

Dr. S. M. Moosavi

Data Sets

inear Geometry

Mathematics for Data Science

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Dr. S. M

Data Sets

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



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



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What is a dataset

Definition 1.1

Geometrically, a dataset is a sample of N points x_1, x_2, \dots, 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:

matrix = CSV file = spreadsheet = SQL table = array = 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.



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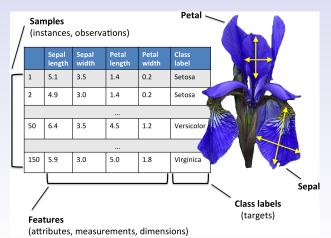
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ris dataset

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.





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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.

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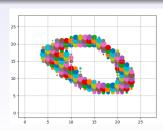
Exercises

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.





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ntroduction

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

$$1 = [x_1, x_2, \dots, x_N]$$

The total population is the population or the sample space.

Example 1.1

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

$$1 = [3.95, 3.20, 3.10, 5.55, 6.93]$$

Example 1.2

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

$$1 = [35, -32, -8, 45, -8]$$



Averages and Vector

Example 1.3

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

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

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
3
  def hexcolor():
    return "#" + ''.join([choice('0123456789abcdef') for
                                _ in range(6)])
  for i in range(5): plt.scatter(i,0, c=hexcolor())
  plt.show()
```



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Mean

Let 1 be a list as above. The goal is to compute the sample average or mean of the list, which is

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

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.



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/ector 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) = 0);
- **5** 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;
- r(sv) = (rs)v.



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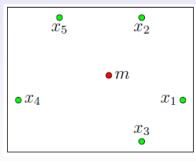
Centered dataset

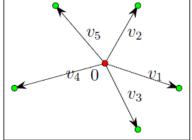
Definition 1.5 (Centered Versus Non-Centered)

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

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

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







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ome note:

- 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.
- ullet The set of all real numbers $\mathbb R$ is a vector space.
- ullet 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(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.

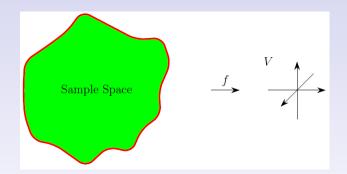


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In general, a statistic need not be a number. A statistic can be anything that "behaves like a number". For example, f(item) can be a vector or a matrix. More generally, a statistic's values may be anything that lives in a vector space V.



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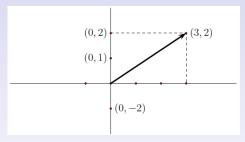
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artesian plane

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

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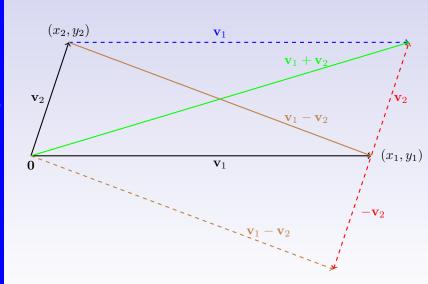
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2d example

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```
Example 1.6
```

```
import numpy as np
   v1 = (1.2)
4 v2 = (3,4)
   print(v1 + v2 == (1+3,2+4)) # returns False
6
   v1 = [1,2]
8
   v2 = [3.4]
9
   print(v1 + v2 == [1+3,2+4]) # returns False
10
11
   v1 = np.array([1,2])
12
   v2 = np.array([3,4])
13
   print(v1 + v2 == np.array([1+3,2+4]))
14
   # returns [ True True]
15
   print(3*v1 == np.array([3,6]))
16
   # returns [ True True]
17
   print(-v1 == np.array([-1,-2]))
18
   # returns [ True True]
19
   print(v1 - v2 == np.array([1-3,2-4]))
20
   # returns [ True True]
```



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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

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



Example 1.8

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Mean and Covariance

```
Generate a 2 dimensional dataset of random points and their mean
```

```
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)])
6
   mean = np.mean(dataset,axis=0)
   plt.grid()
8
   X, Y = dataset[:,0], dataset[:,1]
   plt.scatter(X,Y)
10
   plt.scatter(*mean)
11
   plt.annotate('$m$', xy=mean+0.01)
12
   plt.show()
                                1.0
                                0.8
```

0.6

0.0

0.2

0.4

0.6

0.8

1.0



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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 ${\bf v}=(x,y)$ to the origin ${\bf 0}=(0,0)$ 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 $\mathbf{v}_2 = (3, 4)$

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

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

```
1  import numpy as np
2  
3  v1 = np.array([1,2])
4  v2 = np.array([3,4])
5  print(np.linalg.norm(v1)) #returns 2.23606797749979
6  print(np.linalg.norm(v1-v2)) #returns 2.
```



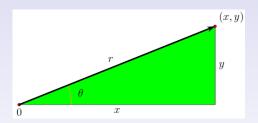
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Polar representation

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



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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 $\mathit{center}\ (a,b)$ 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.



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nner 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)

$$x_1x_2 + y_1y_2 = \mathbf{v}_1 \cdot \mathbf{v}_2 = |\mathbf{v}_1||\mathbf{v}_2|\cos\theta,$$

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.



