyser eruption dataset.

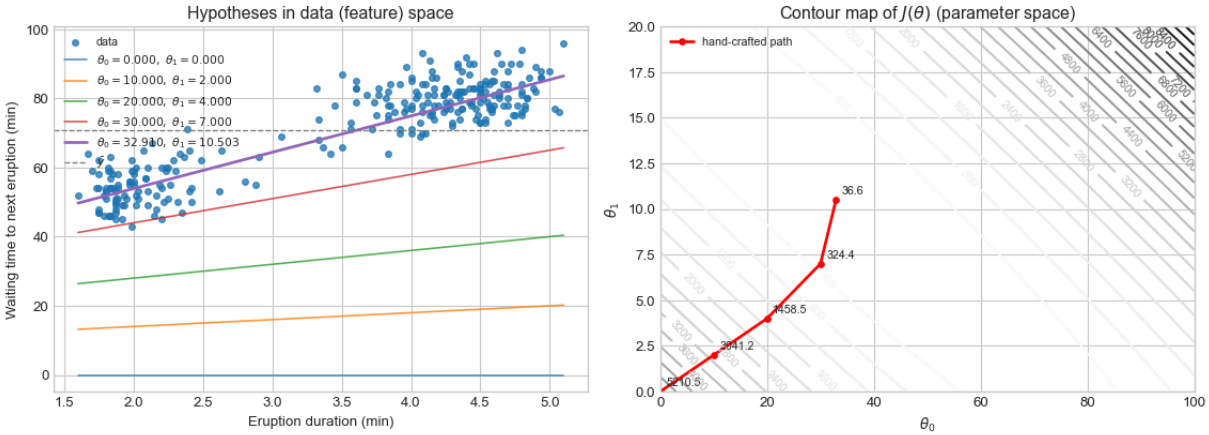
The figure on the left illustrates the data within its feature space, where each line represents a distinct hypothesis. For instance, the horizontal blue line corresponds to the hypothesis defined by parameters $(\theta_0 = 0, \theta_1 = 0)$, while the orange line corresponds to $(\theta_0 = 10, \theta_1 = 2)$. The sequence of model parameters, or hypotheses, has been deliberately designed to elucidate the underlying concepts.

Conversely, the figure on the right depicts the parameter space, which is where optimization is performed. In this space, the vertical axis indicates the Mean Squared Error (MSE) for all combinations of θ_0 and θ_1. Specifically, a model characterized by these parameters would incur this level of error with the specified training data. During the training process, the data remains constant, whereas the parameters θ_0 and θ_1 are adjusted to minimize the error.

In the figure on the right, the progression of model parameters, denoted as (θ_0, θ_1) with the sequence $\{(0.000, 0.000), (10.000, 2.000), (20.000, 4.000), (30.000, 7.000), (32.910, 10.503)\}$, illustrates a reduction in the mean squared error (MSE), $J(\theta)$.

Hypothesis vs Parameter Space

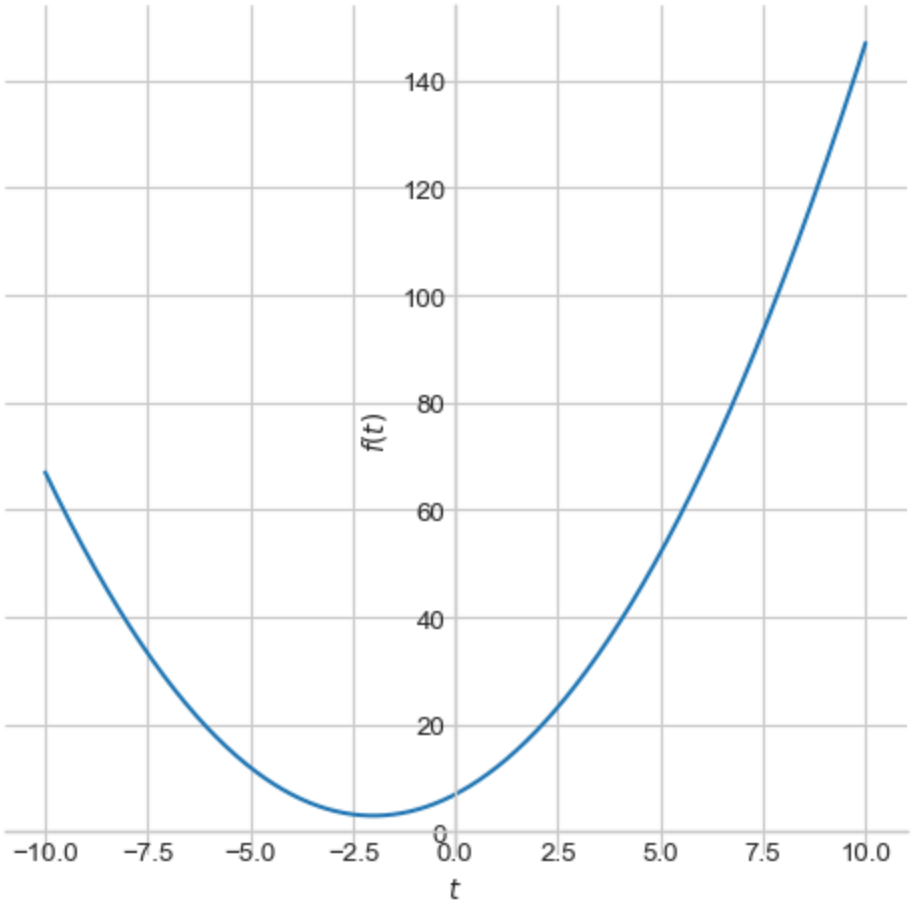
In [6]:



Thes figures illustrate the same concept, but using a contour plot.

Derivative

Derivative



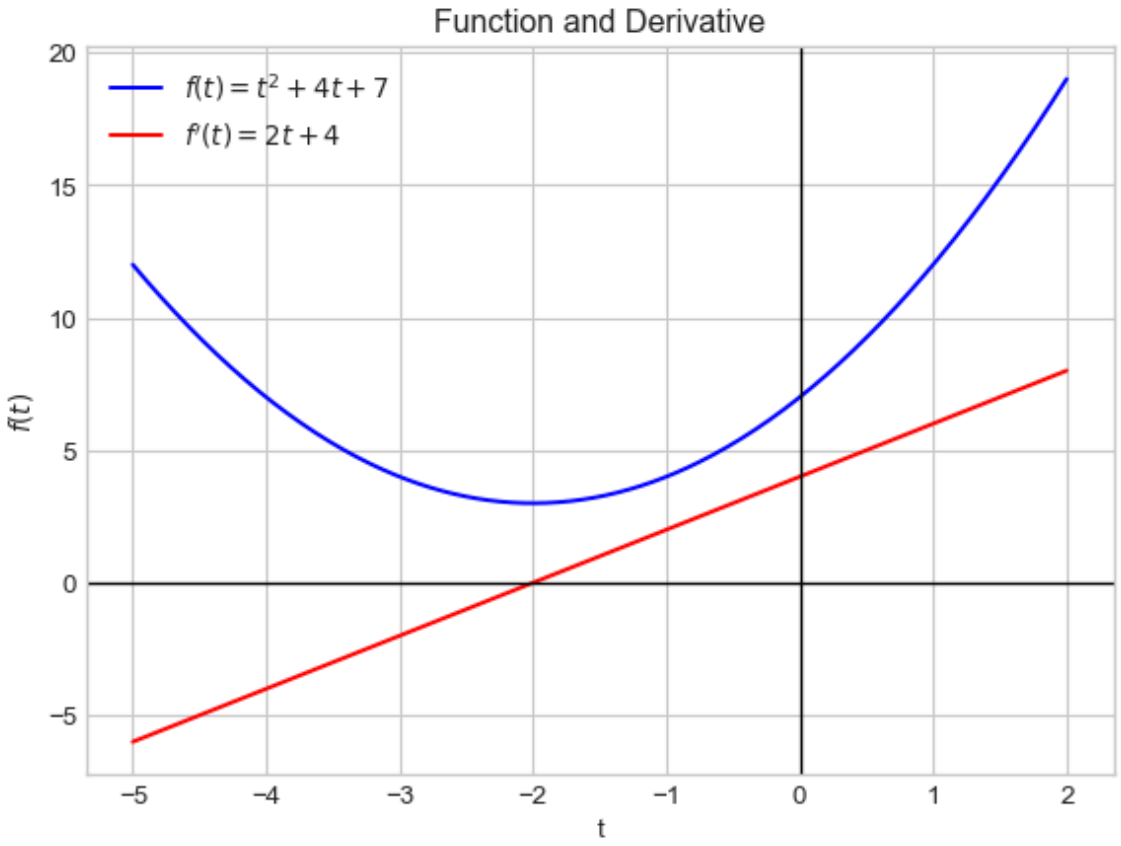
- We will start with a **single-variable function**.
- Think of this as our **loss function**, which we aim to minimize; to reduce the average discrepancy between expected and predicted values.
- Here, I am using t to avoid any confusion with the attributes of our training examples.

