Math for Data

Dr. S. M. Moosavi

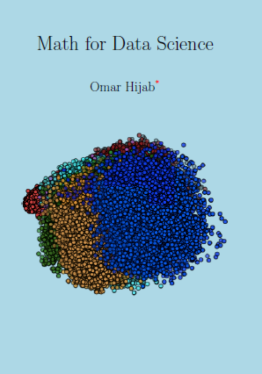
Mathematics for Data Science

Dr. S. M. Moosavi

smohsenmoosavi2009@gmail.com

September 9, 2024

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

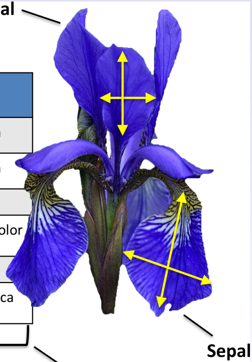
Sometimes one of the features is separated out as the label. In this case, the dataset is a labelled dataset.

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



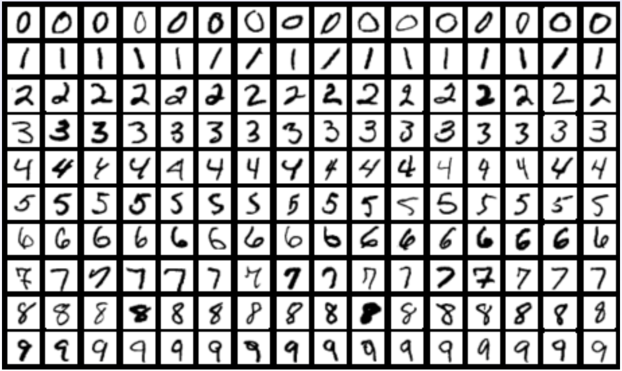
Class labels
(targets)

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.



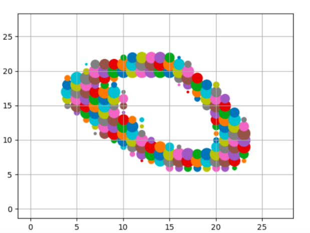
Exercises

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.

Math for Data

Dr. S. M. Moosavi

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 $\mathbf{0}$ $(\mathbf{0} + v = v)$;*
5. *vectors v have negatives (or opposites) $-v$ $(v + (-v) = \mathbf{0})$;*
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 $0v = \mathbf{0}$;*
9. *$r(sv) = (rs)v$.*

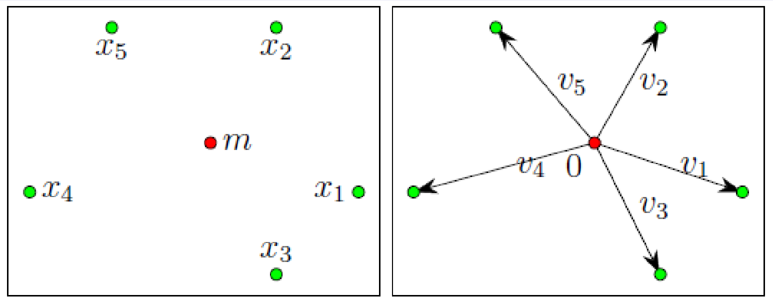
Centered dataset

Definition 1.5 (Centered Versus Non-Centered)

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

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

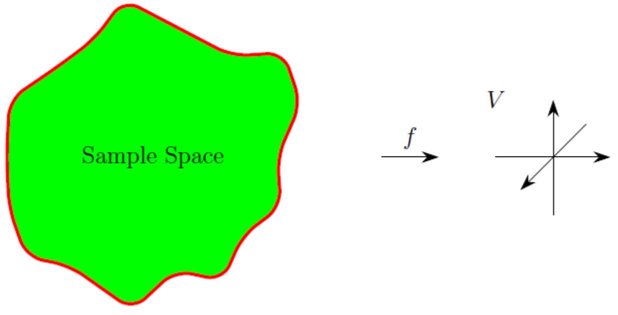
then $v_1, v_2, \cdots, v_N$ *is a centered dataset of vectors where its mean is zero.*



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 over $\mathbb{Q}$ but not over $\mathbb{R}$.
- 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



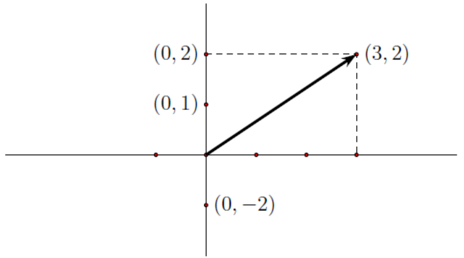
In general, a statistic need not be a number. A statistic can be anything that "behaves like a number". For example, $f(\text{item})$ can be a vector or a matrix. More generally, a statistic's values may be anything that lives in a vector space V.

Math for Data

Dr. S. M. Moosavi

Cartesian plane

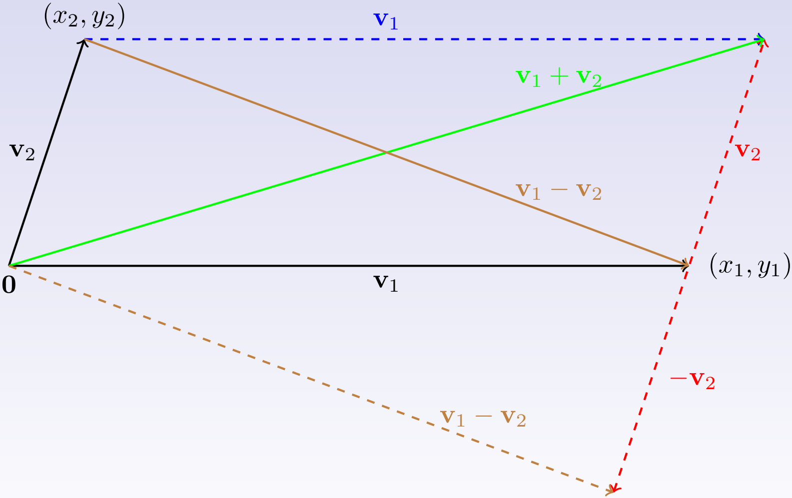
The *cartesian plane* $\mathbb{R}^2$, also called the 2-dimensional real space is a vector space.