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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
```



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Recall that $-1 \le \cos \theta \le 1$. 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

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

Exercise 1.4

Prove the "Cauchy-Schwarz Inequality".



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2d linear equations system

Consider the homogeneous system

$$\begin{cases}
ax + by = 0 \\
cx + dy = 0
\end{cases}$$
(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+du=ad-bc=0.

Definition 1.8 (Determinant)

The determinant of A is

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



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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

$$\begin{cases} ax + by = e \\ cx + dy = f \end{cases}$$
 (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 syster

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Mean and Covaria Linear Geometr 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).



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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).



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xample

Example 1.11

- \bullet (1,2) + (3,4) = (4,6).
- \bullet (0,0) + (1,2) = (1,2).
- 3(1,2) = (3,6).
- (1,0)(1,2) = (1-0,2+0) = (1,2).
- \bullet (1,2)(3,4) = (3-8,4+6) = (-5,10).
- \bullet (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

- \bullet 0 = (0,0).
- 1 = (1, 0).
- \bullet -1 = (-1,0).



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



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Complex Numbers

Example 1.13

In complex numbers:

- $\sqrt{-1} = i$.
- $\sqrt{-4} = 2i$.

•
$$(1,2)(3,4) = (1+2i)(3+4i)$$

= $3+4i+6i+8i^2$
= $3+10i-8$
= $-5+10i$
= $(-5,10)$.

•
$$(1,2)^3 = (1+2i)^3$$

= $(1)^3 + 3(1)^2(2i) + 3(1)(2i)^2 + (2i)^3$
= $1 + 6i + 12i^2 + 8i^3$
= $1 + 6i - 12 - 8i$
= $-11 - 2i$
= $-(11,2)$.



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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.

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

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

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

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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,

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

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 $0 \neq z_2 \in \mathbb{C}$

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



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

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

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

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```
import matplotlib.pyplot as plt
    import numpy as np
    np.random.seed(1)
   N = 20
6 rnd = np.random.random
    dataset = np.array([ [rnd(), rnd()] for _ in range(N) ])
    # Mean
    m = np.mean(dataset, axis=0)
10
    #Random point
11
    p = np.array([rnd(), rnd()])
12
13
    plt.grid()
14
    X, Y = dataset[:,0], dataset[:,1]
15
    plt.scatter(X,Y)
16
    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')
17
18
    plt.show()
19
20
21
    # Comparison of MSD of the mean and a random point
22
    MSD_m = np.sum(np.abs(dataset-m)**2)/N
23
    MSD_p = np.sum(np.abs(dataset-p)**2)/N
24
    print (MSD_m, MSD_p) # 0.160478187272121 0.5984208474157081
```



Point of Best-fi

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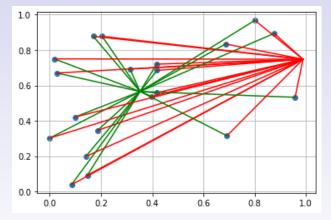


Figure 1.1: MSD for the mean (green) versus MSD for a random point (red).



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ensor 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 ${\bf u}$ and ${\bf text}$ 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} :

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

In square case:

•
$$\det(\mathbf{u} \otimes \mathbf{v}) = 0$$
.

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

•
$$trace(\mathbf{u} \otimes \mathbf{u}) = |\mathbf{u}|^2$$
.

$$\bullet (\mathbf{u} \otimes \mathbf{v})\mathbf{w} = (\mathbf{v} \cdot \mathbf{w})\mathbf{u}.$$



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Covariance

Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ 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

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

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

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



Example 1.16

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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

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



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```
import numpy as np
   def tensor(u.v):
     return np.array([ [ a*b for b in v] for a in u ])
5
   np.random.seed(1)
   N = 20
   rnd = np.random.random
   dataset = np.array([[rnd(), rnd()] for _ in range(N)])
10
   # mean
11
   m = np.mean(dataset,axis=0)
12
   # center dataset
13
   vectors = dataset - m
14
   # covariance
15
   Q = np.mean([ tensor(v,v) for v in vectors ],axis=0)
16
   print(Q)
```



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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

```
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)
```



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Total variance

Definition 1.17 (Total variance)

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

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

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

```
import numpy as np

np.random.seed(1)

np.random.seed(1)

n = 20

rnd = np.random.random

dataset = np.array([[rnd(), rnd()] for _ in range(N)])

covariance

np.cov(dataset.T,bias=True)

print(Q.trace()) # returns 0.16047818727212101
```



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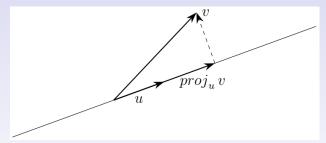
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rojections

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



When a vector ${\bf v}$ is projected onto the line through ${\bf u}$, 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

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



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Hence,

Definition 1.18 (Reduced dataset)

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

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

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

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

which is in \mathbb{R} .

Exercise 1.7

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

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 $\mathbf{u} \cdot Q\mathbf{u}$:

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



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Covariance ellipse

Hence,

Definition 1.19 (Covariance ellipse)

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

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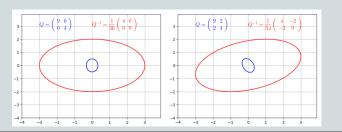
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Example 1.20

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

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```
import matplotlib.pyplot as plt
   import numpy as np
3
4
   def ellipse(a, b, c, levels, color):
5
     L. delta = 4...1
6
     x = np.arange(-L,L,delta)
     y = np.arange(-L,L,delta)
8
     X,Y = np.meshgrid(x, y)
9
     plt.contour(X, Y, a*X**2 + 2*b*X*Y + c*Y**2, levels,
                                  colors=color)
10
11
   # Q1 Covariance entities
12
   a, b, c = 9, 0, 4
13
14
   # Inverse Covariance entities
15
   det = a*c - b**2
16
   A, B, C = c/det, -b/det, a/det
17
18
   plt.grid()
19
   ellipse(a, b, c, [20], 'blue')
20
   ellipse(A, B, C, [1], 'red')
21
   plt.show()
```



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plt.show()

```
23
   # Q2 Covariance entities
24
   a, b, c = 9, 2, 4
25
26
   # Inverse Covariance entities
27
   det = a*c - b**2
28
   A, B, C = c/det, -b/det, a/det
29
30
   plt.grid()
31
   ellipse(a, b, c, [1], 'blue')
32
   ellipse(A, B, C, [1], 'red')
```



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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

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

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

where

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



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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:

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

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.

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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*.

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



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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.



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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

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



Matrices

Example 2.1

Apple 2.1
$$A = \begin{pmatrix} 1 & 6 & 11 \\ 2 & 7 & 12 \\ 3 & 8 & 13 \\ 4 & 9 & 14 \\ 5 & 10 & 15 \end{pmatrix} \Rightarrow A^t = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 6 & 7 & 8 & 9 & 10 \\ 11 & 12 & 13 & 14 & 15 \end{pmatrix}.$$

```
1
     import numpy as np
2
     A = np.array([[1,6,11],[2,7,12],[3,8,13],[4,9,14],[5,10,15]))
4
     print(A)
5
     print (A. shape)
6
     print (len(A))
7
     print (A[1])
8
     print (A[1,2])
9
     print (A[1:3])
10
11
     # transpose
12
     A_t = np.transpose(A)
13
     print (A-t)
14
     print (A-t.shape)
15
     print (len (A_t))
16
     print (A_t[1])
17
     print (A_t[1,2])
18
     print (A_t[1:3])
```



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Definition 2.2

A d-dimensional vector ${\bf v}$ 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 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 v a column vector.