Source code

In [8]:
```
from sympy import *

x = symbols('t')

f = t**2 + 4*t + 7

plot(f)
```

On the previous slide, I've used **SymPy**, a library for **symbolic mathematics**.

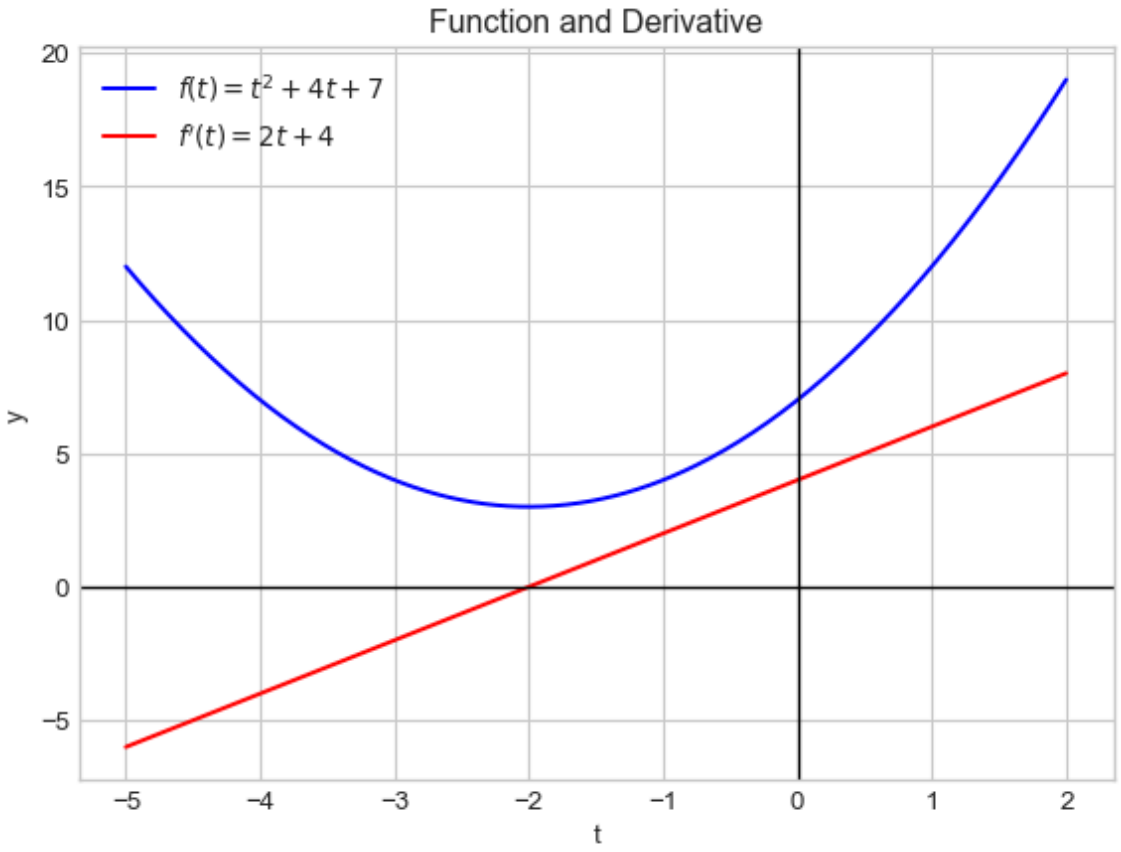
Derivative



- The graph of the **derivative**, $f^{'}(t)$, is depicted in **red**.
- The **derivative** indicates how changes in the input affect the output, $f(t)$.
- The magnitude of the **derivative** at $t = -2$ is 0.
- This point corresponds to the **minimum** of our function.

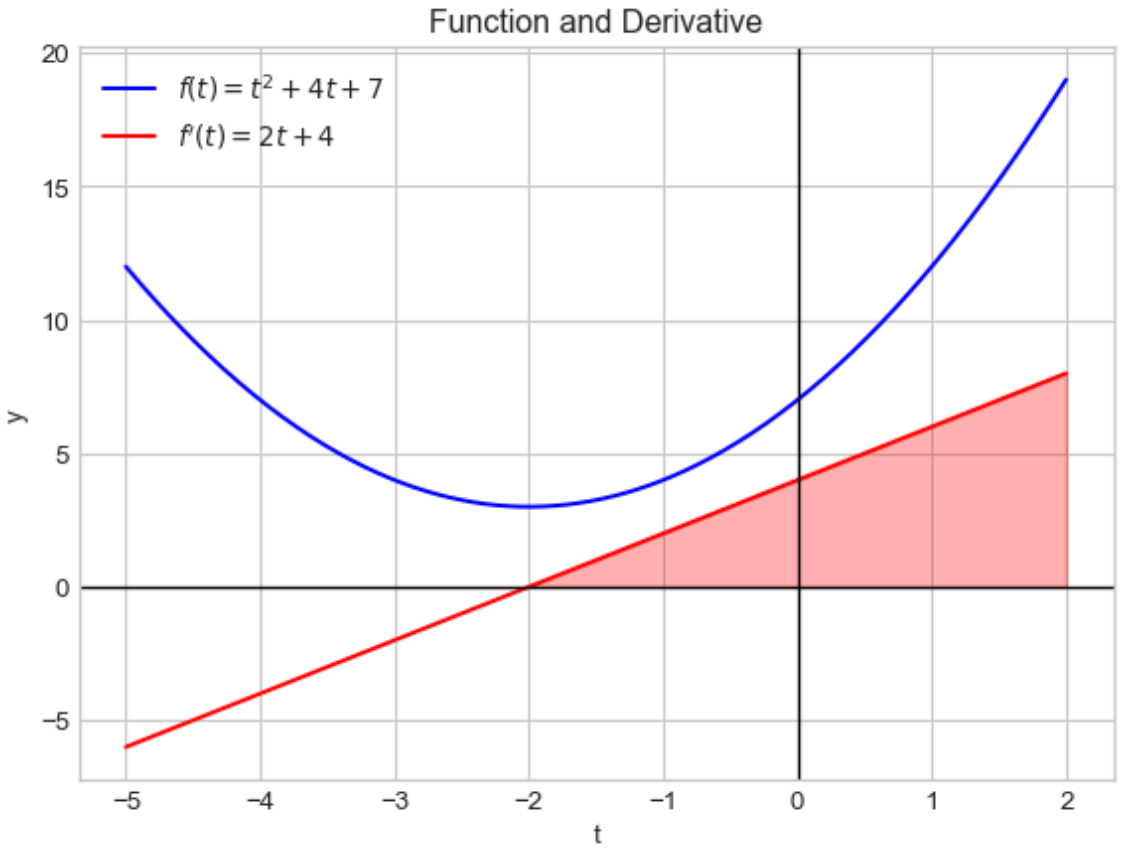
Near $t = -2$, variations in t have minimal impact on the output, $f(t)$.

Derivative



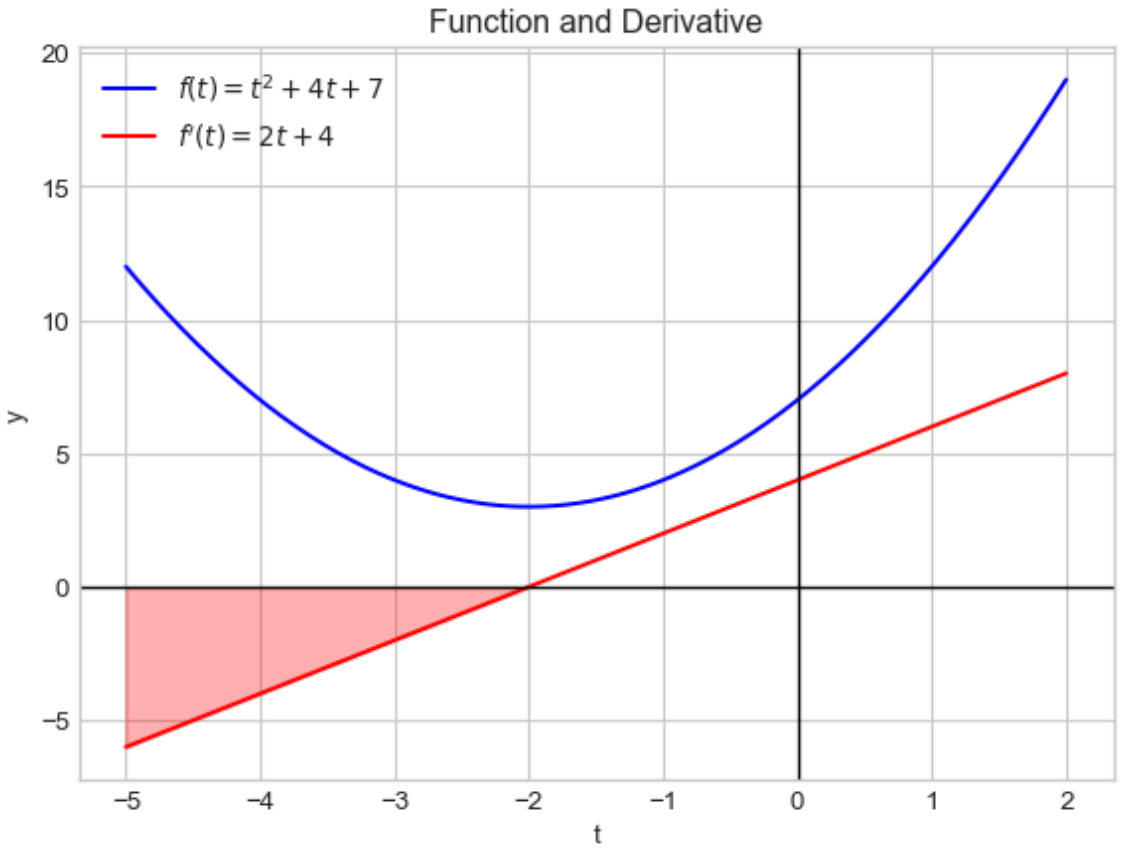
- When evaluated at a **specific point**, the derivative indicates the **slope** of the **tangent line** to the graph of the function at that point.
- At $t = -2$, the **slope** of the **tangent line** is 0.