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

```
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

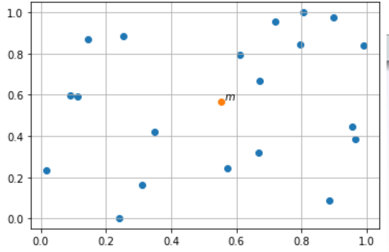
```python
import numpy as np

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 $\mathbf{v}_2 = (3, 4)$

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

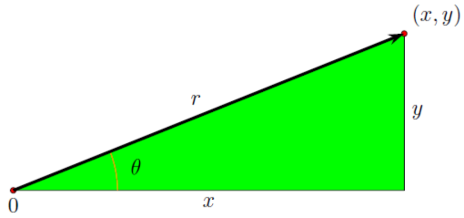
$$|\mathbf{v}_1 - \mathbf{v}_2| = \sqrt{(1-3)^2 + (2-4)^2} = \sqrt{4+4} = \sqrt{8} \simeq 2.828.$$

```python
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 $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ be a dataset, say D, in $\mathbb{R}^d$, and let $\mathbf{x} \in \mathbb{R}^d$. The mean-squared distance of $\mathbf{x}$ to D is

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

Definition 1.13 (Mean)

Let $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ be a dataset in $\mathbb{R}^d$. The mean or sample mean is

$$\mathbf{m} = \bar{\mathbf{x}}_N = \frac{1}{N} \sum_{k=1}^{N} \mathbf{x}_k = \frac{\mathbf{x}_1 + \mathbf{x}_2 + \cdots + \mathbf{x}_N}{N}.$$

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

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

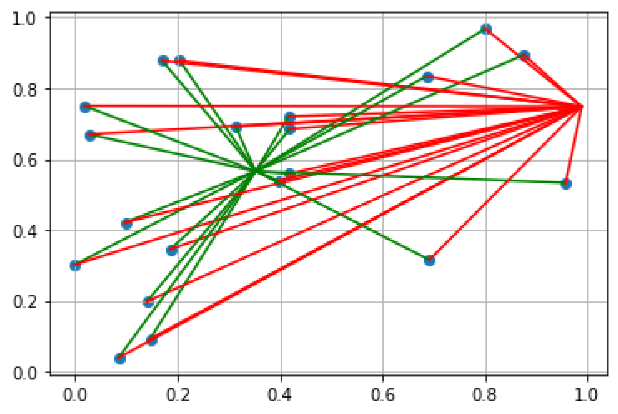


Figure 1.1: MSD for the mean (green) versus MSD for a random point (red).

Tensor product

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

Definition 1.14 (Tensor product)

The tensor product of $\mathbf{u}$ *and* **text** *is the matrix*

$$\mathbf{u} \otimes \mathbf{v} = \begin{pmatrix} ac & ad & ae \\ bc & bd & be \end{pmatrix} = \begin{pmatrix} c\mathbf{u} & d\mathbf{u} & e\mathbf{u} \end{pmatrix} = \begin{pmatrix} a\mathbf{v} \\ b\mathbf{v} \end{pmatrix}$$

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 $\mathbf{u}, \mathbf{v}$ and $\mathbf{w}$:

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

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

Covariance

Let $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ be a dataset in $\mathbb{R}^d$ with $\mathbf{m}$ 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

$$\mathbf{v}_1 = \mathbf{x}_1 - \mathbf{m}, \mathbf{v}_2 = \mathbf{x}_2 - \mathbf{m}, \ldots, \mathbf{v}_N = \mathbf{x}_N - \mathbf{m}.$$

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

$$Q = \frac{\mathbf{v}_1 \otimes \mathbf{v}_1 + \mathbf{v}_2 \otimes \mathbf{v}_2 + \ldots + \mathbf{v}_N \otimes \mathbf{v}_N}{N}. \tag{1.4}$$

Example

Example 1.16

Suppose $N = 5$ and

$$\mathbf{x}_1 = (1, 2), \quad \mathbf{x}_2 = (3, 4), \quad \mathbf{x}_3 = (5, 6), \quad \mathbf{x}_4 = (7, 8), \quad \mathbf{x}_5 = (9, 10).$$

Then $m = (5, 6)$ and

$$\mathbf{v}_1 = \mathbf{x}_1 - \mathbf{m} = (-4, -4), \quad \mathbf{v}_2 = \mathbf{x}_2 - \mathbf{m} = (-2, -2),$$
$$\mathbf{v}_3 = \mathbf{x}_3 - \mathbf{m} = (0, 0), \quad \mathbf{v}_4 = \mathbf{x}_4 - \mathbf{m} = (2, 2), \quad \mathbf{v}_5 = \mathbf{x}_5 - \mathbf{m} = (4, 4).$$

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