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ntroductio

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

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



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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:

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



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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:

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



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Definition 2.6

A dataset is a collection of points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ in \mathbb{R}^d . After centering the mean to the origin, the dataset becomes a collection of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$. 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



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Example 2.4

For the Iris dataset:

```
import numpy as np
   import pandas as pd
   from sklearn import datasets
4
   iris = datasets.load_iris()
6
7
8
9
   # The dataset
   dataset = iris["data"]
10
   # To center the dataset
11
   m = np.mean(dataset,axis=0)
12
   vectors = dataset - m
13
14
   # To make a data frame
15
   centered_df = pd.DataFrame(data=vectors)
```



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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

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

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

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Example 2.5

```
import numpy as np
    A = np.zeros((4,3))
    print(A)
   B = np.eye(3)
   print(B)
7
8
    C = np.eye(4,3)
   print(C)
    D = np.array([[1,2,3],[4,5,6],[7,8,9],[10,11,12]])
10
    print(D)
11
    E = np.diag([1,2,3,4])
12
    print(E)
13
14
    print(A+C)
15
    print(C+D)
16
    print(4*D)
17
    print(-D)
18
    print(-2*D)
```



Introduction

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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.



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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,

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



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Dot produc

Example 2.6

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

```
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_)

print(u_dot_v_)
```



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Dot product

As we mentioned in 2 dimensions, we have the following generalizations in \boldsymbol{d} dimension:

Definition 2.7

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

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

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:

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



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Corollary 2.2 (Cauchy-Schwarz Inequality)

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

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

Definition 2.8

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

Vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$ 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.



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



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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:

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

4 5

import numpy as no

$$Av = np.dot(A, v)$$

 $print(Av)$



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Matrix-matrix produc

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.
- $\bullet (AB)^t = B^t A^t.$



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Products

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:

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

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

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

import numpy as no

5



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Orthonormal Rows and Columns

Assume the rows of a matrix A are $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$. 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 $U^tU=I$.



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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 v_1, v_2, \dots, v_N . Then

$$A^t A = \mathbf{v}_1 \otimes \mathbf{v}_1 + \mathbf{v}_2 \otimes \mathbf{v}_2 + \dots + \mathbf{v}_N \otimes \mathbf{v}_N.$$

Exercise 2.2

Prove the tensor identity.



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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

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



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lorm 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 $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$. Then

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

and

$$||A||^2 = trace(A^tA).$$

Exercise 2.5

Prove Theorem (2.3).



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If $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ is a dataset of points in \mathbb{R}^d with mean \mathbf{m} , and $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$ is the corresponding centered dataset, then we saw

that the covariance matrix Q is the average of tensor products

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

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

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



Iris

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Example 2.10

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

```
import numpy as no
2
     from sklearn import datasets
     iris = datasets.load_iris()
5
6
     # The dataset
7
     dataset = iris["data"]
8
9
     # Mean
10
    m = np.mean(dataset.axis=0)
11
12
     # Centered dataset
13
     vectors = dataset - m
14
15
     # Covariance
16
    N = len(vectors)
17
         Biased
18
     Q = np.dot(vectors.T, vectors)/N
     Q = np.cov(dataset,rowvar=False,ddof=0) # ddof = delta degrees of freedom
19
20
     Q = np.cov(dataset.T,ddof=0)
21
22
         Unbiased
23
     Q = np.dot(vectors.T, vectors)/(N-1)
24
     Q = np.cov(dataset,rowvar=False)
25
     Q = np.cov(dataset.T)
26
27
     # Total Variance
28
     TV = np.trace(Q)
```



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Standardized dataset

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

Let $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_d$ be the standard basis in \mathbb{R}^d , and, for each $j=1,2,\dots,d$, project the dataset onto \mathbf{e}_j , obtaining the scalar dataset $\mathbf{x}_1 \cdot \mathbf{e}_j, \mathbf{x}_2 \cdot \mathbf{e}_j, \dots, \mathbf{x}_N \cdot \mathbf{e}_j$, consisting of the j-th feature of the samples. If q_{jj} is the variance of this scalar dataset, then $q_{11}, q_{22}, \dots, q_{dd}$ 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 $\mathbf{m}=(m_1,m_2,\dots,m_d)$ be the dataset mean. For each sample point $\mathbf{x}=(t_1,t_2,\dots,t_d)$, the standardized vector is

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

Then the standardized dataset is v_1, v_2, \dots, v_N .



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Standardized datase

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

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

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).



ris

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Example 2.11

For the Iris dataset check Theorem (2.4).

```
import numpy as np
   from sklearn import datasets
   from sklearn.preprocessing import StandardScaler
4
5
6
7
   iris = datasets.load iris()
   # The dataset
8
   dataset = iris["data"]
9
10
   # standardize dataset
11
   vectors = StandardScaler().fit_transform(dataset)
12
   Qcorr = np.corrcoef(dataset.T)
13
   Qcov = np.cov(vectors.T,bias=True)
14
   np.allclose(Qcov,Qcorr)
```



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Matrix Invers

Definition 2.16

Given a square matrix A, the inverse matrix is the matrix B satisfying

$$AB = I = BA$$
.

When A has an inverse, we say A is invertible. If a matrix is $d \times d$, then the inverse is also $d \times d$. We write $B = A^{-1}$ for the inverse matrix of A.

Here I is the identity matrix. Not every square matrix has an inverse. For example, the zero matrix does not have an inverse.

Example 2.12

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \Rightarrow A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

Since we can't divide by zero, a 2×2 matrix is invertible only if $ad-bc\neq 0$.



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Exercise 2.7

Prove that $(AB)^{-1} = B^{-1}A^{-1}$.

Exercise 2.8

Prove that for a linear system $A\mathbf{x} = \mathbf{b}$, if A is invertible then $\mathbf{x} = A^{-1}\mathbf{b}$.

