Mathematics for Data Science

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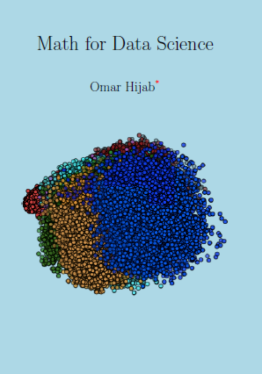
The following slides are arranged (with some modifications) based on the book "*Math for Data Science*" by "**Omar Hijab**".



You can follow me on Linkedin. Also, for course materials such as slides and the related python codes, see this Github repository.

Outline

Outline

What is a dataset?

Definition 1.1

Geometrically, a dataset is a sample of N points $x_1, x_2, \cdots, x_N$ in d-dimensional space $\mathbb{R}^d$. Algebraically, a dataset is an N $\times$ d matrix.

Practically speaking, the following are all representations of datasets:

$$\text{matrix} = \text{CSV file} = \text{spreadsheet} = \text{SQL table} = \text{array} = \text{dataframe}$$

Definition 1.2

Each point $x = (t_1, t_2, \cdots, t_d)$ in the dataset is a sample or an example, and the components $t_1, t_2, \cdots, t_d$ of a sample point x are its features or attributes. As such, d-dimensional space $\mathbb{R}^d$ is feature space.

Definition 1.3

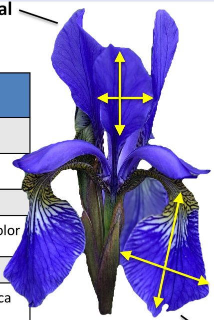
Sometimes one of the features is separated out as the label. In this case, the dataset is a labelled dataset.

Iris dataset

The *Iris dataset* contains 150 examples of four features of Iris flowers, and there are three classes of Irises, *Setosa*, *Versicolor* and *Virginica*, with 50 samples from each class.

Samples
(instances, observations)

	Sepal length	Sepal width	Petal length	Petal width	Class label
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
...					
50	6.4	3.5	4.5	1.2	Versicolor
...					
150	5.9	3.0	5.0	1.8	Virginica



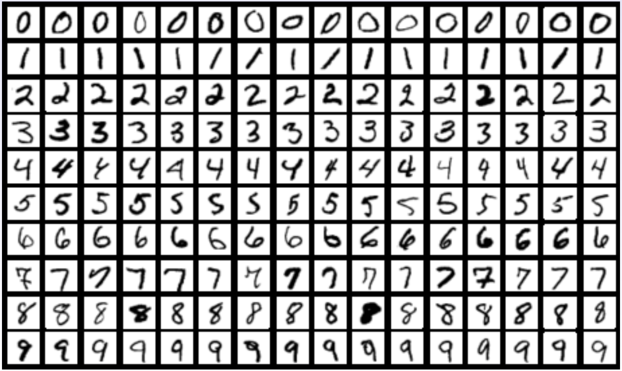
Class labels
(targets)

Features
(attributes, measurements, dimensions)

MNIST dataset

The *MNIST dataset* consists of $60,000$ images of hand-written digits. There are 10 classes of images, corresponding to each digit $0, 1, \cdots, 9$. We seek to compress the images while preserving as much as possible of the images' characteristics.

Each image is a grayscale 28×28 pixel image. Since $28^2 = 784$, each image is a point in $d = 784$ dimensions. Here there are $N = 60000$ samples and $d = 784$ features.



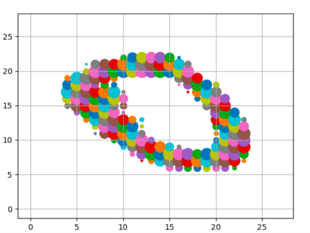
Exercises

Exercise 1.1

Use `sklearn` *to download Iris dataset.*

Exercise 1.2

- *From* `keras` *read the MNIST dataset.*
- *Let* `(train_X, train_y), (test_X, test_y) = mnist.load_data()`
- *Let* `pixels = train_X[1]`.
- *Do* `for` *loops over* `i` *and* `j` *in* `range(28)` *and use* `scatter` *to plot points at location* `(i,j)` *with size given by* `pixels[i,j]`, *then show the following image.*



Introduction

Suppose we have a population of things (people, tables, numbers, vectors, images, etc.) and we have a sample of size N from this population:

```
l = [x_1,x_2,...,x_N]
```

The total population is the *population* or the *sample space*.