```python
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
rnd = np.random.random
dataset = np.array([[rnd(), rnd()] 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

```python
import numpy as np

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

Total variance

Definition 1.17 (Total variance)

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

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

We call (1.5) the total variance of the dataset. Thus the total variance equals $MSD(\mathbf{m})$*.*

Example 1.19

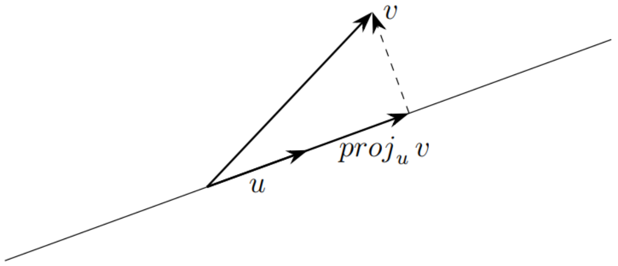
```python
import numpy as np

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

Math for Data

Dr. S. M. Moosavi

Projections

We would like to project a $2d$ dataset onto a line. Let $\mathbf{u}$ be a unit vector (a vector of length one, $|\mathbf{u}| = 1$), and let $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ be a $2d$ dataset, assumed for simplicity to be centered. We wish to project this dataset onto the line through $\mathbf{u}$. This will result in a $1d$ dataset.



When a vector $\mathbf{v}$ is projected onto the line through $\mathbf{u}$, the length of the projected vector reads

$$|proj_{\mathbf{u}}\mathbf{v}| = |\mathbf{v}| \cos\theta,$$

where θ is the angle between the vectors $\mathbf{v}$ and $\mathbf{u}$. Since $|\mathbf{u}| = 1$, this length equals the dot product $\mathbf{v} \cdot \mathbf{u}$. Hence the projected vector is

$$proj_{\mathbf{u}}\mathbf{v} = (\mathbf{v} \cdot \mathbf{u})\mathbf{u}.$$

Projections

Hence,

Definition 1.18 (Reduced dataset)

The projected dataset of $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ onto the line through $\mathbf{u}$ is the dataset

$$(\mathbf{v}_1 \cdot \mathbf{u})\mathbf{u}, (\mathbf{v}_2 \cdot \mathbf{u})\mathbf{u}, \ldots (\mathbf{v}_N \cdot \mathbf{u})\mathbf{u}.$$

The projected datasetc is in $\mathbb{R}^2$. The reduced dataset is

$$(\mathbf{v}_1 \cdot \mathbf{u}), (\mathbf{v}_2 \cdot \mathbf{u}), \ldots (\mathbf{v}_N \cdot \mathbf{u}),$$

which is in $\mathbb{R}$.

Exercise 1.7

Show that when a $2d$ dataset is centered then the mean of the reduced dataset is 0.

Exercise 1.8

Prove that if Q is the covariance matrix of a $2d$ dataset, then the variance of the projected dataset onto the line through the vector $\mathbf{u}$ equals the quadratic function $\mathbf{u} \cdot Q\mathbf{u}$:

$$q = \frac{1}{N} \sum_{k=1}^{N} \mathbf{u} \cdot (\mathbf{v}_k \otimes \mathbf{v}_k)\mathbf{u} = \mathbf{u} \cdot Q\mathbf{u}.$$

Covariance ellipse

Hence,

Definition 1.19 (Covariance ellipse)

The contour of all points $\mathbf{x}$ satisfying $\mathbf{x} \cdot Q\mathbf{x} = 1$ is the covariance ellipsoid. In two dimensions $d = 2$, this is the covariance ellipse. The contour of all points $\mathbf{x}$ satisfying $\mathbf{x} \cdot Q^{-1}\mathbf{x} = 1$ is the inverse covariance ellipsoid. In two dimensions $d = 2$, this is the inverse covariance ellipse.

In two dimensions $d = 2$, a covariance matrix has the form

$$Q = \begin{pmatrix} a & b \\ b & c \end{pmatrix}.$$

If we write $\mathbf{u} = (x, y)$ for a vector in the plane, the covariance ellipse is

$$\mathbf{u} \cdot Q\mathbf{u} = (x, y) \cdot \begin{pmatrix} a & b \\ b & c \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = ax^2 + 2bxy + cy^2 = 1.$$

The covariance ellipse and inverse covariance ellipses described above are centered at the origin $(0, 0)$. When a dataset has mean $\mathbf{m}$ and covariance Q, the ellipses are drawn centered at $\mathbf{m}$.

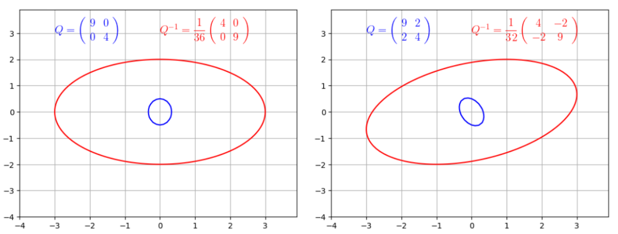
In particular, when $a = c$ and $b = 0$, then $Q = aI$ is a multiple of the identity, the inverse covariance ellipse is the circle of radius $\sqrt{a}$, and the covariance ellipse is the circle of radius $\frac{1}{\sqrt{a}}$.