Example 2.13

Solve the following linear system

$$\begin{cases} x + 2y + 3z = 1 \\ -3x + 6y = 2 \\ 10x - 5y + 23z = 3 \end{cases}$$

```
import numpy as np

A = np.array([[1,2,3],[-3,6,0], [10,-5,23]])
b = np.array([1,2,3])
b = np.array([1,2,3])

# Determinant of A
np.linalg.det(A)
f # Inverse of A
np.linalg.inv(A)
# Solution of Ax=b
v = np.dot(np.linalg.inv(A),b)
```



inear combination

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Definition 2.17 (Linear combination)

A linear combination of vectors $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ is

$$t_1\mathbf{v}_1+t_2\mathbf{v}_2+\ldots+t_d\mathbf{v}_d,$$

where t_1, t_2, \ldots, t_d are scalars.

Example 2.14

Let $\mathbf{u}, \mathbf{v}, \mathbf{w}$ be three vectors. Then

$$3\mathbf{u} - \frac{1}{6}\mathbf{v} + 9\mathbf{w}$$
, $5\mathbf{u} + 0\mathbf{v} - \mathbf{w}$, $0\mathbf{u} + 0\mathbf{v} + 0\mathbf{w}$,

are linear combinations of u, v, w.

Example 2.15

Let A be a matrix with columns $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$, and let $\mathbf{x} = (t_1, t_2, \dots, t_d)$. Then $A\mathbf{x}$ is a linear combination of the columns of A as:

$$A\mathbf{x} = t_1\mathbf{v}_1 + t_2\mathbf{v}_2 + \ldots + t_d\mathbf{v}_d.$$



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Span

Definition 2.18 (Span)

The span of $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ is the set S of all linear combinations of $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$, and we write

$$S = span(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d).$$

Exercise 2.9

Let A be the matrix with columns $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$. Then $S = span(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d)$ is the set S of all vectors of the form $A\mathbf{x}$.

Exercise 2.10

If each vector \mathbf{v}_k of $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ is a linear combination of vectors $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_N$, then

$$span(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d) \subseteq span(\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_N).$$



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column spa

Definition 2.19

Let A be a matrix. The column space of A is the span of its columns.

Example 2.16

```
import sympy as sp
     import scipy as sc
     import numpy as no
5
    A = sp.Matrix([[1, 6, 11], [2, 7, 12], [3, 8, 13], [4, 9, 14], [5, 10, 15]])
6
7
    # column vectors
8
     u = sp. Matrix([1,2,3,4,5])
     v = sp. Matrix([6,7,8,9,10])
9
    w = sp. Matrix([11,12,13,14,15])
10
    A = sp. Matrix. hstack(u, v, w)
12
13
    # returns minimal spanning set for column space of A
    A. columnspace()
14
15
    # returns minimal spanning orthonormal set for column space of A
     A = np. array([[1, 6, 11], [2, 7, 12], [3, 8, 13], [4, 9, 14], [5, 10, 15]])
16
17
     sc.linalg.orth(A)
```

A. columnspace() returns a minimal set of vectors spanning the column space of A. The *column rank* of A is the number of vectors returned: for A in the above example, the column rank is 2. sc.linalg.orth(A) returns a minimal orthonormal set of vectors spanning the column space of A.



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Exercise 2.11

As in example 2.16, show that if

$$\mathbf{v}_1 = (1, 2, 3, 4, 5), \quad \mathbf{v}_2 = (6, 7, 8, 9, 10), \quad \mathbf{v}_3 = (11, 12, 13, 14, 15)$$

then $span(\mathbf{v}_1, \mathbf{v}_2) = span(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$.

Exercise 2.12

Show that: the column space of a matrix A consists of all vectors of the form Ax. A vector **b** is in the column space of A when Ax = b has a solution.

The augmented matrix $\bar{A} = (A, \mathbf{b})$ is obtained by adding \mathbf{b} as an extra column next to the columns of A.

Exercise 2.13

Let A be the matrix A augmented by a vector b. Then b is in the column space of A iff

$$column \ rank(A) = column \ rank(\bar{A}).$$



Notes

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Exercise 2.14

Show that the vectors

$$\mathbf{e}_1 = (1, 0, 0, \dots, 0, 0)$$

$$\mathbf{e}_2 = (0, 1, 0, \dots, 0, 0)$$

$$\mathbf{e}_3 = (0, 0, 1, \dots, 0, 0)$$

$$\mathbf{e}_d = (0, 0, 0, \dots, 0, 1)$$

span \mathbb{R}^d .

The set $\{e_1, e_2, \dots, e_d\}$ is the *standard basis* for \mathbb{R}^d .



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Definition 2.20

The row space of a matrix is the span of its rows.

Example 2.17

```
import sympy as sp
2
     import scipy as sc
3
     import numpy as no
4
5
    A = sp. Matrix([[1, 6, 11], [2, 7, 12], [3, 8, 13], [4, 9, 14], [5, 10, 15]))
6
     Α
7
8
    # returns minimal spanning set for row space of A
    A. rowspace()
9
10
11
    # returns minimal spanning orthonormal set for column space of A
    A = np. array([[1, 6, 11], [2, 7, 12], [3, 8, 13], [4, 9, 14], [5, 10, 15]])
13
     sc.linalg.orth(A.T)
```

The *row rank* of a matrix is the number of vectors returned by A.rowspace(). This is the minimal number of vectors spanning the row space of A which for the above example is 2. sc.linalg.orth(A.T) returns a minimal orthonormal set of vectors spanning the row space of A.



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Definition 2.21

A linear combination $t_1\mathbf{v}_1 + t_2\mathbf{v}_2 + \ldots + t_d\mathbf{v}_d$ is trivial if all the coefficients are zero: $t_1 = t_2 = \ldots = t_d = 0$. Otherwise it is non-trivial: if at least one coefficient is not zero.

A linear combination t_1 **v**₁ + t_2 **v**₂ + . . . + t_d **v**_d vanishes if it equals the zero vector:

$$t_1\mathbf{v}_1+t_2\mathbf{v}_2+\ldots+t_d\mathbf{v}_d=\mathbf{0}.$$

We say $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ are linearly dependent if there is a non-trivial vanishing linear combination of $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$. Otherwise, we say $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ are linearly independent.