Derivative



- A **positive derivative** indicates that **increasing the input variable** will **increase the output value**.
- Additionally, the **magnitude** of the derivative quantifies how **rapidly** the output changes.

Derivative



- A **negative derivative** indicates that **increasing the input variable** will **decrease the output value**.
- Additionally, the **magnitude** of the derivative quantifies how **rapidly** the output changes.

Source code

In [13]:

```
import sympy as sp
import numpy as np
import matplotlib.pyplot as plt

# Define the variable and function
t = sp.symbols('t')
f = t**2 + 4*t + 7

# Compute the derivative
f_prime = sp.diff(f, t)

# Lambdify the functions for numerical plotting
f_func = sp.lambdify(t, f, "numpy")
f_prime_func = sp.lambdify(t, f_prime, "numpy")

# Generate t values for plotting
t_vals = np.linspace(-5, 2, 400)
```

```python
# Get y values for the function and its derivative
f_vals = f_func(t_vals)
f_prime_vals = f_prime_func(t_vals)

# Plot the function and its derivative
plt.plot(t_vals, f_vals, label=r'$f(t) = t^2 + 4t + 7$', color='blue')
plt.plot(t_vals, f_prime_vals, label=r"$f'(t) = 2t + 4$", color='red')

# Fill the area below the derivative where it's negative
plt.fill_between(t_vals, f_prime_vals, where=(f_prime_vals > 0), color='red'

# Add labels and legend
plt.axhline(0, color='black',linewidth=1)
plt.axvline(0, color='black',linewidth=1)
plt.title('Function and Derivative')
plt.xlabel('t')
plt.ylabel('y')
plt.legend()

# Show the plot
plt.grid(True)
plt.show()
```

Gradient Descent

Gradient Descent — Single Feature

- **Model** (hypothesis):

$$h(x_i;\theta) = \theta_0 + \theta_1 x_i^{(1)}$$

- **Loss/cost function**:

$$J(\theta_0,\theta_1) = \frac{1}{N}\sum_{i=1}^{N}[h(x_i;\theta) - y_i]^2$$

Gradient descent - intuition

https://youtu.be/i62czvwDlsw

Gradient Descent - Step-by-Step

https://www.youtube.com/watch?v=sDv4f4s2SB8

Gradient descent - single value

- **Initialization:** θ_0 and θ_1 - either with random values or zeros.
- **Loop:**
  - repeat until convergence:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1), \text{for } j = 0 \text{ and } j = 1$$

- α is called the **learning rate** - this is the size of each step.
- $\frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1)$ is the **partial derivative** with respect to θ_j.

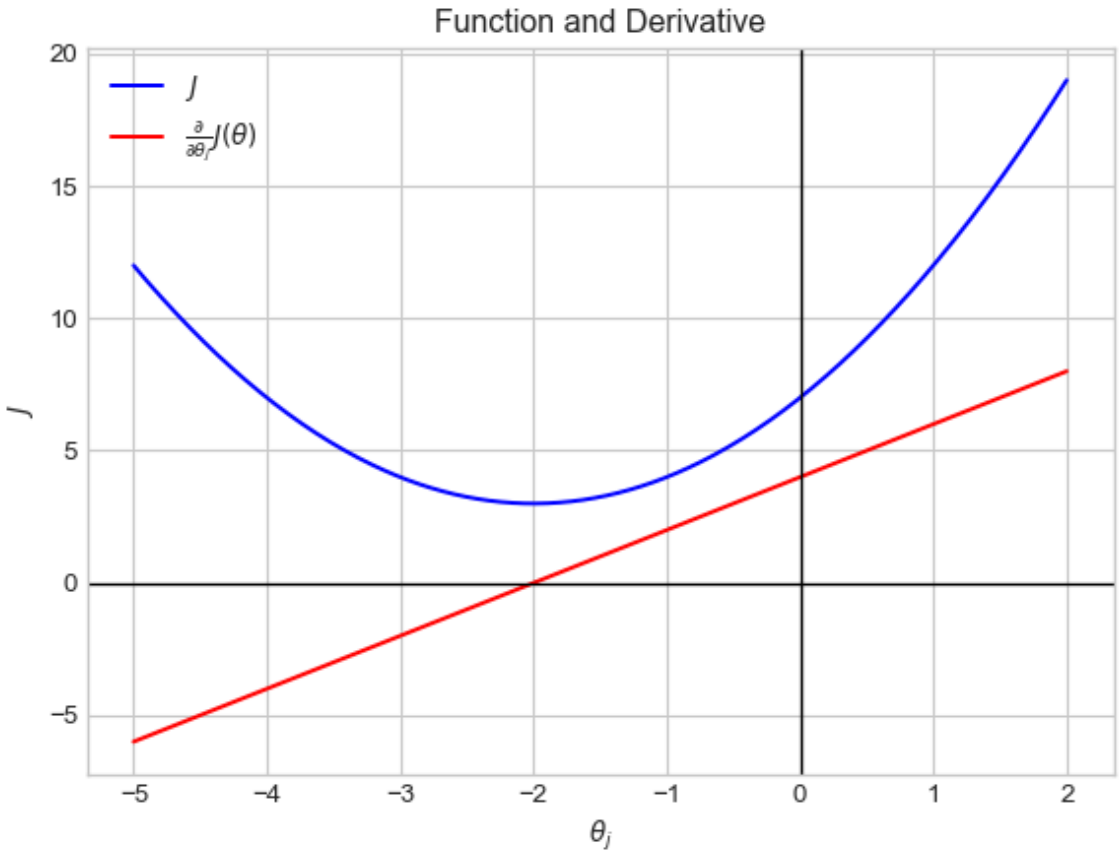
A **partial derivative** represents the rate of change of a multivariable function **with respect to one of its variables**, while **keeping the other variables constant**.

For the algorithm to be mathematically sound, all the θ_j must be updated **simultaneously**.

Gradient Descent - Single Value

```
import sympy as sp
import numpy as np
import matplotlib.pyplot as plt

# Define the variable and function
t = sp.symbols('t')
f = t**2 + 4*t + 7

# Compute the derivative
f_prime = sp.diff(f, t)

# Lambdify the functions for numerical plotting
f_func = sp.lambdify(t, f, "numpy")
f_prime_func = sp.lambdify(t, f_prime, "numpy")

# Generate t values for plotting
t_vals = np.linspace(-5, 2, 400)

# Get y values for the function and its derivative
f_vals = f_func(t_vals)
f_prime_vals = f_prime_func(t_vals)

# Plot the function and its derivative
plt.plot(t_vals, f_vals, label=r'$J$', color='blue')
plt.plot(t_vals, f_prime_vals, label=r"$\frac {\partial}{\partial
\theta_j}J(\theta)$", color='red')

# Add labels and legend
plt.axhline(0, color='black',linewidth=1)
plt.axvline(0, color='black',linewidth=1)
plt.title('Function and Derivative')
```

```
plt.xlabel(r'$\theta_j$')
plt.ylabel(r'$J$')
plt.legend()

# Show the plot
plt.grid(True)
plt.show()
```