Covariance ellipse I

Example 1.20

Plot the contour ellipses for

$$Q_1 = \begin{pmatrix} 9 & 0 \\ 0 & 4 \end{pmatrix}, \quad Q_2 = \begin{pmatrix} 9 & 2 \\ 2 & 4 \end{pmatrix}.$$



Covariance ellipse II

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

def ellipse(a, b, c, levels, color):
  L, delta = 4, .1
  x = np.arange(-L,L,delta)
  y = np.arange(-L,L,delta)
  X,Y = np.meshgrid(x, y)
  plt.contour(X, Y, a*X**2 + 2*b*X*Y + c*Y**2, levels, colors=color)

# Q1 Covariance entities
a, b, c = 9, 0, 4

# Inverse Covariance entities
det = a*c - b**2
A, B, C = c/det, -b/det, a/det

plt.grid()
ellipse(a, b, c, [20], 'blue')
ellipse(A, B, C, [1], 'red')
plt.show()
```

Math for Data

Dr. S. M. Moosavi

Covariance ellipse III

```

# Q2 Covariance entities
a, b, c = 9, 2, 4

# Inverse Covariance entities
det = a*c - b**2
A, B, C = c/det, -b/det, a/det

plt.grid()
ellipse(a, b, c, [1], 'blue')
ellipse(A, B, C, [1], 'red')
plt.show()
```

Standardization

Here, we describe how to standardize datasets in $\mathbb{R}^2$. *Standardizing* the dataset means to center the dataset and to place the x and y features on the same scale.

Consider the dataset $\mathbf{x}_1 = (x_1, y_1), \mathbf{x}_2 = (x_2, y_2), \ldots, \mathbf{x}_N = (x_N, y_N)$ with mean $\mathbf{m} = (m_x, m_y)$. Then the covariance matrix is

$$Q = \begin{pmatrix} a & b \\ b & c \end{pmatrix},$$

where

$$a = \frac{1}{N}\sum_{k=1}^{N}(x_k - m_x)^2, \quad b = \frac{1}{N}\sum_{k=1}^{N}(x_k - m_x)(y_k - m_y),$$

$$c = \frac{1}{N}\sum_{k=1}^{N}(y_k - m_y)^2.$$

Standardization

If a and c differ, the different scales of x's and y's distorts the relation between them, and b may not accurately reflect the correlation. To correct for this, we center and re-scale

$$x_1, x_2, \dots, x_N \to x_1' = \frac{x_1 - m_x}{\sqrt{a}}, x_2' = \frac{x_2 - m_x}{\sqrt{a}}, \dots, x_N' = \frac{x_N - m_x}{\sqrt{a}}$$

and

$$y_1, y_2, \dots, y_N \to y_1' = \frac{y_1 - m_y}{\sqrt{c}}, y_2' = \frac{y_2 - m_y}{\sqrt{c}}, \dots, y_N' = \frac{y_N - m_y}{\sqrt{c}}$$

This results in a new dataset

$\mathbf{v}_1 = (x_1', y_1'), \mathbf{v}_2 = (x_2', y_2'), \dots, \mathbf{v}_N = (x_N', y_N')$ that is centered:

$$\frac{\mathbf{v}_1 + \mathbf{v}_2 + \dots + \mathbf{v}_N}{N} = 0,$$

with each feature standardized to have unit variance,

$$\frac{1}{N}\sum_{k=1}^{N} x_k' = 1, \quad \frac{1}{N}\sum_{k=1}^{N} y_k' = 1.$$

This is the *standardized dataset*.

Standardization

The covariance matrix of the standardized dataset has the form

$$Q' = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix},$$

where

$$\rho = \frac{1}{N}\sum_{k=1}^{N} x'_k y'_k = \frac{b}{\sqrt{ac}} = \frac{\sum_{k=1}^{N}(x_k - m_x)(y_k - m_y)}{\sqrt{\left(\sum_{k=1}^{N}(x_k - m_x)^2\right)\left(\sum_{k=1}^{N}(y_k - m_y)^2\right)}}$$

is the *Pearson correlation coefficient* of the dataset. The matrix Q' is the *correlation matrix*, or the *standardized covariance matrix*.

Example 1.21

$$Q = \begin{pmatrix} 9 & 2 \\ 2 & 4 \end{pmatrix} \quad \Rightarrow \quad \rho = \frac{b}{\sqrt{ac}} = \frac{1}{3} \quad \Rightarrow \quad Q' = \begin{pmatrix} 1 & 1/3 \\ 1/3 & 1 \end{pmatrix}.$$

Standardization

From the Cauchy-Schwarz inequality, the correlation coefficient ρ is always between -1 and 1 . When $\rho = \pm 1$, the dataset samples are perfectly correlated and lie on a line passing through the mean. When $\rho = 1$, the line has slope 1, and when $\rho = -1$, the line has slope -1. When $\rho = 0$, the dataset samples are completely uncorrelated and are considered two independent one-dimensional datasets (In standardized case).

In Python numpy, the correlation matrix is returned by

```
import numpy as np
np.corrcoef(dataset.T)
```

Here again, we input the transpose of the dataset if our default is vectors as rows.

Notice the $1/N$ cancels in the definition of ρ. Because of this, corrcoef is the same whether we deal with biased or unbiased covariance matrices.

Math for Data

Dr. S. M. Moosavi

Outline

Introduction

Definition 2.1

A matrix is a listing arranged in a rectangle of rows and columns. Specifically, an $N \times d$ *matrix* A *has* N *rows and* d *columns,*

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1d} \\ a_{21} & a_{22} & \dots & a_{2d} \\ \vdots & \vdots & \dots & \vdots \\ a_{N1} & a_{N2} & \dots & a_{Nd} \end{pmatrix}$$

The transpose of A *is*

$$A^t = \begin{pmatrix} a_{11} & a_{21} & \dots & a_{N1} \\ a_{12} & a_{22} & \dots & a_{N2} \\ \vdots & \vdots & \dots & \vdots \\ a_{1d} & a_{2d} & \dots & a_{Nd} \end{pmatrix}$$

Introduction

Example 2.1

$$A = \begin{pmatrix} 1 & 6 & 11 \\ 2 & 7 & 12 \\ 3 & 8 & 13 \\ 4 & 9 & 14 \\ 5 & 10 & 15 \end{pmatrix} \Rightarrow A^t = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 6 & 7 & 8 & 9 & 10 \\ 11 & 12 & 13 & 14 & 15 \end{pmatrix}.$$