Example 1.1

The sample space consists of all real numbers and we take $N = 5$ samples from

```
l = [3.95, 3.20, 3.10, 5.55, 6.93]
```

Example 1.2

The sample space consists of all integers and we take $N = 5$ samples from

```
l = [35, -32, -8, 45, -8]
```

Introduction

Example 1.3

The sample space consists of all Python strings and we take $N = 5$ samples from

```
l = ['a2e?','#%T','7y5,','kkk>><</','[[)*+']
```

Example 1.4

The sample space consists of all HTML colors and we take $N = 5$ samples from

```
from random import choice
import matplotlib.pyplot as plt

def hexcolor():
  return "#" + ''.join([choice('0123456789abcdef') for _ in range(6)])

for i in range(5): plt.scatter(i,0, c=hexcolor())
plt.show()
```

Mean

Let `l` be a list as above. The goal is to compute the sample *average* or *mean* of the list, which is

$$mean = average = \frac{x_1 + x_2 + \cdots + x_N}{N}.$$

In the Example (1.1), the average is

$$\frac{3.95 + 3.20 + 3.10 + 5.55 + 6.93}{5} = 4.546.$$

Example 1.5

```
import numpy as np

dataset = np.array([3.95, 3.20, 3.10, 5.55, 6.93])
print(np.mean(dataset))

output: 4.546
```

In the Example (1.2), the average is $\frac{32}{5}$. In the Example (1.3), while we can add strings, we can't divide them by 5, so the average is undefined. Similarly for colors: the average is undefined.

Vector space

A sample space or population V is called a *vector space* if, roughly speaking, one can compute means or averages in V . In this case, we call the members of the population "*vectors*".

Definition 1.4 (Vector space)

Let V be a set. V is a vector space (over $\mathbb{R}$) if for every $u, v, w \in V$ and $r, s \in \mathbb{R}$:

1. *vectors can be added (and the sum $v + w$ is back in V);*
2. *vector addition is commutative $v + w = w + v$*
3. *vector addition is associative $u + (v + w) = (u + v) + w$;*
4. *there is a zero vector 0 $(0 + v = v)$;*
5. *vectors v have negatives (or opposites) $-v$ $(v + (-v) = 0)$;*
6. *vectors can be multiplied by real numbers (and the product rv is back in V);*
7. *multiplication is distributive over addition $(r + s)v = rv + sv$ and $r(u + v) = ru + rv$;*
8. *$1v = v$ and $0v = 0$;*
9. *$r(sv) = (rs)v$.*

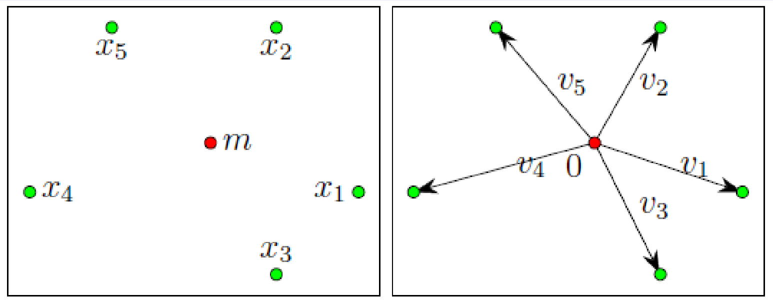
Centered dataset

Definition 1.5 (Centered Versus Non-Centered)

If $x_1, x_2, \cdots, x_N$ is a dataset of points with mean m and

$$v_1 = x_1 - m, v_2 = x_2 - m, \cdots, v_N = x_N - m,$$

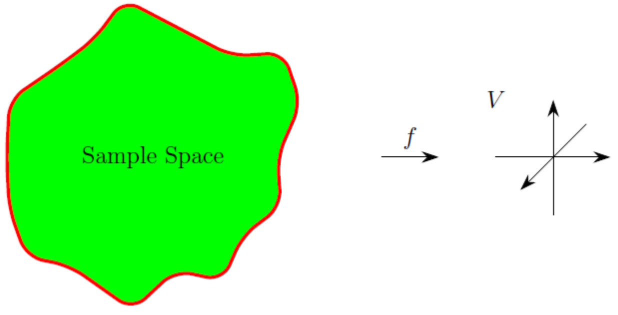
then $v_1, v_2, \cdots, v_N$ is a centered dataset of vectors where its mean is zero.