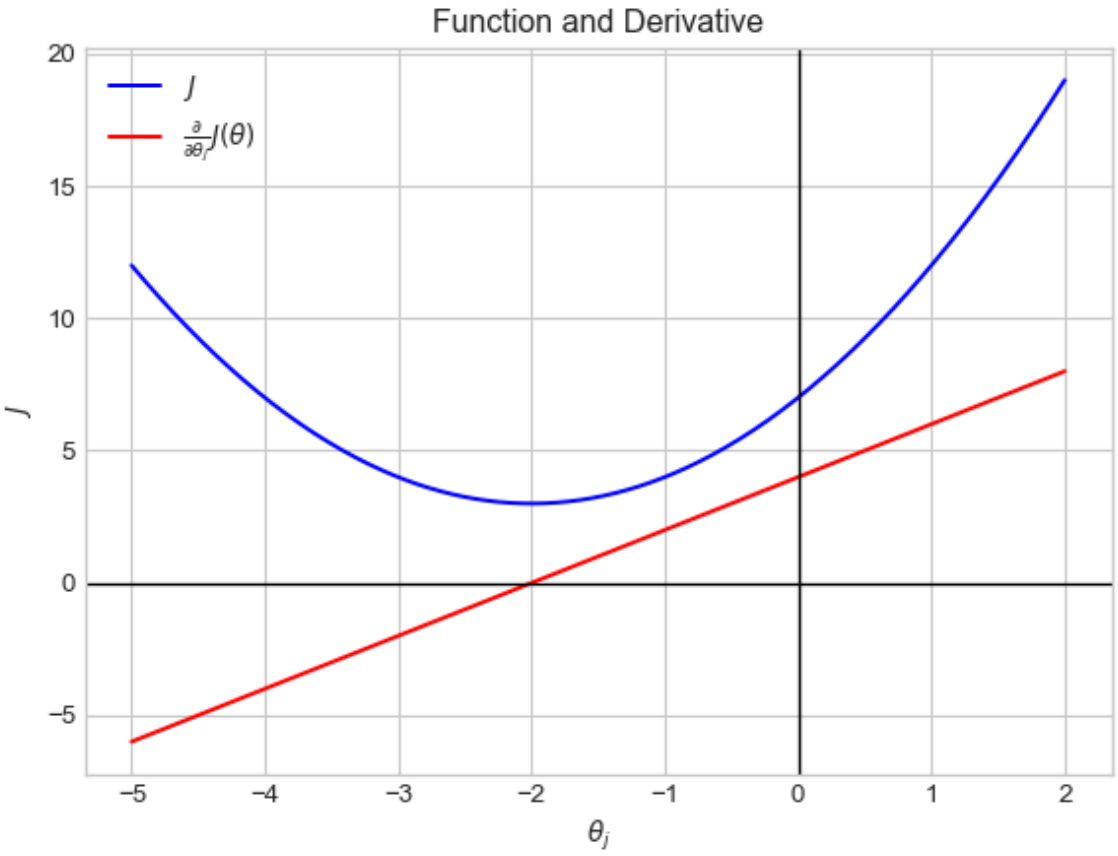
- When the value of θ_j is in the range $[-\inf, -2)$, $\frac{\partial}{\partial\theta_j}J(\theta)$ has a **negative** value.
- Therefore, $-\alpha\frac{\partial}{\partial\theta_j}J(\theta)$ is **positive**.
- Accordingly, the value of θ_j is **increased**.

Updating rule: $\theta_j := \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta_0, \theta_1)$, for $j = 0$ and $j = 1$.

Gradient Descent - Single Value

```
import sympy as sp
import numpy as np
import matplotlib.pyplot as plt

# Define the variable and function
t = sp.symbols('t')
f = t**2 + 4*t + 7
```

```python
# Compute the derivative
f_prime = sp.diff(f, t)

# Lambdify the functions for numerical plotting
f_func = sp.lambdify(t, f, "numpy")
f_prime_func = sp.lambdify(t, f_prime, "numpy")

# Generate t values for plotting
t_vals = np.linspace(-5, 2, 400)

# Get y values for the function and its derivative
f_vals = f_func(t_vals)
f_prime_vals = f_prime_func(t_vals)

# Plot the function and its derivative
plt.plot(t_vals, f_vals, label=r'$J$', color='blue')
plt.plot(t_vals, f_prime_vals, label=r"$\frac {\partial}{\partial
\theta_j}J(\theta)$", color='red')

# Add labels and legend
plt.axhline(0, color='black',linewidth=1)
plt.axvline(0, color='black',linewidth=1)
plt.title('Function and Derivative')
plt.xlabel(r'$\theta_j$')
plt.ylabel(r'$J$')
plt.legend()

# Show the plot
plt.grid(True)
plt.show()
```



- When the value of θ_j is in the range $(-2, \infty]$, $\frac{\partial}{\partial\theta_j}J(\theta)$ has a **positive** value.
- Therefore, $-\alpha\frac{\partial}{\partial\theta_j}J(\theta)$ is **negative**.
- Accordingly, the value of θ_j is **decreased**.

Updating rule: $\theta_j := \theta_j - \alpha\frac{\partial}{\partial\theta_j}J(\theta_0, \theta_1), \text{for } j = 0 \text{ and } j = 1.$

Partial derivatives

Given

$$J(\theta_0, \theta_1) = \frac{1}{N}\sum_{1}^{N}[h(x_i) - y_i]^2 = \frac{1}{N}\sum_{1}^{N}[\theta_0 + \theta_1 x_i - y_i]^2$$

. . .

We have

$$\frac{\partial}{\partial\theta_0}J(\theta_0, \theta_1) = \frac{2}{N}\sum_{i=1}^{N}[\theta_0 - \theta_1 x_i - y_i]$$

. . .

and

$$\frac{\partial}{\partial \theta_1} J(\theta_0, \theta_1) = \frac{2}{N} \sum_{i=1}^{N} x_i [\theta_0 + \theta_1 x_i - y_i]$$

Partial derivate (SymPy)

In [16]:
```
from IPython.display import Math, display
from sympy import *

# Define the symbols

theta_0, theta_1, x_i, y_i = symbols('theta_0 theta_1 x_i y_i')

# Define the hypothesis function:

h = theta_0 + theta_1 * x_i

print("Hypothesis function:")

display(Math('h(x) = ' + latex(h)))
```

```
Hypothesis function:
```

Partial derivate (SymPy)

In [17]:
```
N = Symbol('N', integer=True)

# Define the loss function (mean squared error)

J = (1/N) * Sum((h - y_i)**2, (x_i, 1, N))

print("Loss function:")

display(Math('J = ' + latex(J)))
```

```
Loss function:
```

Partial derivate (SymPy)

In [18]:
```
# Calculate the partial derivative with respect to theta_0

partial_derivative_theta_0 = diff(J, theta_0)

print("Partial derivative with respect to theta_0:")

display(Math(latex(partial_derivative_theta_0)))
```

```
Partial derivative with respect to theta_0:
```

Partial derivate (SymPy)

In [19]:
```
# Calculate the partial derivative with respect to theta_1

partial_derivative_theta_1 = diff(J, theta_1)

print("\nPartial derivative with respect to theta_1:")

display(Math(latex(partial_derivative_theta_1)))
```

```
Partial derivative with respect to theta_1:
```

Multivariate linear regression

$$h(x_i) = \theta_0 + \theta_1 x_i^{(1)} + \theta_2 x_i^{(2)} + \theta_3 x_i^{(3)} + \cdots + \theta_D x_i^{(D)}$$

$$x_i^{(j)} = \text{value of the feature } j \text{ in the } i\text{th example}$$
$$D = \text{the number of features}$$

Gradient descent - multivariate

The new **loss function** is

$$J(\theta_0, \theta_1, \ldots, \theta_D) = \frac{1}{N} \sum_{i=1}^{N} [h(x_i) - y_i]^2$$

Its **partial derivative**:

$$\frac{\partial}{\partial \theta_j} J(\theta) = \frac{2}{N} \sum_{i=1}^{N} x_i^{(j)} [\theta x_i - y_i]$$

where θ, x_i and y_i are vectors, and θx_i is a vector operation!

Gradient vector

The vector containing the partial derivative of J (with respect to θ_j, for $j \in \{0, 1 \ldots D\}$) is called the **gradient vector**.

$$\nabla_\theta J(\theta) = \begin{pmatrix} \frac{\partial}{\partial \theta_0} J(\theta) \\ \frac{\partial}{\partial \theta_1} J(\theta) \\ \vdots \\ \frac{\partial}{\partial \theta_D} J(\theta) \end{pmatrix}$$

. . .

- This vector gives the direction of the **steepest ascent**.
- It gives its name to the **gradient descent** algorithm:

$$\theta' = \theta - \alpha \nabla_\theta J(\theta)$$

Gradient descent - multivariate

The gradient descent algorithm becomes:

Repeat until convergence:

$$\begin{aligned}
&\{ \\
\theta_j :=& \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta_0, \theta_1, \ldots, \theta_D) \\
&\text{for } j \in [0, \ldots, D] \ \textbf{(update simultaneously)} \\
&\}
\end{aligned}$$

Gradient descent - multivariate

Repeat until convergence:

$$\begin{aligned}
&\{ \\
&\theta_0 := \theta_0 - \alpha \frac{2}{N} \sum_{i=1}^{N} x_i^0 [h(x_i) - y_i] \\
&\theta_1 := \theta_1 - \alpha \frac{2}{N} \sum_{i=1}^{N} x_i^1 [h(x_i) - y_i] \\
&\theta_2 := \theta_2 - \alpha \frac{2}{N} \sum_{i=1}^{N} x_i^2 [h(x_i) - y_i] \\
&\ldots \\
&\}
\end{aligned}$$

Where $x_0 = 1$.