```python
import numpy as np

A = np.array([[1,6,11],[2,7,12],[3,8,13],[4,9,14],[5,10,15]])
print(A)
print(A.shape)
print(len(A))
print(A[1])
print(A[1,2])
print(A[1:3])

# transpose
A_t = np.transpose(A)
print(A_t)
print(A_t.shape)
print(len(A_t))
print(A_t[1])
print(A_t[1,2])
print(A_t[1:3])
```

Introduction

Definition 2.2

A d-dimensional vector $\mathbf{v}$ may be written as a $1 \times d$ matrix

$$\mathbf{v} = \begin{pmatrix} t_1 & t_2 & \cdots & t_d \end{pmatrix}.$$

In this case, we call $\mathbf{v}$ a row vector.

Definition 2.3

An N-dimensional vector $\mathbf{v}$ may be written as an $N \times 1$ matrix

$$\mathbf{v} = \begin{pmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{pmatrix}.$$

In this case, we call $\mathbf{v}$ a column vector.

Introduction

Vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_d$ with the same dimension may be stacked as columns (`np.column_stack` in `Python`) of a matrix,

$$A = \begin{pmatrix} \mathbf{v}_1 & \mathbf{v}_2 & \cdots & \mathbf{v}_d \end{pmatrix}.$$

Similarly, vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ with the same dimension may be stacked as rows (`np.row_stack` in `Python`) of a matrix,

$$A = \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \vdots \\ \mathbf{v}_N \end{pmatrix}.$$

Introduction

Example 2.2

The row stack of $\mathbf{v}_1 = (1, 6, 11)$, $\mathbf{v}_2 = (2, 7, 12)$, $\mathbf{v}_3 = (3, 8, 13)$, $\mathbf{v}_4 = (4, 9, 14)$ and $\mathbf{v}_5 = (5, 10, 15)$ reads:

$$A = \begin{pmatrix} 1 & 6 & 11 \\ 2 & 7 & 12 \\ 3 & 8 & 13 \\ 4 & 9 & 14 \\ 5 & 10 & 15 \end{pmatrix},$$

and the column stack of them is:

$$A^t = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 6 & 7 & 8 & 9 & 10 \\ 11 & 12 & 13 & 14 & 15 \end{pmatrix}.$$

```python
import numpy as np

v1 = [1,6,11]
v2 = [2,7,12]
v3 = [3,8,13]
v4 = [4,9,14]
v5 = [5,10,15]
A = np.row_stack((v1,v2,v3,v4,v5))
print(A)
A_t = np.column_stack((v1,v2,v3,v4,v5))
print(A_t)
```

Introduction

Definition 2.4

A matrix is square if the number of rows equals the number of columns.

Definition 2.5

A matrix is diagonal if the off-diagonal entities are zero.

Example 2.3

The matrix

$$\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{pmatrix},$$

is square and diagonal.
The following matrices are not square but they are diagonal:

$$\begin{pmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \end{pmatrix}, \quad \begin{pmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \\ 0 & 0 & 0 \end{pmatrix}.$$

Datasets

Definition 2.6

A dataset is a collection of points $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ *in* $\mathbb{R}^d$*. After centering the mean to the origin, the dataset becomes a collection of vectors* $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$*. Usually the vectors are presented as the rows of an* $N \times d$ *matrix* A*.*

Corresponding to this, datasets are often provided as a CSV file. The matrix A is the dataset matrix. In excel, this is called a spreadsheet. In SQL, this is called a table. In `numpy`, it's an array. In `pandas`, it's a dataframe. So, effectively,

matrix = dataset = CSV file = spreadsheet = table = array = dataframe

Datasets

Example 2.4

For the Iris dataset:

```python
import numpy as np
import pandas as pd
from sklearn import datasets

iris = datasets.load_iris()

# The dataset
dataset = iris["data"]

# To center the dataset
m = np.mean(dataset,axis=0)
vectors = dataset - m

# To make a data frame
centered_df = pd.DataFrame(data=vectors)
```

Addition & scalar multiplication

Matrices consisting of numbers are added and multiplied by scalars as follows. With t as an scalar and the matrices

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1d} \\ a_{21} & a_{22} & \dots & a_{2d} \\ \vdots & \vdots & \dots & \vdots \\ a_{N1} & a_{N2} & \dots & a_{Nd} \end{pmatrix} \quad \text{and} \quad A' = \begin{pmatrix} a'_{11} & a'_{12} & \dots & a'_{1d} \\ a'_{21} & a'_{22} & \dots & a'_{2d} \\ \vdots & \vdots & \dots & \vdots \\ a'_{N1} & a'_{N2} & \dots & a'_{Nd} \end{pmatrix}$$

we have

$$A + A' = \begin{pmatrix} a_{11} + a'_{11} & a_{12} + a'_{12} & \dots & a_{1d} + a'_{1d} \\ a_{21} + a'_{21} & a_{22} + a'_{22} & \dots & a_{2d} + a'_{2d} \\ \vdots & \vdots & \dots & \vdots \\ a_{N1} + a'_{N1} & a_{N2} + a'_{N2} & \dots & a_{Nd} + a'_{Nd} \end{pmatrix},$$

and

$$tA = \begin{pmatrix} ta_{11} & ta_{12} & \dots & ta_{1d} \\ ta_{21} & ta_{22} & \dots & ta_{2d} \\ \vdots & \vdots & \dots & \vdots \\ ta_{N1} & ta_{N2} & \dots & ta_{Nd} \end{pmatrix}.$$

Matrices may be added only if they have the same shape.

Addition & scalar multiplication

Example 2.5