Example 2.18

The vectors $\mathbf{v}_1 = (1, 2, 3, 4, 5)$, $\mathbf{v}_2 = (6, 7, 8, 9, 10)$, $\mathbf{v}_3 = (11, 12, 13, 14, 15)$ are linearly dependent, because

$$\mathbf{v}_3 + \mathbf{v}_1 - 2\mathbf{v}_2 = \mathbf{0}.$$

We can see $\mathbf{v}_3 = 2\mathbf{v}_2 - \mathbf{v}_1$.



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Exercise 2.15

Show that if $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ are linearly dependent then at least one of the vectors is a linear combination of the remaining vectors.

Exercise 2.16 (Homogeneous Linear Systems)

Let A be the matrix with columns $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$. Then $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$

- \bullet are linearly dependent when $A\mathbf{x}=\mathbf{0}$ has a nonzero solution $\mathbf{x},$ and
- are linearly independent when $A\mathbf{x} = \mathbf{0}$ has only the zero solution $\mathbf{x} = 0$.

Exercise 2.17

Show that if $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_d$ are orthonormal then they are linearly independent.



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Null space

Definition 2.22

The set of vectors \mathbf{x} satisfying $A\mathbf{x} = \mathbf{0}$, or the set of solutions \mathbf{x} of $A\mathbf{x} = \mathbf{0}$, is the null space of the matrix A.

The cardinality of a minimal set of vectors spanning the null space of A is called the nullity of A.

Example 2.19

Show that the nullity of the following matrix is 1.

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

```
import sympy as sp
import scipy as sc
import numpy as np

# using sympy
A = sp. Matrix([[1, 6, 11], [2, 7, 12], [3, 8, 13], [4, 9, 14], [5, 10, 15]])
A nullspace()

# using numpy and scipy
A = np.array([[1, 6, 11], [2, 7, 12], [3, 8, 13], [4, 9, 14], [5, 10, 15]])
Isc.linale, null.space(A)
```



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Exercise 2.18

Let A be any matrix. Show that the null space, row space and column space of A equals the null space, row space and column space of A^tA , respectively.

Definition 2.23 (Orthogonal complements)

Let S and T be spans. We say S and T are orthogonal complements if every vector in S is orthogonal to every vector in T. In symbols, we write $S=T^\perp$ and $T=S^\perp$ (pronounced "T-perp" and "S-perp").

Exercise 2.19

Show that, if $S = span(\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N)$, and A is the matrix with rows $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$, then S^{\perp} equals the null space of A.

Exercise 2.20

For a matrix A, show that $(null space^{\perp} = row space)$ and $(row space^{\perp} = null space)$



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Definition 2.24 (Subspace)

A subspace is a set of vectors closed under addition and scalar multiplication. precisely: A subset $S \subseteq V$ is a subspace of the vector space V whenever for every $\mathbf{x}_1, \mathbf{x}_2 \in S$ and every scalar t we have

- \bullet $\mathbf{x}_1 + \mathbf{x}_2 \in S$ and
- $t\mathbf{x}_1 \in S$.

or equivalently: $t\mathbf{x}_1 + \mathbf{x}_2 \in S$.

Exercise 2.21

If V is a vector space then \emptyset and V are the trivial subspaces of V.

Exercise 2.22

Show that

- the null space: all x's satisfying Ax = 0,
- the row space: the span of the rows of A, and
- the column space: the span of the columns of A

are subspaces, but

is not a subspace.

• the solution space: the solutions x of Ax = b



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Projected datase

Let $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$ be the centered dataset of the dataset $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N$ in \mathbb{R}^d with mean \mathbf{m} . Then the covariance is

$$Q = \frac{\mathbf{v}_1 \otimes \mathbf{v}_1 + \mathbf{v}_2 \otimes \mathbf{v}_2 + \ldots + \mathbf{v}_N \otimes \mathbf{v}_N}{N} = \frac{1}{N} A^t A,$$

where A is the matrix with rows $\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N$.

If **b** is a vector, the projection of the centered dataset onto the line through **b** results in the reduced dataset

$$\mathbf{v}_1 \cdot \mathbf{b}, \mathbf{v}_2 \cdot \mathbf{b}, \dots, \mathbf{v}_N \cdot \mathbf{b}.$$

The mean of this projected dataset is zero, and its variance is

$$\frac{(\mathbf{v}_1 \cdot \mathbf{b})^2 + (\mathbf{v}_2 \cdot \mathbf{b})^2 + \ldots + (\mathbf{v}_N \cdot \mathbf{b})^2}{N} = \frac{1}{N} \mathbf{b}^t A^t A \mathbf{b} = \mathbf{b} \cdot Q \mathbf{b}.$$



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Zero variance direction

Definition 2.25

Let m be a point in \mathbb{R}^d and b a vector in \mathbb{R}^d . The hyperplane passing through m and orthogonal to b is the set of points x satisfying the equation

$$\mathbf{b} \cdot (\mathbf{x} - \mathbf{m}) = 0.$$

Example 2.20

In \mathbb{R}^3 , a hyperplane is a plane, and in \mathbb{R}^2 , a hyperplane is a line. In general, in \mathbb{R}^d , a hyperplane is (d-1)-dimensional, always one less than the ambient dimension.



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Hyperplane

Definition 2.26

A vector \mathbf{b} is a zero variance direction of Q if the projected variance is zero:

$$\mathbf{b} \cdot Q\mathbf{b} = 0.$$

Theorem 2.5

Let \mathbf{m} and Q be the mean and covariance of a dataset in \mathbb{R}^d . Then $\mathbf{b} \cdot Q\mathbf{b} = 0$ is the same as saying every point in the dataset lies in the hyperplane passing through \mathbf{m} and orthogonal to $\mathbf{b} \colon \mathbf{b} \cdot (\mathbf{x} - \mathbf{m}) = 0$.

Theorem 2.6

Let Q be a covariance matrix. Then the null space of Q equals the zero variance directions of Q.