Assumptions

What were our **assumptions**?

. . .

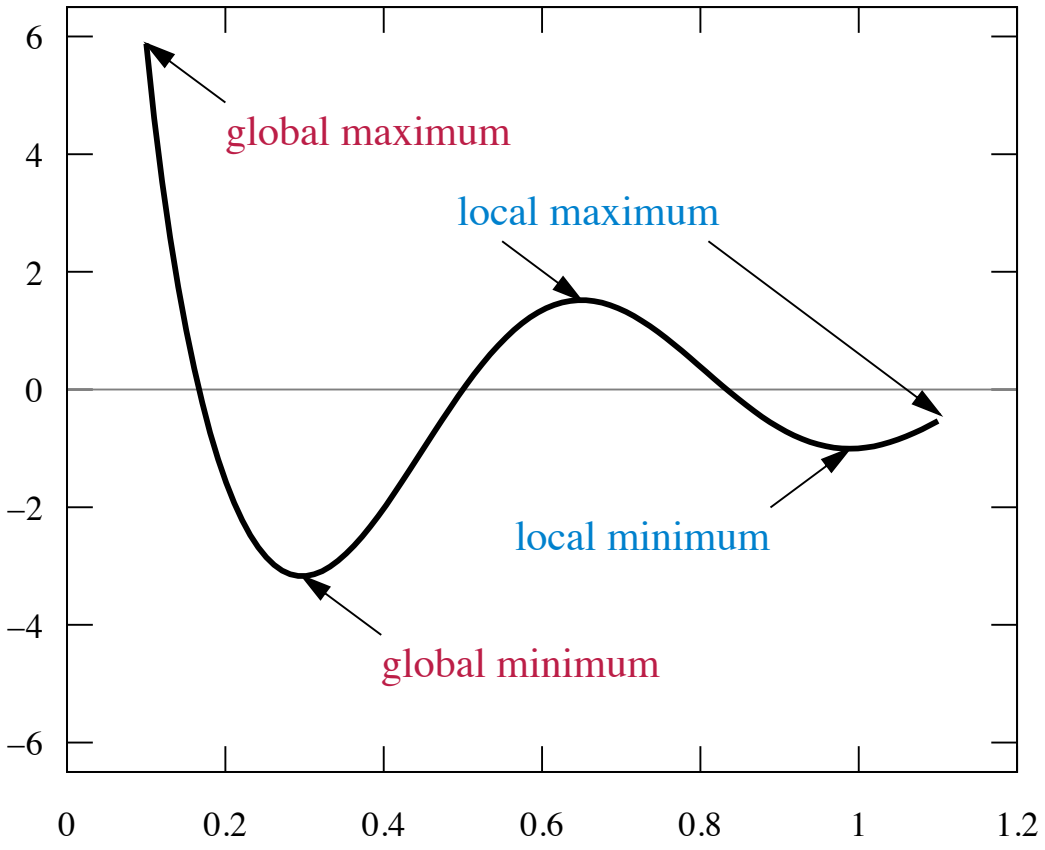
- The (objective/loss) function is **differentiable**.

Local vs. global

- A function is **convex** if for any pair of points on the graph of the function, the line connecting these two points lies above or on the graph.
    - A **convex** function has a **single** minimum.
        - The loss function for the linear regression (MSE) is convex.
- For functions that are not convex, the gradient descent algorithm converges to a **local** minimum.
- The loss function generally used with linear or logistic regressions, and Support Vector Machines (SVM) are convex, but not the ones for artificial neural networks.

A function would be convex downward or concave if those lines were below or on the graph of the function.

Local vs. global

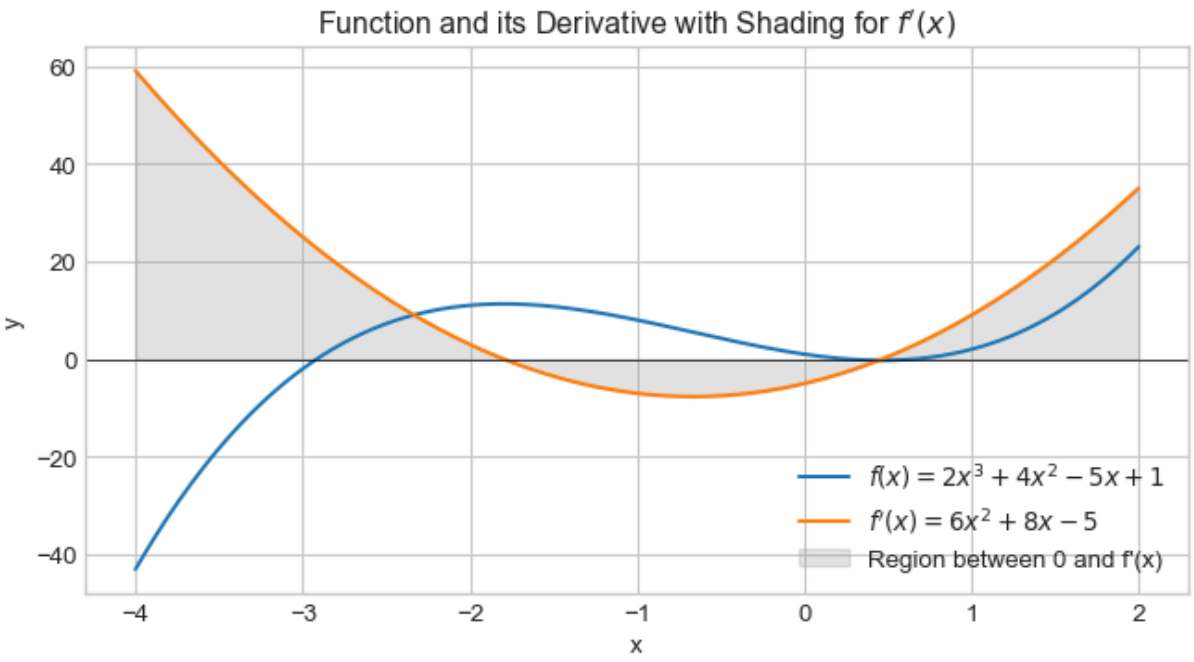


Attribution: commons.wikimedia.org/wiki/File:Extrema_example.svg

Convergence

In [20]:

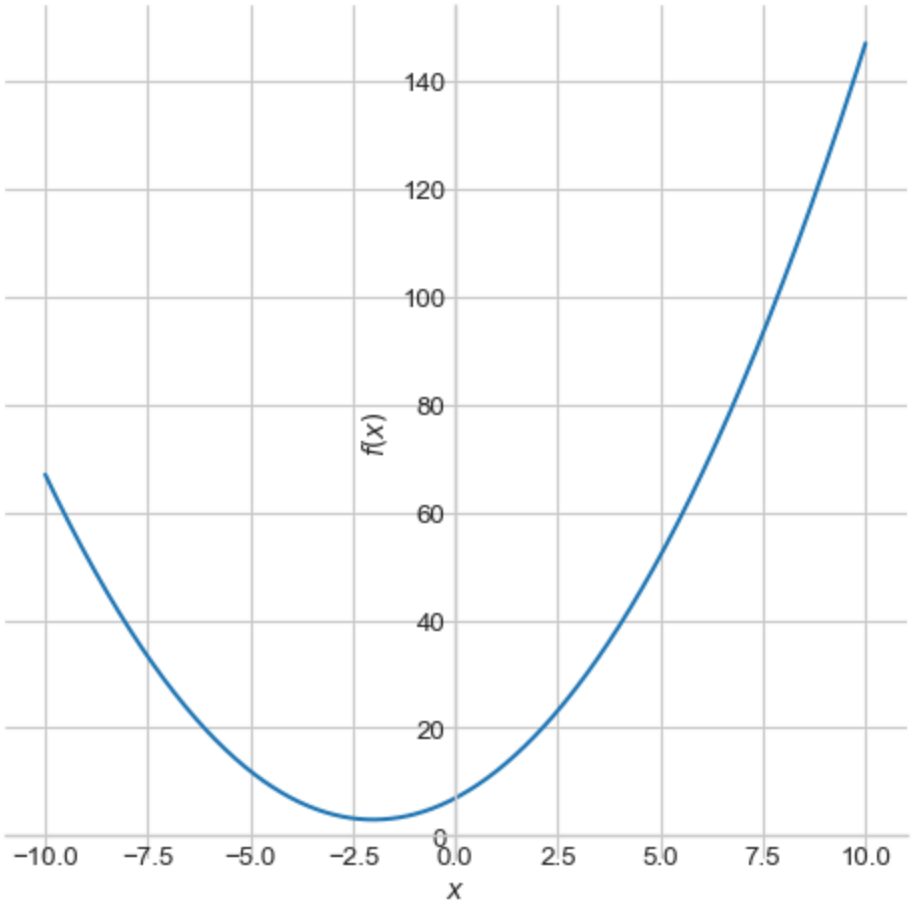
```python
# 1. Define the symbolic variable and the function
x = sp.Symbol('x', real=True)
f_expr = 2*x**3 + 4*x**2 - 5*x + 1

# 2. Compute the derivative of f
f_prime_expr = sp.diff(f_expr, x)

# 3. Convert symbolic expressions to Python functions
f = sp.lambdify(x, f_expr, 'numpy')
f_prime = sp.lambdify(x, f_prime_expr, 'numpy')

# 4. Generate a range of x-values
x_vals = np.linspace(-4, 2, 1000)

# 5. Compute f and f' over this range
y_vals = f(x_vals)
y_prime_vals = f_prime(x_vals)

# 6. Prepare LaTeX strings for legend
f_label = rf'$f(x) = {sp.latex(f_expr)}$'
f_prime_label = rf'$f^\prime(x) = {sp.latex(f_prime_expr)}$'

# 7. Plot f and f', with equations in the legend
plt.figure(figsize=(8, 4))
plt.plot(x_vals, y_vals, label=f_label)
plt.plot(x_vals, y_prime_vals, label=f_prime_label)

# 8. Shade the region between x-axis and f'(x) for the entire domain
plt.fill_between(x_vals, y_prime_vals, 0, color='gray', alpha=0.2, interpola
                 label='Region between 0 and f\'(x)')

# 9. Add reference line, labels, legend, etc.
plt.axhline(0, color='black', linewidth=0.5)
plt.title(rf'Function and its Derivative with Shading for $f^\prime(x)$')
plt.xlabel('x')
plt.ylabel('y')
plt.legend()
plt.grid(True)
plt.show()
```