```
import numpy as np

A = np.zeros((4,3))
print(A)
B = np.eye(3)
print(B)
C = np.eye(4,3)
print(C)
D = np.array([[1,2,3],[4,5,6],[7,8,9],[10,11,12]])
print(D)
E = np.diag([1,2,3,4])
print(E)

print(A+C)
print(C+D)
print(4*D)
print(-D)
print(-2*D)
```

Introduction

Let t be a scalar, $\mathbf{u}, \mathbf{v}, \mathbf{w}$ be vectors, and let A, B be matrices. We already know how to compute $t\mathbf{u}$, $t\mathbf{v}$, and tA, tB. In this section, we compute the *dot product* $\mathbf{u} \cdot \mathbf{v}$, the *matrix-vector product* $A\mathbf{v}$, and the *matrix-matrix product* AB.

Dot product

In the first chapter, we defined the dot product in two dimensions. We now generalize it to any dimension d. Suppose $\mathbf{u}, \mathbf{v}$ are vectors in $\mathbb{R}^d$. Then their dot product $\mathbf{u} \cdot \mathbf{v}$ is the scalar obtained by multiplying corresponding features and then summing the products. This only works if the dimensions of $\mathbf{u}$ and $\mathbf{v}$ agree.

In other words, if $\mathbf{u} = (u_1, u_2, \ldots, u_d)$ and $\mathbf{v} = (v_1, v_2, \ldots, v_d)$, then

$$\mathbf{u} \cdot \mathbf{v} = u_1 v_1 + u_2 v_2 + \ldots + u_d v_d.$$

It's best to think of this as "row-times-column" multiplication,

$$\mathbf{u} \cdot \mathbf{v} = \begin{pmatrix} u_1 & u_2 & \cdots & u_d \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_d \end{pmatrix} = u_1 v_1 + u_2 v_2 + \ldots + u_d v_d.$$

Dot product

Example 2.6

In Python, calculate the dot product of $\mathbf{u} = (1, 2, 3)$ and $\mathbf{v} = (4, 5, 6)$.

```python
import numpy as np

u = np.array([1,2,3])
v = np.array([4, 5, 6])

u_dot_v = np.dot(u,v)
print(u_dot_v)

u_dot_v_ = u[0]*v[0] + u[1]*v[1] + u[2]*v[2]
print(u_dot_v_)

print(u_dot_v == u_dot_v_)
```

Dot product

As we mentioned in 2 dimensions, we have the following generalizations in d dimension:

Definition 2.7

The length or norm or magnitude of a vector $\mathbf{v}$ *is the square root of the dot product* $\mathbf{v} \cdot \mathbf{v}$,

$$|\mathbf{v}| = \sqrt{\mathbf{v} \cdot \mathbf{v}}$$

Theorem 2.1 (Dot Product)

The dot product $\mathbf{u} \cdot \mathbf{v}$ *satisfies*

$$\mathbf{u} \cdot \mathbf{v} = |\mathbf{u}||\mathbf{v}| \cos\theta,$$

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

Corollary 2.1

To calculate the angle θ *between* $\mathbf{u}$ *and* $\mathbf{v}$ *we have:*

$$\cos\theta = \frac{\mathbf{u} \cdot \mathbf{v}}{\sqrt{|\mathbf{u}||\mathbf{v}|}} = \frac{\mathbf{u} \cdot \mathbf{v}}{\sqrt{(\mathbf{u} \cdot \mathbf{u})(\mathbf{v} \cdot \mathbf{v})}}.$$

Dot product

Corollary 2.2 (Cauchy-Schwarz Inequality)

The dot product of two vectors is absolutely less or equal to the product of their lengths,

$$|\mathbf{u} \cdot \mathbf{v}| \leq |\mathbf{u}||\mathbf{v}| \quad \textit{or} \quad |\mathbf{u} \cdot \mathbf{v}| \leq (\mathbf{u} \cdot \mathbf{u})(\mathbf{v} \cdot \mathbf{v}).$$

Definition 2.8

Vectors $\mathbf{u}$ and $\mathbf{v}$ are said to be perpendicular or orthogonal if $|\mathbf{u} \cdot \mathbf{v}| = 0$. A collection of vectors is orthogonal if any pair of vectors in the collection are orthogonal.

Vectors $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ are said to be orthonormal if they are both unit vectors and orthogonal.

Exercise 2.1

The zero vector is orthogonal to every vector. The converse is true as well: if a vector is orthogonal to every vector then it is the zero vector.

Matrix-vector product

Definition 2.9

Suppose $\mathbf{v}$ is a vector and A is a matrix. If the rows of A have the same dimension as that of $\mathbf{v}$, we can take the dot product of each row of A with $\mathbf{v}$, obtaining the matrix-vector product $A\mathbf{v}$: $A\mathbf{v}$ is the vector whose features are the dot products of the rows of A with $\mathbf{v}$.

Note:

- In Python we use again `np.dot(A,v)` for matrix-vector product.
- If $\mathbf{u}$ and $\mathbf{v}$ are vectors, we can think of $\mathbf{u}$ as a row vector, or a matrix consisting of a single row. With this interpretation, the matrix-vector product $\mathbf{u}\mathbf{v}$ equals the dot product $\mathbf{u} \cdot \mathbf{v}$.
- If $\mathbf{u}$ and $\mathbf{v}$ are vectors, we can think of $\mathbf{u}$ as a column vector, or a matrix consisting of a single column. With this interpretation, $\mathbf{u}^t$ is a single row, and the matrix-vector product $\mathbf{u}^t\mathbf{v}$ equals the dot product $\mathbf{u} \cdot \mathbf{v}$.
- $(A\mathbf{v})^t = \mathbf{v}^t A^t$.
- $(A\mathbf{u}) \cdot \mathbf{v} = \mathbf{u} \cdot (A^t\mathbf{v})$.

Matrix-vector product

Example 2.7

Calculate $A\mathbf{v}$, when

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{pmatrix} \quad \text{and} \quad \mathbf{v} = (1, 2, 3, 4).$$

Answer:

$$A\mathbf{v} = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}$$

$$= \begin{pmatrix} (1 \times 1) + (2 \times 2) + (3 \times 3) + (4 \times 4) \\ (5 \times 1) + (6 \times 2) + (7 \times 3) + (8 \times 4) \\ (9 \times 1) + (10 \times 2) + (11 \times 3) + (12 \times 4) \end{pmatrix} = \begin{pmatrix} 30 \\ 70 \\ 110 \end{pmatrix}$$