Some notes

- When we work with vector spaces, numbers are referred to as *scalars*.
- When we multiply a vector v by a scalar r to get the scaled vector rv, we call it *scalar multiplication*.
- The set of all real numbers $\mathbb{R}$ is a vector space.
- The set of all integers $\mathbb{Z}$ is not a vector space.
- The set of all rational numbers $\mathbb{Q}$ is a vector space.
- The set of all Python strings is not a vector space.
- Usually, we can't take sample means from a population, we instead take the sample mean of a *statistic* associated to the population. A statistic is an assignment of a number $f(\text{item})$ to each item in the population. For example, the human population on Earth is not a vector space (they can't be added), but their heights is a vector space (heights can be added). For the Python strings, a statistic might be the length of the strings. For the HTML colors, a statistic is the HTML code of the color.

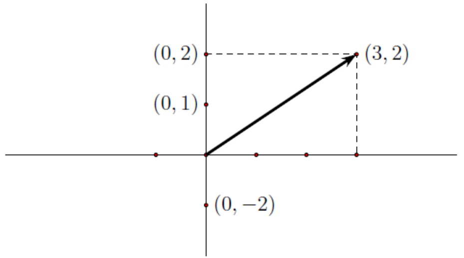
Statistic



In general, a statistic need not be a number. A statistic can be anything that "behaves like a number". For example, $f(\text{item})$ can be a vector or a matrix. More generally, a statistic's values may be anything that lives in a vector space V.

Cartesian plane

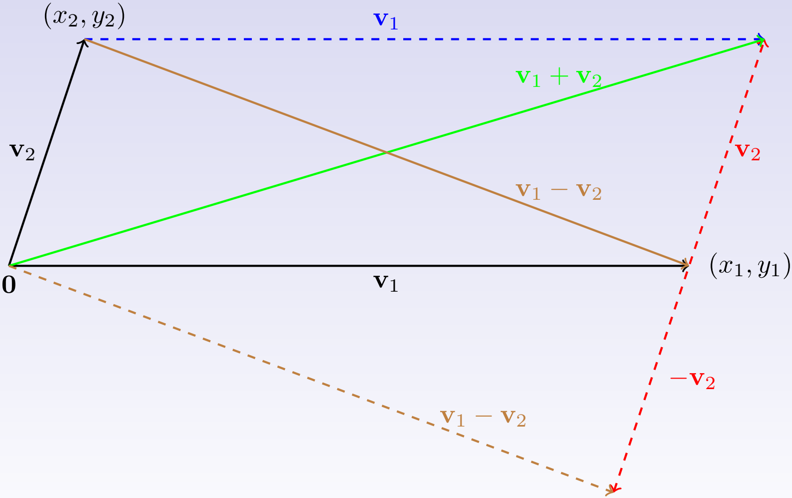
The *cartesian plane* $\mathbb{R}^2$, also called 2-dimensional real space is a vector space.



For $\mathbf{v}_1 = (x_1, y_1), \mathbf{v}_2 = (x_2, y_2) \in \mathbb{R}^2$ and $t \in \mathbb{R}$ define

- $\mathbf{v}_1 + \mathbf{v}_2 = (x_1 + x_2, y_1 + y_2)$ (Addition).
- $\mathbf{0} = (0, 0)$ (Zero).
- $t\mathbf{v}_1 = (tx_1, ty_1)$ (Scaling).
- $-\mathbf{v}_1 = (-1)\mathbf{v}_1$ (Negative).
- $\mathbf{v}_1 - \mathbf{v}_2 = \mathbf{v}_1 + (-\mathbf{v}_2) = (x_1 - x_2, y_1 - y_2)$ (Subtraction).

Operations



(x_2, y_2)
$\mathbf{v}_1$
$\mathbf{v}_1 + \mathbf{v}_2$
$\mathbf{v}_2$
$\mathbf{v}_2$
$\mathbf{v}_1 - \mathbf{v}_2$
(x_1, y_1)
$\mathbf{0}$
$\mathbf{v}_1$
$-\mathbf{v}_2$
$\mathbf{v}_1 - \mathbf{v}_2$

2d example

Example 1.6

```python
import numpy as np

v1 = (1,2)
v2 = (3,4)
print(v1 + v2 == (1+3,2+4)) # returns False

v1 = [1,2]
v2 = [3,4]
print(v1 + v2 == [1+3,2+4]) # returns False

v1 = np.array([1,2])
v2 = np.array([3,4])
print(v1 + v2 == np.array([1+3,2+4]))
# returns [ True  True]
print(3*v1 == np.array([3,6]))
# returns [ True  True]
print(-v1 == np.array([-1,-2]))
# returns [ True  True]
print(v1 - v2 == np.array([1-3,2-4]))
# returns [ True  True]
```