For **functions lacking a global minimum**, gradient descent can **continue descending indefinitely**, preventing convergence.

- The first objective of this example is to illustrate that gradient descent is applicable to functions of arbitrary complexity, provided that the gradient can be computed or approximated at each iteration.
- Furthermore, the function must possesses at least one local minimum within the interval of interest.

Learning Rate

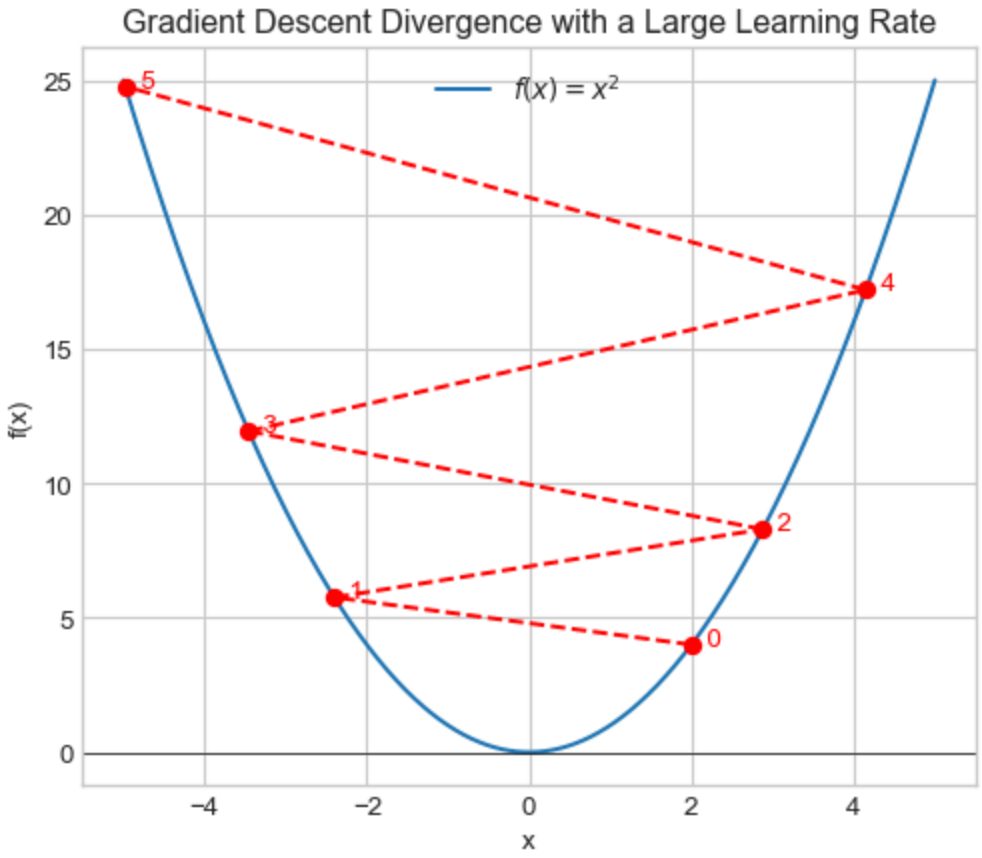


- **Small steps**, low values for α, will make the algorithm **converge slowly**.
- **Large steps** might cause the algorithm to **diverge**.
- Notice how the algorithm **slows down** naturally when approaching a minimum.

Learning Rate

In [22]:
```python
import numpy as np
import matplotlib.pyplot as plt

def f(x):
    return x**2

def grad_f(x):
    return 2*x

# Initial guess, learning rate, and number of gradient-descent steps
x_current = 2.0
learning_rate = 1.1  # Too large => divergence
num_iterations = 5   # We'll do five updates

# Store each x value in a list (trajectory) for plotting
trajectory = [x_current]

# Perform gradient descent
for _ in range(num_iterations):
```

```
    g = grad_f(x_current)
    x_current = x_current - learning_rate * g
    trajectory.append(x_current)

# Prepare data for plotting
x_vals = np.linspace(-5, 5, 1000)
y_vals = f(x_vals)

# Plot the function f(x)
plt.figure(figsize=(6, 5))
plt.plot(x_vals, y_vals, label=r"$f(x) = x^2$")
plt.axhline(0, color='black', linewidth=0.5)

# Plot the trajectory, labeling each iteration
for i, x_t in enumerate(trajectory):
    y_t = f(x_t)
    # Plot the point
    plt.plot(x_t, y_t, 'ro')
    # Label the iteration number
    plt.text(x_t, y_t, f"  {i}", color='red')
    # Connect consecutive points
    if i > 0:
        x_prev = trajectory[i - 1]
        y_prev = f(x_prev)
        plt.plot([x_prev, x_t], [y_prev, y_t], 'r--')

# Final touches
plt.title("Gradient Descent Divergence with a Large Learning Rate")
plt.xlabel("x")
plt.ylabel("f(x)")
plt.legend()
plt.grid(True)
plt.show()
```



Batch gradient descent

- To be more precise, this algorithm is known as **batch gradient descent** since for each iteration, it processes the “whole batch” of training examples.

. . .

- Literature suggests that the algorithm might take more time to converge if the features are on different scales.

Batch gradient descent - drawback

- The **batch gradient descent** algorithm becomes very **slow** as the **number of training examples increases**.

. . .

- This is because **all** the training data is seen at **each iteration**. The algorithm is generally run for a fixed number of iterations, say 1000.

Stochastic Gradient Descent

The **stochastic gradient descent** algorithm randomly selects **one** training instance to calculate its gradient.

```
epochs = 10
for epoch in range(epochs):
   for i in range(N):
         selection = np.random.randint(N)
         # Calculate the gradient using selection
         # Update the parameters
```

- This allows it to work with large training sets.
- Its trajectory is not as regular as the batch algorithm.
  - Because of its bumpy trajectory, it is often better at finding the **global minima**, when compared to batch.
  - Its bumpy trajectory makes it bounce around the local minima.

To mitigate the issue of oscillating around local minima, it is advisable to progressively reduce the learning rate as the number of epochs increases. This technique, known as a **learning schedule**, helps achieve more stable convergence.