Corollary 2.4

Let Q be a covariance matrix of a centered dataset A. Then the null space of A equals the zero variance directions of Q.



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Example 2<u>.21</u>

Suppose the dataset

	t_1	t_2	t_3	t_4	t_5
\mathbf{x}_1	1	2	3	4	5
\mathbf{x}_2	6	7	8	9	10
\mathbf{x}_3	11	12	13	14	15
\mathbf{x}_4	16	17	18	19	20

Here we have 5 features. By the following code the null space of the covariance matrix, say Q, has 4 vectors which means it is 4-dimensional (or the nullity of Q is 4). Hence the dataset is a 1-dimensional dataset (5-4=1). It means that there is a hyperplane (here a line) in \mathbb{R}^5 which we can project the dataset on it without loosing any information.

```
1
2
3
4
5
6
```

```
import numpy as np
import scipy as sc

dataset = np.array([[1,2,3,4,5],[6,7,8,9,10],[11,12,13,14,15],[16,17,18,19,20]])
Q = np.cov(dataset.T)
N = sc.linalg.null.space(Q)
nullity = N.shape[1]
```



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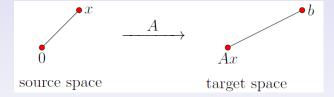
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Think of ${\bf b}$ and $A{\bf x}$ as points, and measure the distance between them, and think of ${\bf x}$ and the origin ${\bf 0}$ as points, and measure the distance between them.



If $A\mathbf{x} = \mathbf{b}$ is solvable, then, among all solutions \mathbf{x}^* , select the solution \mathbf{x}^+ closest to $\mathbf{0}$. More generally, if $A\mathbf{x} = \mathbf{b}$ is not solvable, select the points \mathbf{x}^* so that $A\mathbf{x}^*$ is closest to \mathbf{b} , then, among all such \mathbf{x}^* , select the point \mathbf{x}^+ closest to the origin.

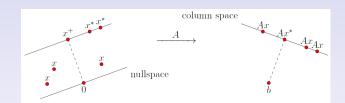


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Even though the point \mathbf{x}^+ may not solve $A\mathbf{x} = \mathbf{b}$, this procedure results in a uniquely determined \mathbf{x}^+ : While there may be several points \mathbf{x}^* , there is only one \mathbf{x}^+ .



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Concept

The results in this section are as follows. Let A be any matrix. There is a unique matrix A^+ — the *pseudo-inverse* of A — with the following properties:

- the linear system $A\mathbf{x} = \mathbf{b}$ is solvable, when $\mathbf{b} = AA^{+}\mathbf{b}$.
- $\mathbf{x}^+ = A^+ \mathbf{b}$ is a solution of
 - 1 the linear system $A\mathbf{x} = \mathbf{b}$, if $A\mathbf{x} = \mathbf{b}$ is solvable.
 - 2 the regression equation $A^t A \mathbf{x} = A^t \mathbf{b}$, always.
- In either case,
 - 1 there is exactly one solution with minimum norm.
 - 2 Among all solutions, x^+ has minimum norm.
 - **3** Every other solution is $\mathbf{x} = \mathbf{x}^+ + \mathbf{v}$ for \mathbf{v} in the null space of A.

Key concepts in this section are the residual

$$|A\mathbf{x} - \mathbf{b}|^2$$

and the regression equation

$$A^t A \mathbf{x} = A^t \mathbf{b}.$$

Exercise 2.23

x is a solution of Ax = b iff the residual is zero.



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Example 2.22

For A and b as below

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

the linear system $A\mathbf{x} = \mathbf{b}$ and the regression equation $A^t A \mathbf{x} = A^t \mathbf{b}$ are

$$\begin{cases} x + 6y + 11z = -9 \\ 2x + 7y + 12z = -3 \\ 3x + 8y + 13z = 3 \\ 4x + 9y + 14z = 9 \\ 5x + 10y + 15z = 10 \end{cases}, \begin{cases} 11x + 26y + 41z = 16 \\ 13x + 33y + 53z = 13 \\ 41x + 106y + 171z = 36 \end{cases}$$

respectively.



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Residual minimize

Let \mathbf{b} be any vector, not necessarily in the column space of A. To see how close we can get to solving $A\mathbf{x} = \mathbf{b}$, we minimize the residual $|A\mathbf{x} - \mathbf{b}|^2$.

Definition 2.27 (Residual minimizer)

We say x^* is a residual minimizer if

$$|A\mathbf{x}^* - \mathbf{b}|^2 = \min_x |A\mathbf{x} - \mathbf{b}|^2.$$

Theorem 2.7 (Existence of Residual Minimizer)

There is a residual minimizer x^* in the row space of A.

Exercise 2.24

Prove Theorem 2.7.



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Residual minimizer

Theorem 2.8

 \mathbf{x}^* is a residual minimizer iff \mathbf{x}^* solves the regression equation.

Proof: let \mathbf{v} be any vector, and t a scalar. Insert $\mathbf{x} = \mathbf{x}^* + t\mathbf{v}$ into the residual:

$$|A\mathbf{x} - \mathbf{b}|^2 = |A(\mathbf{x}^* + t\mathbf{v}) - \mathbf{b}|^2$$

$$= |(A\mathbf{x}^* - \mathbf{b}) + At\mathbf{v}|^2$$

$$= |A\mathbf{x}^* - \mathbf{b}|^2 + 2t(A\mathbf{x}^* - \mathbf{b}) \cdot A\mathbf{v} + t^2|A\mathbf{v}|^2$$

$$:= f(t).$$

If \mathbf{x}^* is a residual minimizer, then f(t) is minimized when t=0. But a parabola $f(t)=a+2bt+ct^2$ is minimized at t=0 only when b=0. Thus the linear coefficient vanishes, $(A\mathbf{x}^*-\mathbf{b})\cdot A\mathbf{v}=0$. This implies

$$A^{t}(A\mathbf{x}^{*} - \mathbf{b}) \cdot \mathbf{v} = (A\mathbf{x}^{*} - \mathbf{b}) \cdot A\mathbf{v} = 0.$$

Since v is any vector, this implies

$$A^t(A\mathbf{x}^* - \mathbf{b}) = \mathbf{0},$$

which is the regression equation. Conversely, if the regression equation holds, then the linear coefficient in the parabola f(t) vanishes, so t=0 is a minimum, establishing that \mathbf{x}^* is a residual minimizer.