```python
import numpy as np

A = np.arange(1,13).reshape(3,4)
v = np.array([1,2,3,4])

Av = np.dot(A, v)
print(Av)
```

Matrix-matrix product

Definition 2.10

Let A and B be two matrices. If the row dimension of A equals the column dimension of B, the matrix-matrix product AB is defined. When this condition holds, the entries in the matrix AB are the dot products of the rows of A with the columns of B.

Note:

- In Python we use again `np.dot(A,B)` for matrix-vector product.
- $(AB)^t = B^t A^t$.

Matrix-vector product

Example 2.8

Calculate AB, when

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 13 & 14 \\ 15 & 16 \\ 17 & 18 \\ 19 & 20 \end{pmatrix}.$$

Answer:

$$AB = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{pmatrix} \begin{pmatrix} 13 & 14 \\ 15 & 16 \\ 17 & 18 \\ 19 & 20 \end{pmatrix}$$

$$= \begin{pmatrix} (1 \times 13) + (2 \times 15) + (3 \times 17) + (4 \times 19) & (1 \times 14) + (2 \times 16) + (3 \times 18) + (4 \times 20) \\ (5 \times 13) + (6 \times 15) + (7 \times 17) + (8 \times 19) & (5 \times 14) + (6 \times 16) + (7 \times 18) + (8 \times 20) \\ (9 \times 13) + (10 \times 15) + (11 \times 17) + (12 \times 19) & (9 \times 14) + (10 \times 16) + (11 \times 18) + (12 \times 20) \end{pmatrix}$$

$$= \begin{pmatrix} 170 & 180 \\ 426 & 452 \\ 682 & 724 \end{pmatrix}$$

```python
import numpy as np

A = np.arange(1,13).reshape(3,4)
B = np.arange(13,21).reshape(4,2)