2d example

For the two-dimensional dataset

$$\mathbf{x}_1 = (1,2), \mathbf{x}_2 = (3,4), \mathbf{x}_3 = (-2,11), \mathbf{x}_4 = (0,66),$$

or, equivalently,

$$\mathbf{x} = \begin{pmatrix} 1 & 2 \\ 3 & 4 \\ -2 & 11 \\ 0 & 66 \end{pmatrix},$$

the average is

$$\frac{(1,2)+(3,4)+(-2,11)+(0,66)}{4} = (0.5, 20.75).$$

Example 1.7

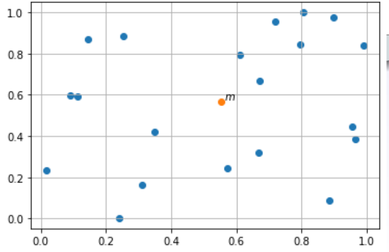
```
import numpy as np

dataset = np.array([[1,2], [3,4], [-2,11], [0,66]])
print(np.mean(dataset, axis=0))
# returns [ 0.5 , 20.75]
```

2d example

Example 1.8

Generate a 2 dimensional dataset of random points and their mean

```python
import numpy as np
from numpy.random import random as rd
import matplotlib.pyplot as plt
N = 20
dataset = np.array([[rd(), rd()] for _ in range(N)])
mean = np.mean(dataset,axis=0)
plt.grid()
X, Y = dataset[:,0], dataset[:,1]
plt.scatter(X,Y)
plt.scatter(*mean)
plt.annotate('$m$', xy=mean+0.01)
plt.show()
```



Magnitude

Definition 1.6 (Distance Formula)

If $\mathbf{v}_1 = (x_1, y_1)$ *and* $\mathbf{v}_2 = (x_2, y_2)$, *then the distance between* $\mathbf{v}_1$ *and* $\mathbf{v}_2$ *is*

$$|\mathbf{v}_1 - \mathbf{v}_2| = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}.$$

The distance of $\mathbf{v} = (x, y)$ *to the origin* $\mathbf{0} = (0, 0)$ *is its magnitude or norm or length*

$$r = |\mathbf{v}| = |\mathbf{v} - \mathbf{0}| = \sqrt{x^2 + y^2}.$$

Example 1.9

For $\mathbf{v}_1 = (1, 2)$ and $\mathbf{v}_2 = (3, 4)$

$$|\mathbf{v}_1| = \sqrt{1^2 + 2^2} = \sqrt{5} \simeq 2.236,$$

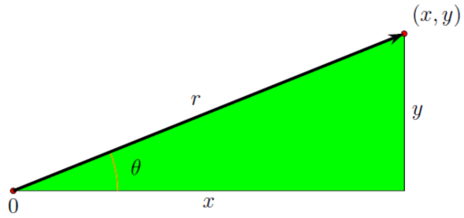
$$|\mathbf{v}_1 - \mathbf{v}_2| = \sqrt{(1-3)^2 + (2-4)^2} = \sqrt{4+4} = \sqrt{8} \simeq 2.828.$$

```
import numpy as np

v1 = np.array([1,2])
v2 = np.array([3,4])
print(np.linalg.norm(v1)) #returns 2.23606797749979
print(np.linalg.norm(v1-v2)) #returns 2.
                              8284271247461903
```

Polar representation

In terms of r and θ, the *polar representation* of (x, y) is

$$x = r\cos\theta, \quad y = r\sin\theta.$$



The *unit circle* consists of the vectors which are distance 1 from the origin $\mathbf{0}$. When $\mathbf{v}$ is on the unit circle, the magnitude of $\mathbf{v}$ is 1, and we say $\mathbf{v}$ is a *unit vector*. In this case, the line formed by the scalings of $\mathbf{v}$ intersects the unit circle at $\pm\mathbf{v}$.

When $\mathbf{v}$ is a unit vector, then $r = 1$ and $\mathbf{v} = (x, y) = (\cos\theta, \sin\theta)$.