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Exercise 2.25

Any two residual minimizers differ by a vector in the nullspace of A.

Definition 2.28

We say \mathbf{x}^+ is a minimum norm residual minimizer if \mathbf{x}^+ is a residual minimizer and

$$|\mathbf{x}^+|^2 \le |\mathbf{x}^*|^2$$

for any residual minimizer x^* .

Theorem 2.9

Let x^* be a residual minimizer. Then x^* is a minimum norm residual minimizer iff x^* is in the row space of A.

Exercise 2.26

Prove Theorem 2.9.



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Residual minimizer

Theorem 2.10 (Uniqueness of Residual Minimizer)

There is exactly one minimum norm residual minimizer \mathbf{x}^+ .

Proof: If \mathbf{x}_1^+ and \mathbf{x}_2^+ are minimum norm residual minimizers, then $\mathbf{v} = \mathbf{x}_1^+ - \mathbf{x}_2^+$ is both in the row space and in the null space of A, $\mathbf{x}_1^+ - \mathbf{x}_2^+ = \mathbf{0}$. Hence $\mathbf{x}_1^+ = \mathbf{x}_2^+$.

Putting the above all together, each vector \mathbf{b} leads to a unique \mathbf{x}^+ . Defining A^+ by setting

$$\mathbf{x}^+ = A^+ \mathbf{b},$$

we obtain A^+ , the pseudo-inverse of A.

Notice if A is, for example, 5×4 , then $A\mathbf{x} = \mathbf{b}$ implies \mathbf{x} is a 4-vector and \mathbf{b} is a 5-vector. Then from $\mathbf{x}^+ = A^+\mathbf{b}$, it follows A^+ is 4×5 . Thus the shape of A^+ equals the shape of A^t .

Theorem 2.11 (Regression Equation is Always Solvable)

The regression equation $A^t A \mathbf{x} = A^t \mathbf{b}$ is always solvable. The solution of minimum norm is $\mathbf{x}^+ = A^+ \mathbf{b}$. Any other solution differs by a vector in the null space of A.



Example

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Example 2.23

For A and \mathbf{b} as below

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

the minimum norm solution of the regression equation $A^t A \mathbf{x} = A^t \mathbf{b}$ is

$$\mathbf{x}^{+} = A^{+}\mathbf{b} = \frac{1}{150} \begin{pmatrix} -37 & -20 & -3 & 14 & 31 \\ -10 & -5 & 0 & 5 & 10 \\ 17 & 10 & 3 & -4 & -11 \end{pmatrix} \begin{pmatrix} -9 \\ -3 \\ 3 \\ 9 \\ 10 \end{pmatrix} = \frac{1}{15} \begin{pmatrix} 82 \\ 25 \\ -32 \end{pmatrix}.$$

import sympy as sm

A. pinv()

9 10 b = sm. Matrix([-9,-3,3,9,10])

11 A. pinv()*b

5 6 7

8



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Linear systems

Returning to the linear system, we have

Theorem 2.12

If the linear system is solvable, then every solution of the regression equation is a solution of the linear system, and vice-versa.

Corollary 2.5

The linear system $A\mathbf{x} = \mathbf{b}$ is solvable iff $\mathbf{b} = AA^+\mathbf{b}$. When this happens, $\mathbf{x}^+ = A^+\mathbf{b}$ is the solution of minimum norm.

Example 2.24

For A and b as in Example 2.23, since

$$AA^{+}\mathbf{b} = \begin{pmatrix} -8\\ -3\\ 2\\ 7\\ 12 \end{pmatrix}$$

is not equal to \mathbf{b} , the linear system $A\mathbf{x} = \mathbf{b}$ is not solvable.



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Corollary 2.6

If A is invertible, then $A^+ = A^{-1}$.

Theorem 2.13 (Properties of Pseudo-Inverse)

- $2 A^+AA^+ = A^+.$
- \blacksquare AA^+ and A^+A are symmetric.
- If A has orthonormal columns or orthonormal rows, then $A^+ = A^t$.

Exercise 2.27

Prove Theorem 2.12, Corollary 2.5, Corollary 2.6 and Theorem 2.13.



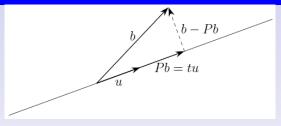
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Projections

Projection onto a line



Let ${\bf u}$ be a unit vector, and let ${\bf b}$ be any vector. Let $span({\bf u})$ be the line through ${\bf u}$. The *projection* of ${\bf b}$ onto $span({\bf u})$ is the vector ${\bf v}$ in $span({\bf u})$ that is closest to ${\bf b}$ (Exercise). It turns out this closest vector ${\bf v}$ equals $P{\bf b}$ for some matrix P, the *projection matrix*. Since $span({\bf u})$ is a line, the projected vector $P{\bf b}$ is a multiple $t{\bf u}$ of ${\bf u}$. We have ${\bf b}-P{\bf b}$ is orthogonal to ${\bf u}$, so

$$0 = (\mathbf{b} - P\mathbf{b}) \cdot \mathbf{u} = \mathbf{b} \cdot \mathbf{u} - P\mathbf{b} \cdot \mathbf{u} = \mathbf{b} \cdot \mathbf{u} - t\mathbf{u} \cdot \mathbf{u} = \mathbf{b} \cdot \mathbf{u} - t.$$

Solving for t, this implies $t = \mathbf{b} \cdot \mathbf{u}$. If U is the matrix with column \mathbf{u}

$$P\mathbf{b} = (\mathbf{b} \cdot \mathbf{u})\mathbf{u} = (\mathbf{u} \otimes \mathbf{u})\mathbf{b} = UU^t\mathbf{b}.$$

We call $\mathbf{b} \cdot \mathbf{u} = U^t \mathbf{b}$ the reduced vector.



