



Python Meets Mathematics:

Linear Algebra

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Programming meets Mathematics

~~■~~ ~~Calculus~~ **Differentiation**

- Visualization using [Matplotlib](#)
- Differentiation
 - Meaning: The **slope** of a tangent line (\sim linear approximation) of a function
 - Finding a **derivative** using [rules](#), [SymPy](#), and numerical differentiation

■ **Linear Algebra**

■ **Optimization**

■ **Probability**

■ **Information Theory**

Getting Started from Line Fitting

Q) How about finding a line from three points?

(1, 4)



(4, 2)



(7, 1)



- Line representation: $y = ax + b$ ($y = -\frac{2}{3}x + \frac{14}{3}$)
- Slope $a = \frac{2-4}{4-1} = -\frac{2}{3}$
- Y intercept $b = 4 - a \cdot 1 = \frac{14}{3}$

Getting Started from Line Fitting

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Q) Can it represent a vertical line such as $x = 1$?

- Line representation: $ax + by + c = 0$
($2x + 3y - 14 = 0$; $4x + 6y - 28 = 0$)
→ additional constraint $a^2 + b^2 = 1$
- Its shorter form: $\mathbf{n}^T \mathbf{x} + c = 0$
($\mathbf{n} = \begin{bmatrix} a \\ b \end{bmatrix}$ and $\mathbf{x} = \begin{bmatrix} x \\ y \end{bmatrix}$)

Normal vector

Linear Algebra

- [Algebra](#) is the study of mathematical objects and their manipulating rules (e.g. arithmetic operations).
- [Linear algebra](#) is the mathematical branch on [linear equations](#) represented in [vector spaces](#).

- [Linear equation](#)

- e.g. $ax + b = 0$ (one-variable), $ax + by + c = 0$ (two-variable), ..., $a_1x_1 + a_2x_2 + \dots + a_nx_n + b = 0$ (n -variable)
- Note) Nonlinear equations: $y = 0.1x^3 - 0.8x^2 - 1.5x + 5.4$, $y = \sin x$

- [Vector space](#) (a.k.a. linear space): A set of vectors which can be 1) added together and 2) multiplied by scalars

- [Scalar](#): A single element

- e.g. x (one-dimensional)

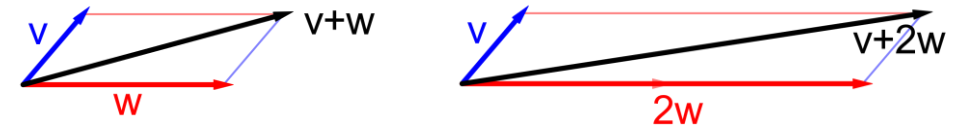
- [Vector](#): A finite ordered list of elements (a.k.a. [tuple](#))

- e.g. $[x, y]$ (two-dimensional row vector), ..., $[x_1, x_2, \dots, x_n]^T$ (n -dimensional column vector)

- [Matrix](#): A rectangular array (table) of elements arranged in **rows** and **columns** (a.k.a. [tensor](#))

- e.g. $m \times n$ matrix

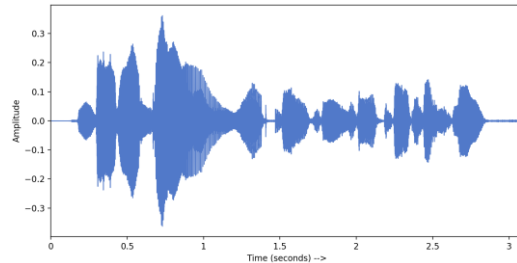
$$\begin{matrix} & \begin{matrix} 1 & 2 & \dots & n \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ \vdots \\ m \end{matrix} & \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ a_{31} & a_{32} & \dots & a_{3n} \\ \vdots & \vdots & \vdots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \end{matrix}$$



Vector

▪ Why a vector?

- To represent physical quantities
 - e.g. [Speed](#) (magnitude; **속력** in Korean) vs. [velocity](#) (magnitude+*direction*; **속도** in Korean)
- To represent data and models
 - e.g. A point $[1, 4]$, a line $2x + 3y - 14 = 0 \rightarrow [2, 3, -14]$, and its **normal vector** $[2, 3]$ or $[0.554 \dots, 8.832 \dots]$
 - e.g. Sound data



▪ Vector operations

- Vector addition (subtraction): $\mathbf{a} + \mathbf{b}$
- Scalar multiplication (division): $a \mathbf{b}$
- [Vector multiplication](#)
 - [Dot product](#) (a.k.a. scalar product): $\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i = a_1 b_1 + a_2 b_2 + \dots + a_n b_n$ or $\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos \theta$
 - [Cross product](#) (a.k.a. vector product): $\mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin \theta \mathbf{n}$

Vector

- **Norm** is a function from a vector space to the non-negative real numbers that behaves as like the distance from the origin (a.k.a. magnitude).