Polar representation

By the distance formula, a vector $\mathbf{v} = (x, y)$ is a unit vector when

$$x^2 + y^2 = 1.$$

More generally, any circle with *center* (a, b) and radius r consists of vectors $\mathbf{v} = (x, y)$ satisfying

$$(x - a)^2 + (y - b)^2 = r^2.$$

Let R be a point on the unit circle, and let $t > 0$. The scaled point tR is on the circle with center $(0, 0)$ and radius t. Moreover, if Q is any point, $Q + tR$ is on the circle with center Q and radius t. It is easy to check that $|t\mathbf{v}| = |t||\mathbf{v}|$ for any real number t and vector $\mathbf{v}$.

From this, if a vector $\mathbf{v}$ is unit and $r > 0$, then $r\mathbf{v}$ has magnitude r. If $\mathbf{v}$ is any vector not equal to the zero vector, then $r = |\mathbf{v}|$ is positive, and

$$\left|\frac{1}{r}\mathbf{v}\right| = \frac{1}{r}|\mathbf{v}| = \frac{1}{r}r = 1$$

so $\mathbf{v}/r$ is a unit vector.

Inner product

Definition 1.7

Let $\mathbf{v}_1 = (x_1, y_1), \mathbf{v}_2 = (x_2, y_2) \in \mathbb{R}^2$. *The inner product or the dot product of* $\mathbf{v}_1$ *and* $\mathbf{v}_2$ *is given algebraically as*

$$\mathbf{v}_1 \cdot \mathbf{v}_2 = x_1 x_2 + y_1 y_2.$$

From the geometric view, we have:

Theorem 1.1 (Dot Product Identity)

$$x_1 x_2 + y_1 y_2 = \mathbf{v}_1 \cdot \mathbf{v}_2 = |\mathbf{v}_1||\mathbf{v}_2| \cos\theta,$$

where θ *is the angle between* $\mathbf{v}_1$ *and* $\mathbf{v}_1$.

Exercise 1.3

Prove the "Dot Product Identity", Theorem (1.1).
Hint: Use Pythagoras' theorem for general triangles.

The angle between two vectors

In Python, the dot product is given by `numpy.dot` and as a consequence of the dot product identity, we have the code for the angle between two vectors:

$$\theta_{\mathbf{v}_1,\mathbf{v}_2} = \arccos\left(\frac{\mathbf{v}_1 \cdot \mathbf{v}_2}{|\mathbf{v}_1||\mathbf{v}_2|}\right).$$

Example 1.10

Find the angle between the vectors $\mathbf{v}_1 = (1, 2)$ and $\mathbf{v}_2 = (3, 4)$.

```
import numpy as np

def angle(u,v):
  a = np.dot(u,v)
  b = np.dot(u,u)
  c = np.dot(v,v)
  theta = np.arccos(a / np.sqrt(b*c))
  return np.degrees(theta)

v1 = np.array([1,2])
v2 = np.array([3,4])
print(angle(v1,v2)) #returns 10.304846468766044 in degree
```

Cauchy-Schwarz Inequality

Recall that $-1 \leq \cos\theta \leq 1$. Using the dot product identity, we obtain the important inequality:

Theorem 1.2 (Cauchy-Schwarz Inequality)

If u and v are any two vectors, then

$$-|u||v| \leq u \cdot v \leq |u||v|.$$

Exercise 1.4

Prove the "Cauchy-Schwarz Inequality".

2d linear equations system

Consider the homogeneous system

$$\begin{cases} ax + by = 0 \\ cx + dy = 0 \end{cases} \tag{1.1}$$

and let A be the 2×2 matrix

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{1.2}$$

$(x, y) = (-b, a)$ is a solution of the first equation in (1.1). If we want this to be a solution of the second equation as well, we must have $cx + dy = ad - bc = 0$.

Definition 1.8 (Determinant)

The determinant of A is

$$\det(A) = \det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = ad - bc.$$

2d linear equations system

Theorem 1.3 (Homogeneous System)

When $\det(A) = 0$*, the homogeneous system (1.1) has a nonzero solution, and all solutions are scalar multiples of* $(x, y) = (-b, a)$*. When* $\det(A) \neq 0$*, the only solution is* $(x, y) = (0, 0)$*.*

For the inhomogeneous case

$$\begin{cases} ax + by = e \\ cx + dy = f \end{cases} \tag{1.3}$$

we have

Theorem 1.4 (Inhomogeneous System)