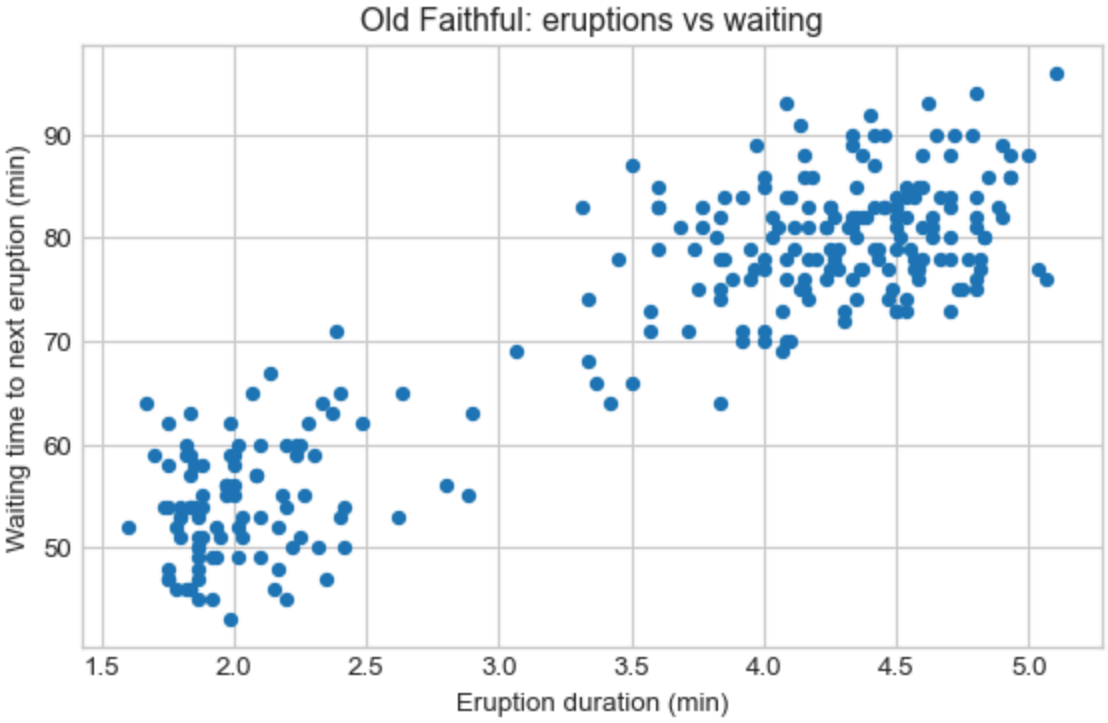
It important that the examples are either **selected randomly** or **shuffled** before running the algorithm to make sure that the algorithm converges towards the global minima.

Mini-batch gradient descent

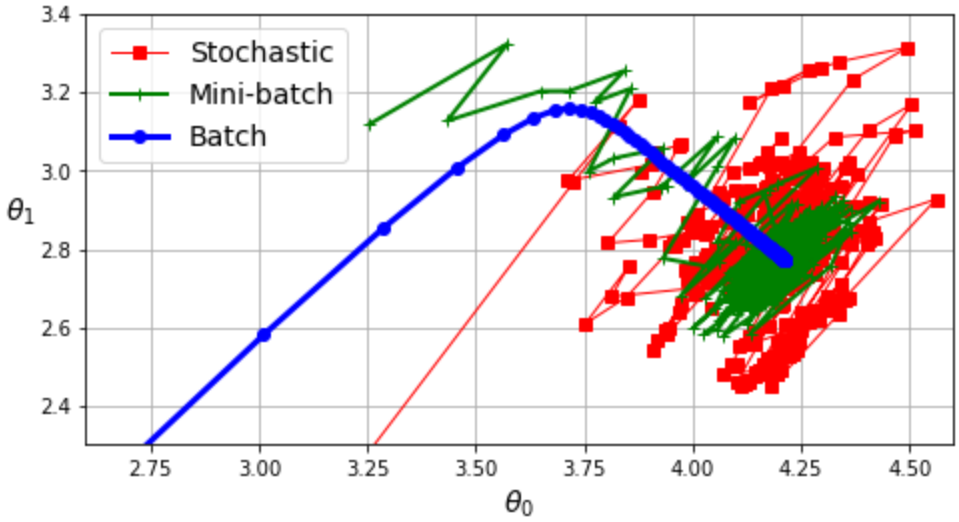
- At each step, rather than selecting one training example as SGD does, **mini-batch gradient descent** randomly selects a **small number** of training examples to compute the gradients.
- Its trajectory is more regular compared to SGD.
  - As the size of the mini-batches increases, the algorithm becomes increasingly similar to batch gradient descent, which uses all the examples at each step.
- It can take advantage of the hardware acceleration of matrix operations, particularly with GPUs.

Quick Visualization

In [23]:
```
import matplotlib.pyplot as plt

plt.figure(figsize=(6,4))
plt.scatter(df["eruptions"], df["waiting"], s=20)
plt.xlabel("Eruption duration (min)")
plt.ylabel("Waiting time to next eruption (min)")
plt.title("Old Faithful: eruptions vs waiting")
plt.tight_layout()
plt.show()
```



Stochastic, Mini-Batch, Batch



Attribution: Géron (2022), Figure 4.10, 04_training_linear_models.ipynb

Summary

- **Batch gradient descent** is inherently **slow** and impractical for large datasets requiring **out-of-core** support, though it is capable of handling a substantial number of features.
- **Stochastic gradient descent** is **fast** and well-suited for processing a large volume of examples efficiently.

- **Mini-batch gradient descent** combines the benefits of both batch and stochastic methods; it is **fast**, capable of managing large datasets, and leverages hardware acceleration, particularly with GPUs.

The typical size of a mini-batch when applying stochastic gradient descent (SGD) can vary depending on the specific application and dataset, but common sizes often range between 32 and 512 samples. Here are some common mini-batch sizes used in practice:

1. **Small Mini-Batches**: Sizes such as 16, 32, or 64 are often used when working with smaller datasets or when memory constraints are a concern.
2. **Medium Mini-Batches**: Sizes like 128, 256, or 512 are commonly used and can provide a good balance between computational efficiency and convergence speed.
3. **Large Mini-Batches**: Sizes like 1024, 2048, or larger might be used in large-scale machine learning tasks, especially when sufficient computational resources are available.

The choice of mini-batch size can influence several factors such as:

- **Training Speed**: Larger mini-batches can make better use of parallel processing capabilities, potentially speeding up training.
- **Convergence**: Smaller mini-batches can introduce more noise in the gradient estimation, which can sometimes help escape local minima and improve generalization.
- **Memory Usage**: Larger mini-batches require more memory, which might be a limiting factor, especially on GPUs with limited VRAM.

Ultimately, the optimal mini-batch size is task-specific and often determined empirically through experimentation.

All three are implemented by `SGDRegressor` in `Scikit-Learn`.

Optimization and deep nets

We will briefly revisit the subject when discussing **deep artificial neural networks**, for which **specialized optimization algorithms** exist.

- Momentum Optimization
- Nesterov Accelerated Gradient
- AdaGrad
- RMSProp
- Adam and Nadam

Final word

- Optimization is a vast subject. Other algorithms exist and are used in other contexts.

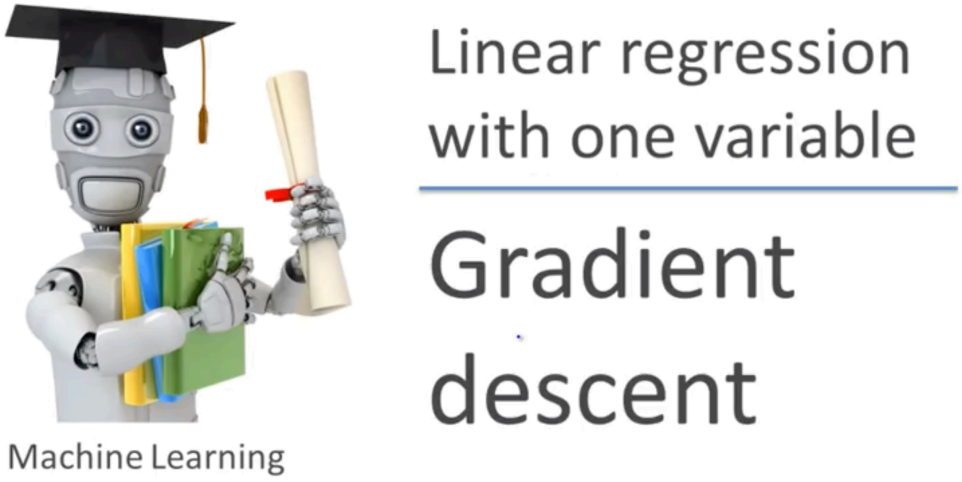
- Including:
  - Particle swarm optimization (PSO), genetic algorithms (GAs), and artificial bee colony (ABC) algorithms.

Prologue

Linear regression - summary

- A **linear model** assumes that the value of the label, $\hat{y}_i$, can be expressed as a **linear combination** of the feature values, $x_i^{(j)}$:
  $\hat{y}_i = h(x_i) = \theta_0 + \theta_1 x_i^{(1)} + \theta_2 x_i^{(2)} + \ldots + \theta_D x_i^{(D)}$
- The **Mean Squared Error (MSE)** is: $\frac{1}{N}\sum_1^N [h(x_i) - y_i]^2$
- **Batch**, **stochastic**, or **mini-batch gradient descent** can be used to find "optimal" values for the parameters, θ_j for $j \in 0, 1, \ldots, D$.
- The result is a **regressor**, a function that can be used to predict the y value (the label) for some unseen example x.