Projecting onto a plane

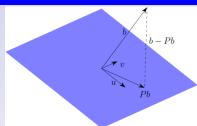
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Let \mathbf{u}, \mathbf{v} be an orthonormal pair of vectors, so $\mathbf{u} \cdot \mathbf{v} = 0$, $\mathbf{u} \cdot \mathbf{u} = 1 = \mathbf{v} \cdot \mathbf{v}$. We project a vector \mathbf{b} onto $span(\mathbf{u}, \mathbf{v})$. As before, there is a matrix P, the projection matrix, such that the projection of \mathbf{b} onto the plane equals $P\mathbf{b}$. Then $\mathbf{b} - P\mathbf{b}$ is orthogonal to the plane:

$$(\mathbf{b} - P\mathbf{b}) \cdot \mathbf{u} = 0$$
 and $(\mathbf{b} - P\mathbf{b}) \cdot \mathbf{v} = 0$.

Since $P\mathbf{b}$ lies in the plane, $P\mathbf{b} = r\mathbf{u} + s\mathbf{v}$ is a linear combination of \mathbf{u} and \mathbf{v} . So:

$$r = \mathbf{b} \cdot \mathbf{u}, \quad s = \mathbf{b} \cdot \mathbf{v}.$$

If U is the matrix with columns \mathbf{u}, \mathbf{v} , then

$$P\mathbf{b} = (\mathbf{b} \cdot \mathbf{u})\mathbf{u} + (\mathbf{b} \cdot \mathbf{v})\mathbf{v} = (\mathbf{u} \otimes \mathbf{u} + \mathbf{v} \otimes \mathbf{v})\mathbf{b} = UU^t\mathbf{b}.$$

We call $(\mathbf{b} \cdot \mathbf{u}, \mathbf{b} \cdot \mathbf{v}) = U^t \mathbf{b}$ the reduced vector.



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Projection matrices in general

Definition 2.29

Let S be a span. A matrix P is a projection matrix onto S if

- \blacksquare $P\mathbf{b}$ is in S for any vector \mathbf{b} ,
- 2 Pb = b if b is in S,
- **3** $\mathbf{b} P\mathbf{b}$ is orthogonal to S for any vector \mathbf{b} .

Exercise 2.28

Show that, the projection of a vector onto a span equals the vector itself when the vector is already in the span.

Theorem 2.14 (Projection Onto a Column Space)

Let A be a matrix and \mathbf{v} a vector. Then the projected vector onto the column space of A is $P\mathbf{v} = AA^{\dagger}\mathbf{v}$ and the reduced vector is $\mathbf{x} = A^{\dagger}\mathbf{v}$.

Theorem 2.15 (Projection Onto a Row Space)

Let A be a matrix and \mathbf{v} a vector. Then the projected vector onto the row space of A is $P\mathbf{v} = A^+A\mathbf{v}$.

Exercise 2.29

Prove Theorems 2.14 and 2.15.



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Example 2.25

```
import numpy as np
2 3
   # projection of column vector b onto column space of A
   def project_col(A,b):
5
      Aplus = np.linalg.pinv(A)
6
      x = np.dot(Aplus,b) # reduced
      return np.dot(A,x) # projected
8
9
   # projection of column vector b onto row space of A
10
   def project_row(A,b):
11
      Aplus = np.linalg.pinv(A)
12
      AplusA = np.dot(Aplus,A)
13
      return np.dot(AplusA,b) # projected
14
15
   A = np.array([[1,6,11],[2,7,12],[3,8,13],[4,9,14],[5,10])
                                  .15]])
16
17
   b = np.array([-9, -3, 3, 9, 10])
18
   project_col(A, b.T)
19
20
   b = np.array([-9, -3, 3])
21
   project_row(A, b.T)
```



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Projecting onto Orthonormal Vectors

Theorem 2.16 (Projection Onto Orthonormal Vectors)

If the columns of U are orthonormal and \mathbf{v} is a vector. Then the projected vector onto the column space of U is $P\mathbf{v} = UU^t\mathbf{v}$ and the reduced vector is $\mathbf{x} = U^t\mathbf{v}$.

Example 2.26

```
import numpy as no
     # projection of column vector b onto column space of U
     # with orthonormal columns
     def project_col_ortho(U.b):
       x = np.dot(U.T.b) \# reduced
7
       return np. dot(U.x) # projected
8
     # Matrices with orthnormal columns
     U1 = np. array([[1,0,0],[0,1,0],[0,0,1]])
10
     U2 = np. array([[1,1,1]/np. sqrt(3), [1,-1,0]/np. sqrt(2), [1,1,-2]/np. sqrt(6)])
12
     U3 = np. array([[1.0.0], [0.1.0], [0.0.1], [0.0.0], [0.0.0]))
13
14
     b = np.array([1,2,3]).reshape(3,1)
15
16
     project_col_ortho(U1, b)
17
     project_col_ortho(U2, b)
18
19
     b = np. array([1,2,3,4,5]). reshape(5,1)
20
21
     project_col_ortho(U3, b)
```



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irect sum

Let S and T be spans. Let S+T consist of all sums of vectors $\mathbf{u}+\mathbf{v}$ with \mathbf{u} in S and \mathbf{u} in T. Then a moment's thought shows S+T is itself a span. When the intersection of S and T is the zero vector, we write $S\oplus T$, and we say $S\oplus T$ is the direct sum of S and T.

Theorem 2.17

If S is a span in \mathbb{R}^d , then

$$\mathbb{R}^d = S \oplus S^{\perp}.$$

Theorem 2.18

If A is an $N \times d$ matrix,

$$nullspace \oplus rowspace = \mathbb{R}^d$$
,

and the null space and row space are orthogonal to each other.



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Corollary 2.7

From Theorem 2.18, the projection matrix onto the null space of A is $P = I - A^+A$.

Theorem 2.19 (Projection is the Nearest Point in the Span)

Let $P\mathbf{b}=AA^+\mathbf{b}$ be the projection of \mathbf{b} onto the column space of A, and let $\mathbf{x}^+=A^+\mathbf{b}$ be the reduced vector. Then

$$|A\mathbf{x}^+ - \mathbf{b}|^2 = \min_{\mathbf{x}} |A\mathbf{x} - \mathbf{b}|^2.$$

Exercise 2.30

Prove Theorems 2.17, 2.18, 2.19 and Corollary 2.7.