When $\det(A) \neq 0$*, the inhomogeneous system (1.3) has the unique solution*

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{\det(A)} \begin{pmatrix} de - bf \\ af - ce \end{pmatrix}.$$

When $\det(A) = 0$*, (1.3) has a solution iff* $ce = af$ *and* $de = bf$*.*

2d linear equations system

When $a^2 + b^2 \neq 0$, a solution is

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{a^2 + b^2} \begin{pmatrix} ae \\ be \end{pmatrix}.$$

When $c^2 + d^2 \neq 0$, a solution is

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{c^2 + d^2} \begin{pmatrix} cf \\ df \end{pmatrix}.$$

Any other solution differs from these solutions by a scalar multiple of the homogeneous solution $(x, y) = (-b, a)$.

Exercise 1.5

Prove the Theorems (1.3) and (1.4).

Complex numbers

Roughly speaking, the set of all *complex numbers* is the set of all points in $\mathbb{R}^2$ with different multiplication rule.

Definition 1.9 (Complex numbers)

The complex numbers, $\mathbb{C}$*, is the set*

$$\mathbb{C} = \{(x, y) \in \mathbb{R}^2\}$$

with operations

- *Addition:* $(x_1, y_1) + (x_2, y_2) = (x_1 + x_2, y_1 + y_2)$.
- *Scalar Multiplication:* $t(x, y) = (tx, ty)$
- *Multiplication:* $(x_1, y_1)(x_2, y_2) = (x_1x_2 - y_1y_2, x_1y_2 + x_2y_1)$.

Then, in $\mathbb{C}$, we have

- zero: $0 = (0, 0)$.
- opposite or additive inverse: $-(x, y) = (-x, -y)$.
- one: $1 = (1, 0)$.

Example

Example 1.11

- $(1,2)+(3,4)=(4,6)$.
- $(0,0)+(1,2)=(1,2)$.
- $3(1,2)=(3,6)$.
- $(1,0)(1,2)=(1-0,2+0)=(1,2)$.
- $(1,2)(3,4)=(3-8,4+6)=(-5,10)$.
- $(x,0)+(y,0)=(x+y,0)$.
- $(x,0)(y,0)=(xy,0)$.

Note. By the last two examples, we see that complex numbers with 0 as their second component act like real numbers in addition and multiplication. So, from now on, we set $x=(x,0)$.

Example 1.12

- $0=(0,0)$.
- $1=(1,0)$.
- $-1=(-1,0)$.

Imaginary number

Definition 1.10 (Imaginary number)

$i = (0, 1).$

Note. Python uses the symbol j for imaginary number.

Theorem 1.5

For each $z = (x, y) \in \mathbb{C}$, we can write

$$z = x + iy.$$

We call x as the real part of z, and y the imaginary part of z.

$$x = Re(z), \quad y = Im(z).$$

Proof. $x + iy = (x, 0) + (0, 1)(y, 0) = (x, 0) + (0 - 0, 0 + y) = (x, y).$

Theorem 1.6

$i^2 = -1.$

Proof. $i^2 = (0, 1)(0, 1) = (0 - 1, 0 + 0) = (-1, 0) = -1.$

Example

Example 1.13

In complex numbers:

- $\sqrt{-1} = i.$
- $\sqrt{-4} = 2i.$
- $$\begin{aligned}(1,2)(3,4) &= (1+2i)(3+4i)\\ &= 3+4i+6i+8i^2\\ &= 3+10i-8\\ &= -5+10i\\ &= (-5,10).\end{aligned}$$
- $$\begin{aligned}(1,2)^3 &= (1+2i)^3\\ &= (1)^3+3(1)^2(2i)+3(1)(2i)^2+(2i)^3\\ &= 1+6i+12i^2+8i^3\\ &= 1+6i-12-8i\\ &= -11-2i\\ &= -(11,2).\end{aligned}$$

Conjugate

Definition 1.11 (Conjugate)

For $z = (x, y) \in \mathbb{C}$*, the conjugate is*

$$\bar{z} = (x, -y) = x - iy \in \mathbb{C}.$$

Some properties.