Andrew Ng



- Gradient Descent (Math)
  (11:30 m)
- Intuition
  (11:51 m)

- Linear Regression
  (10:20 m)
- ML-005 | Stanford | Andrew Ng
  (19 videos)

Andrew Ng is presenting the gradient descent algorithm using a linear regression with one variable.

Andrew Ng is Founder of DeepLearning.AI, Founder & CEO of Landing AI, General Partner at AI Fund, Chairman and Co-Founder of Coursera and an Adjunct Professor at Stanford University's Computer Science Department.

Ng was also a cofounder and head of Google Brain and was the former Chief Scientist at Baidu.

Fundamentals by Herman Kamper

https://www.youtube.com/watch?v=BlnLoqn3ZBo&list=PLmZlBIcArwhOr0ysO1Hg4Wfoww0dZnHz4

Mathematics

3Blue1Brown

- Essence of **linear algebra**
  - A series of 16 videos (10 to 15 minutes per video) providing "a geometric understanding of matrices, determinants, eigen-stuffs and more."
    - 6,662,732 views as of September 30, 2019.
- Essence of **calculus**
  - A series of 12 videos (15 to 20 minutes per video): "The goal here is to make calculus feel like something that you yourself could have discovered."
    - 2,309,726 views as of September 30, 2019.

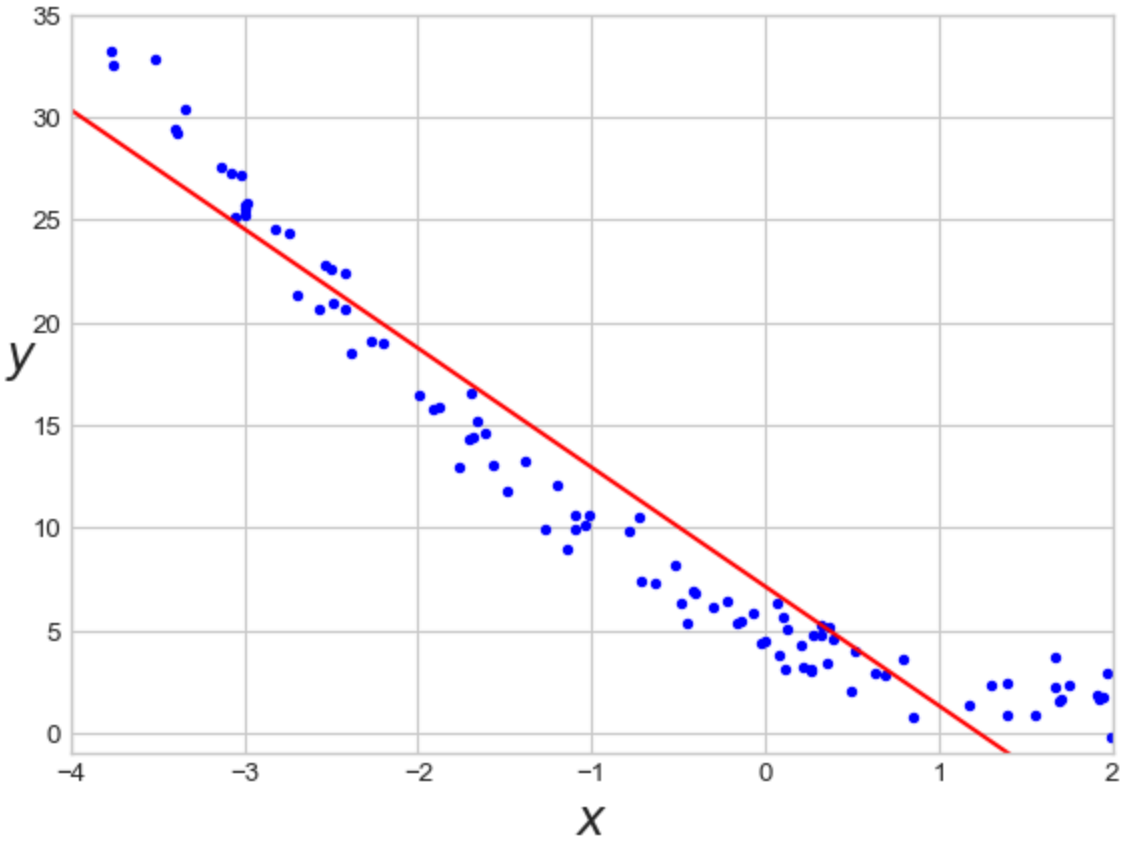
Next lecture

- Logistic regression

Appendix

LinearRegression

In [24]:



In [25]:
```
from sklearn.linear_model import LinearRegression

lin_reg = LinearRegression()
lin_reg.fit(X, y)
```

Herein, we examine a straightforward model involving a single variable.

Source code

In [26]:
```
import numpy as np

X = 6 * np.random.rand(100, 1) - 4
y = X ** 2 - 4 * X + 5 + np.random.randn(100, 1)

from sklearn.linear_model import LinearRegression

lin_reg = LinearRegression()
lin_reg.fit(X, y)

X_new = np.array([[-4], [2]])
y_pred = lin_reg.predict(X_new)
```

This slide contains an anomaly. Can you identify it?

The data have been generated from a quadratic model, $x^2 - 4x + 5$, with Gaussian noise added to make the synthetic data more realistic.

This example illustrates that, in practice, we often have limited knowledge about the underlying model that generated the data.

Despite this uncertainty, we make assumptions—in this case, assuming linearity—when building our models.

Later, we will refer to this as **bias** (distinct from the bias parameter in our regression model). Both bias and variance influence the performance of our models.

GPT 4o interactions (2024-09-14)

User: Explain the code on the previous slide line by line.

. . .

AI: Certainly! Here is a line-by-line explanation of the provided code:

In [27]:
```
import numpy as np
```

- **Explanation**: This line imports the NumPy library, which is a fundamental package for numerical computations in Python. It is commonly used for working with arrays and matrices, as well as for performing a variety of mathematical operations.

In [28]:
```
X = 6 * np.random.rand(100, 1) - 4
```

- **Explanation**: This line generates a NumPy array `X` containing 100 rows and 1 column of random numbers. The `np.random.rand(100, 1)` function generates uniformly distributed random numbers between 0 and 1. Multiplying by 6 scales these numbers to the range [0, 6), and subtracting 4 shifts the range to [-4, 2).

In [29]:
```
y = X ** 2 - 4 * X + 5 + np.random.randn(100, 1)
```

- **Explanation**: This line generates the target variable `y` based on a quadratic equation with some added noise. Specifically:
  - `X ** 2` computes the square of each element in `X`.
  - `- 4 * X` subtracts four times each element in `X`.
  - `+ 5` adds a constant term of 5.
  - `+ np.random.randn(100, 1)` adds Gaussian noise with a mean of 0 and standard deviation of 1 to each element, making the data more realistic by introducing some randomness.

In [30]:
```
from sklearn.linear_model import LinearRegression
```

- **Explanation**: This line imports the `LinearRegression` class from the `sklearn.linear_model` module, which is part of the Scikit-Learn library. Scikit-Learn is widely used for machine learning in Python.

In [31]:
```
lin_reg = LinearRegression()
```

- **Explanation**: This line creates an instance of the `LinearRegression` class and assigns it to the variable `lin_reg`. This object will be used to fit the linear regression model to the data.

In [32]:
```
lin_reg.fit(X, y)
```

- **Explanation**: This line fits the linear regression model to the data by finding the best-fitting line through the points `(X, y)`. The `fit` method trains the model using the provided features `X` and target variable `y`.

In [33]:
```
X_new = np.array([[-4], [2]])
```

- **Explanation**: This line creates a new NumPy array `X_new` with two values: -4 and 2. These values represent new data points for which we want to predict the target variable using the trained model.

In [34]:
```
y_pred = lin_reg.predict(X_new)
```

- **Explanation**: This line uses the trained linear regression model to predict the target variable `y_pred` for the new data points in `X_new`. The `predict` method returns the predicted values based on the fitted model.

In summary, this script generates synthetic data, fits a linear regression model to it, and then uses the model to make predictions on new data points.

Source code (continued)

In [35]:
```
import os
import matplotlib as mpl
import matplotlib.pyplot as plt

def save_fig(fig_id, tight_layout=True, fig_extension="pdf", resolution=300):
    path = os.path.join(fig_id + "." + fig_extension)
    print("Saving figure", fig_id)
    if tight_layout:
```

```
        plt.tight_layout()
    plt.savefig(path, format=fig_extension, dpi=resolution)
```

Source code (continued)

In [36]:
```
plt.plot(X, y, "b.")
plt.plot(X_new, y_pred, "r-")
plt.xlabel("$x$", fontsize=18)
plt.ylabel("$y$", rotation=0, fontsize=18)
plt.axis([-4, 2, -1, 35])
save_fig("regression_linear-01")
plt.show()
```

References

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