AB = np.dot(A, B)
print(AB)
```

Orthonormal Rows and Columns

Assume the rows of a matrix A are $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$. Since matrix-matrix multiplication is $row \times column$, we have

$$AA^t = \begin{pmatrix} \mathbf{v}_1 \cdot \mathbf{v}_1 & \mathbf{v}_1 \cdot \mathbf{v}_2 & \cdots & \mathbf{v}_1 \cdot \mathbf{v}_N \\ \mathbf{v}_2 \cdot \mathbf{v}_1 & \mathbf{v}_2 \cdot \mathbf{v}_2 & \cdots & \mathbf{v}_2 \cdot \mathbf{v}_N \\ \vdots & \vdots & & \vdots \\ \mathbf{v}_N \cdot \mathbf{v}_1 & \mathbf{v}_N \cdot \mathbf{v}_2 & \cdots & \mathbf{v}_N \cdot \mathbf{v}_N \end{pmatrix}.$$

Corollary 2.3

Let U be a matrix.

- *U has orthonormal rows iff $UU^t = I$.*
- *U has orthonormal columns iff $U^tU = I$.*

Tensor product

Definition 2.11

If $\mathbf{u}$ and $\mathbf{v}$ are vectors, the tensor product $\mathbf{u} \otimes \mathbf{v}$ is the matrix-matrix product $\mathbf{u}^t\mathbf{v}$, with $\mathbf{u}$ and $\mathbf{v}$ row vectors. If $\mathbf{u}$ is N-dimensional and $\mathbf{v}$ is d-dimensional, then $\mathbf{u} \otimes \mathbf{v}$ is an $N \times d$ matrix.

Example 2.9

if $\mathbf{u} = (a, b, c)$ and $\mathbf{v}(\alpha, \beta)$, then

$$\mathbf{u} \otimes \mathbf{v} = \begin{pmatrix} a \\ b \\ c \end{pmatrix} \begin{pmatrix} \alpha & \beta \end{pmatrix} = \begin{pmatrix} a\alpha & a\beta \\ b\alpha & b\beta \\ c\alpha & c\beta \end{pmatrix}.$$

Using the tensor product, we have

Theorem 2.2 (Tensor Identity)

Let A be a matrix with rows $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$. Then

$$A^tA = \mathbf{v}_1 \otimes \mathbf{v}_1 + \mathbf{v}_2 \otimes \mathbf{v}_2 + \cdots + \mathbf{v}_N \otimes \mathbf{v}_N.$$

Exercise 2.2

Prove the tensor identity.

Some definitions

Definition 2.12

A matrix Q is symmetric if $Q = Q^t$.
For any matrix A, $Q = AA^t$ and $Q = A^tA$ are symmetric.
A symmetric matrix Q satisfying $\mathbf{v} \cdot Q\mathbf{v} \geq 0$ for every vector $\mathbf{v}$ is nonnegative.
A symmetric matrix Q satisfying $\mathbf{v} \cdot Q\mathbf{v} > 0$ for every nonzero vector $\mathbf{v}$ is positive.

Definition 2.13

The trace of a square matrix is the sum of its diagonal elements.

Even though in general $AB \neq BA$, it is always true that

Exercise 2.3

$trace(AB) = trace(BA)$.

Exercise 2.4

$\mathbf{u} \cdot Q\mathbf{v} = trace(Q(\mathbf{v} \otimes \mathbf{u}))$.

Norm squared

Definition 2.14

If $A = (a_{ij})$ *is any matrix, then the norm squared of* A *is*

$$\| A \|^2 = \sum_{i,j} a_{ij}^2 .$$

Theorem 2.3 (Norm Squared of Matrix)

Let A *be a matrix with rows* $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$. *Then*

$$\| A \|^2 = |\mathbf{v}_1|^2 + |\mathbf{v}_2|^2 + \ldots + |\mathbf{v}_N|^2,$$

and

$$\| A \|^2 = trace(A^t A).$$

Exercise 2.5

Prove Theorem (2.3).

Iris

If $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ is a dataset of points in $\mathbb{R}^d$ with mean m, and $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$ is the corresponding centered dataset, then we saw that the covariance matrix Q is the average of tensor products

$$Q = \frac{\mathbf{v}_1 \otimes \mathbf{v}_1 + \mathbf{v}_2 \otimes \mathbf{v}_2 + \cdots + \mathbf{v}_N \otimes \mathbf{v}_N}{N}.$$

Let A be the matrix with rows $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$. By Theorem (2.2), the last equation is the same as

$$Q = \frac{1}{N} A^t A.$$

Iris

Example 2.10

Calculate the mean, covariance and total variance of the Iris dataset.

```python
import numpy as np
from sklearn import datasets

iris = datasets.load_iris()

# The dataset
dataset = iris["data"]

# Mean
m = np.mean(dataset, axis=0)

# Centered dataset
vectors = dataset - m

# Covariance
N = len(vectors)
#   Biased
Q = np.dot(vectors.T, vectors)/N
Q = np.cov(dataset, rowvar=False, ddof=0) # ddof = delta degrees of freedom
Q = np.cov(dataset.T, ddof=0)

#   Unbiased
Q = np.dot(vectors.T, vectors)/(N-1)
Q = np.cov(dataset, rowvar=False)
Q = np.cov(dataset.T)

# Total Variance
TV = np.trace(Q)
```

Standardized dataset

Let $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ is a dataset of points in $\mathbb{R}^d$. Each sample point $\mathbf{x}$ has d features $(t_1, t_2, \ldots, t_d)$. We compute the variance of each feature separately.

Let $\mathbf{e}_1, e_2, \ldots, e_d$ be the standard basis in $\mathbb{R}^d$, and, for each $j = 1, 2, \ldots, d$, project the dataset onto e_j , obtaining the scalar dataset $\mathbf{x}_1 \cdot \mathbf{e}_j, \mathbf{x}_2 \cdot \mathbf{e}_j, \ldots, \mathbf{x}_N \cdot \mathbf{e}_j$, consisting of the j-th feature of the samples. If q_{jj} is the variance of this scalar dataset, then $q_{11}, q_{22}, \ldots, q_{dd}$ are the diagonal entries of the covariance matrix.

To standardize the dataset, we center it, and rescale the features to have variance one, as follows. Let $\mathbf{m} = (m_1, m_2, \ldots, m_d)$ be the dataset mean. For each sample point $\mathbf{x} = (t_1, t_2, \ldots, t_d)$, the standardized vector is

$$\mathbf{v} = \left(\frac{t_1 - m_1}{\sqrt{q_{11}}}, \frac{t_2 - m_2}{\sqrt{q_{22}}}, \ldots, \frac{t_d - m_d}{\sqrt{q_{dd}}} \right).$$

Then the standardized dataset is $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N$.

Standardized dataset

Definition 2.15

If $Q = (q_{ij})$ is the covariance matrix, then the correlation matrix is the $d \times d$ matrix $Q' = (q'_{ij})$ with entries

$$q'_{ij} = \frac{q_{ij}}{\sqrt{q_{ii}q_{jj}}}, \quad i, j = 1, 2, \ldots, d.$$

Theorem 2.4 (Standardized Covariance Equals Correlation)

The covariance matrix of the standardized dataset equals the correlation matrix of the original dataset.

Exercise 2.6

Prove Theorem (2.4).

Iris

Example 2.11

For the Iris dataset check Theorem (2.4).

```python
import numpy as np
from sklearn import datasets
from sklearn.preprocessing import StandardScaler

iris = datasets.load_iris()

# The dataset
dataset = iris["data"]

# standardize dataset
vectors = StandardScaler().fit_transform(dataset)
Qcorr = np.corrcoef(dataset.T)
Qcov = np.cov(vectors.T,bias=True)
np.allclose(Qcov,Qcorr)
```