- $z + \bar{z} = 2Re(z)$, $z - \bar{z} = 2iIm(z)$.
- $z\bar{z} = Re(z)^2 + Im(z)^2$,

$$\Rightarrow |z| = \sqrt{Re(z)^2 + Im(z)^2} = \sqrt{z\bar{z}}$$

$$\Rightarrow |z|^2 = z\bar{z}.$$

Example 1.14

For $z = (4, -3) \in \mathbb{C}$:

- $\bar{z} = (4, 3) = 4 + 3i$,
- $z + \bar{z} = 2 \times 4 = 8$, $z - \bar{z} = 2i \times (-3) = -6i$.
- $z\bar{z} = (4)^2 + (-3)^2 = 16 + 9 = 25 \Rightarrow |z| = \sqrt{25} = 5$.
- $z^2 = (4 - 3i)^2 = 7 - 24i$.
- $|z|^2 = 25$.

Inverse

Theorem 1.7

For a non-zero $z \in \mathbb{C}$, the inverse of z is

$$z^{-1} = \frac{1}{z} = \frac{\bar{z}}{z\bar{z}} = \frac{\bar{z}}{|z|^2}.$$

Proof. Firstly, if $z = (x, y)$ then $\frac{1}{z} \in \mathbb{C}$, because,

$$\frac{1}{z} = \frac{x - iy}{x^2 + y^2} = (\frac{x}{x^2 + y^2}, \frac{-y}{x^2 + y^2}) \in \mathbb{C}.$$

Secondly,

$$zz^{-1} = (x + iy)\left(\frac{x - iy}{x^2 + y^2}\right) = \frac{x^2 + y^2}{x^2 + y^2} = 1.$$

Corollary 1.1 (Division)

For $z_1 \in \mathbb{C}$ and $0 \neq z_2 \in \mathbb{C}$

$$\frac{z_1}{z_2} = z_1 z_2^{-1}.$$

Definitions

Definition 1.12 (Mean-squared distance)

Let $x_1, x_2, \ldots, x_N$ *be a dataset, say* D, *in* $\mathbb{R}^d$, *and let* $x \in \mathbb{R}^d$. *The mean-square distance of* x *to* D *is*

$$MSD(x) = \frac{1}{N} \sum_{k=1}^{N} |x_k - x|^2.$$

Definition 1.13 (Mean)

Let $x_1, x_2, \ldots, x_N$ *be a dataset in* $\mathbb{R}^d$. *The mean or sample mean is*

$$m = \bar{x}_N = \frac{1}{N} \sum_{k=1}^{N} x_k = \frac{x_1 + x_2 + \cdots + x_N}{N}.$$

Theorem 1.8 (Point of Best-fit)

The mean is the point of best-fit: The mean minimizes the mean-squared distance to the dataset.

Exercise 1.6

Prove the Theorem (1.8).

Point of Best-fit

Example 1.15

```python
import matplotlib.pyplot as plt
import numpy as np

np.random.seed(1)
N = 20
dataset = np.array([ [np.random.random(),np.random.random()]
                                for _ in range(N) ])
# Mean
m = np.mean(dataset, axis=0)
#Random point
p = np.array([np.random.random(),np.random.random()])

plt.grid()
X, Y = dataset[:,0], dataset[:,1]
plt.scatter(X,Y)
for v in dataset:
    plt.plot([m[0],v[0]],[m[1],v[1]],c='green')
    plt.plot([p[0],v[0]],[p[1],v[1]],c='red')
plt.show()

# Comparison of MSD of the mean and a random point
MSD_m = np.sum(np.abs(dataset-m)**2)/N
MSD_p = np.sum(np.abs(dataset-p)**2)/N
print(MSD_m, MSD_p) # 0.160478187272121 0.5984208474157081
```

Point of Best-fit

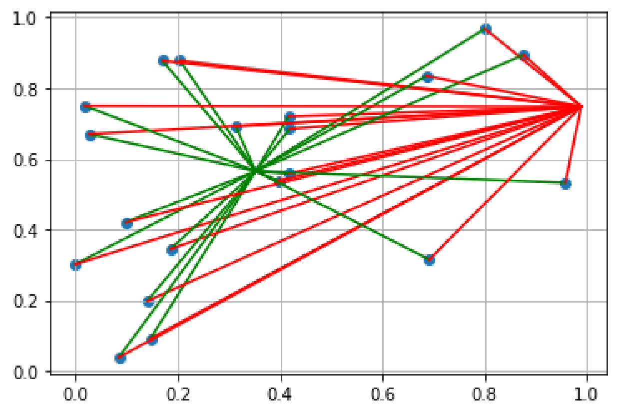


Figure 1.1: MSD for the mean (green) versus MSD for a random point (red).

Tensor product

For simplicity, let $u = (a, b)$ and $v = (c, d, e)$ be two vectors.

Definition 1.14 (Tensor product)

The tensor product of u and v is the matrix

$$u \otimes v = \begin{pmatrix} ac & ad & ae \\ bc & bd & be \end{pmatrix} = \begin{pmatrix} cu & du & eu \end{pmatrix} = \begin{pmatrix} av \\ bv \end{pmatrix}$$

Definition 1.15 (Trace of a matrix)

The trace of a squared matrix A is the sum of the diagonal entries.

Note. For any vectors u, v and w:

- $v \otimes u = (u \otimes v)^t$.

  In square case:
- $\det(u \otimes v) = 0$.
- $trace(u \otimes v) = u \cdot v$.
- $trace(u \otimes u) = |u|^2$.
- $(u \otimes v)w = (v \cdot w)u$.

Covariance

Let $x_1, x_2, \ldots, x_N$ be a dataset in $\mathbb{R}^d$ with m as its mean.

Definition 1.16 (1d Covariance)

When $d = 1$, the covariance q is a scalar

$$q = \frac{1}{N}\sum_{k=1}^{N}(x_k - m)^2 = MSD(m).$$

In the scalar case, the covariance is called the variance of the scalar dataset.

In general, the covariance is a symmetric $d \times d$ matrix Q. We can center the dataset as

$$v_1 = x_1 - m, v_2 = x_2 - m, \ldots, v_N = x_N - m.$$

Then the *covariance matrix* is the $d \times d$ matrix Q as

$$Q = \frac{v_1 \otimes v_1 + v_2 \otimes v_2 + \ldots + v_N \otimes v_N}{N}. \tag{1.4}$$

Example

Example 1.16

Suppose $N = 5$ and

$$x_1 = (1,2), \quad x_2 = (3,4), \quad x_3 = (5,6), \quad x_4 = (7,8), \quad x_5 = (9,10).$$

Then $m = (5,6)$ and

$$v_1 = x_1 - m = (-4,-4), \quad v_2 = x_2 - m = (-2,-2),$$
$$v_3 = x_3 - m = (0,0), \quad v_4 = x_4 - m = (2,2), \quad v_5 = x_5 - m = (4,4).$$

Since

$$(\pm 4, \pm 4) \otimes (\pm 4, \pm 4) = \begin{pmatrix} 16 & 16 \\ 16 & 16 \end{pmatrix},$$
$$(\pm 2, \pm 2) \otimes (\pm 2, \pm 2) = \begin{pmatrix} 4 & 4 \\ 4 & 4 \end{pmatrix},$$
$$(0,0) \otimes (0,0) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix},$$

then

$$Q = \begin{pmatrix} 8 & 8 \\ 8 & 8 \end{pmatrix}.$$

Example

Example 1.17

```
import numpy as np

def tensor(u,v):
  return np.array([ [ a*b for b in v] for a in u ])

np.random.seed(1)
N = 20
dataset = np.array([ [np.random.random(),np.random.random()] for _ in range(N) ])
# mean
m = np.mean(dataset,axis=0)
# center dataset
vectors = dataset - m
# covariance
Q = np.mean([ tensor(v,v) for v in vectors ],axis=0)
print(Q)
```

Standardized

Note. The covariance matrix as written in (1.4) is the *biased covariance matrix*. If the denominator is instead $N - 1$, the matrix is the *unbiased covariance matrix*.
For datasets with large N, it doesn't matter, since N and $N - 1$ are almost equal.

In `numpy`, the Python covariance constructor is

Example 1.18

```
import numpy as np

np.random.seed(1)
N = 20
dataset = np.array([ [np.random.random(),np.random.
                          random()] for _ in range(N
                          ) ])
# covariance
Q = np.cov(dataset,bias=True,rowvar=False)
print(Q)
```

Total variance

Definition 1.17 (Total variance)

From $trace(u \otimes u) = |u|^2$, *if* Q *is the covariance matrix then*

$$trace(Q) = \frac{1}{N} \sum_{k=1}^{N} |x_k - m|^2. \tag{1.5}$$

We call (1.5) the total variance of the dataset. Thus the total variance equals $MSD(m)$.

Example 1.19

```
import numpy as np

np.random.seed(1)
N = 20
dataset = np.array([ [np.random.random(),np.random.random()] for _ in range(N) ])
# covariance
Q = np.cov(dataset.T,bias=True)
print(Q.trace()) # returns 0.16047818727212101
```