- Notation: $\|\mathbf{a}\|$ for a vector \mathbf{a}

- Properties

- Triangle inequality: $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$
- Absolute homogeneity: $\|a \mathbf{x}\| = |a| \|\mathbf{x}\|$
- Positive definiteness: If $\|\mathbf{x}\| = 0$, then $\mathbf{x} = \mathbf{0}$

- Examples

- **Absolute-value norm:** A norm on 1-dimensional vector spaces

$$\|\mathbf{x}\| = |x_1|$$

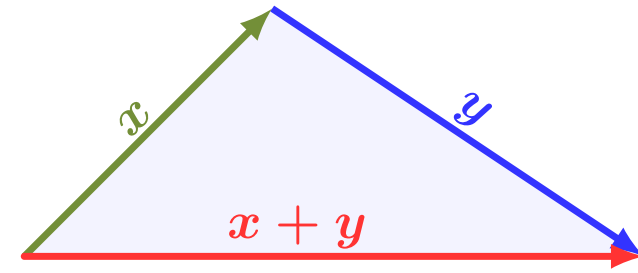
- **Euclidean norm** (a.k.a. L^2 -norm): The most common norm in n-dimensional [Euclidean spaces](#)

$$\|\mathbf{x}\|_2 = \sqrt{x_1^2 + x_2^2 + \cdots + x_n^2}$$

- **Manhattan norm** (a.k.a. L^1 -norm)

$$\|\mathbf{x}\|_1 = |x_1| + |x_2| + \cdots + |x_n|$$

- Note) [A norm can be defined for a matrix.](#)



Vector

- **Vector operations** (cont'd)

- [Vector multiplication](#)

- [Dot product](#) (a.k.a. scalar product)

- Geometric definition: $\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos \theta$

- Algebraic definition: $\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i = a_1 b_1 + a_2 b_2 + \dots + a_n b_n$

- As matrix multiplication: $\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^T \mathbf{b}$ where \mathbf{a} and \mathbf{b} are column vectors.

- $\mathbf{a} \cdot \mathbf{b} = \mathbf{a} \mathbf{b}^T$ where \mathbf{a} and \mathbf{b} are row vectors.

- e.g. $[3, 2] \cdot [5, 1] = 17$

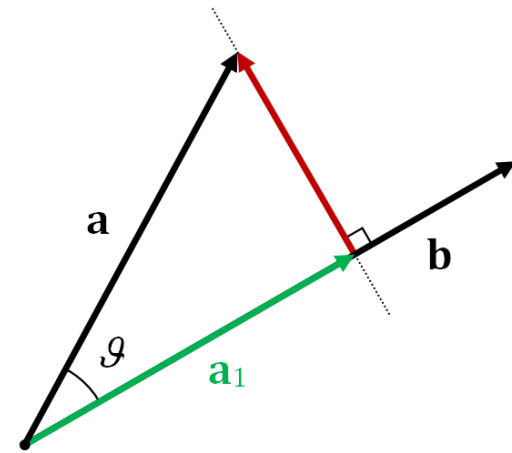
- e.g. $[3, 2, 9] \cdot [5, 1, -2] = -1$

- Applications

- [Scalar projection](#)

- (Directional) similarity of two vectors ([cosine similarity](#))

$$\cos \theta = \frac{\mathbf{a} \cdot \mathbf{b}}{\|\mathbf{a}\| \|\mathbf{b}\|}$$



Vector

▪ Vector operations (cont'd)

– [Vector multiplication](#)

- [Cross product](#) (a.k.a. vector product) is defined **only in a three-dimensional space**.

- Definition: $\mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin \theta \hat{\mathbf{n}}$

where $\hat{\mathbf{n}}$ is a unit vector **orthogonal** (수직 in Korean) to a plane containing \mathbf{a} and \mathbf{b}

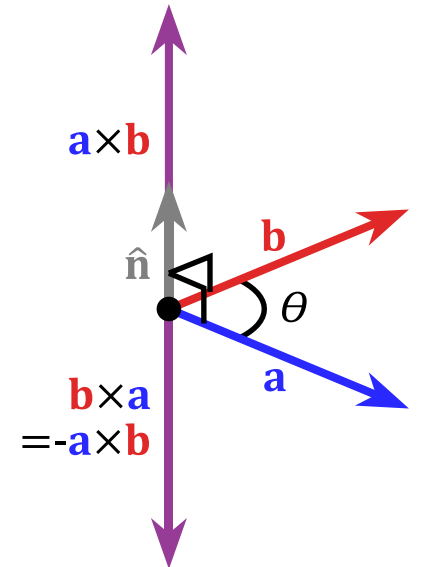
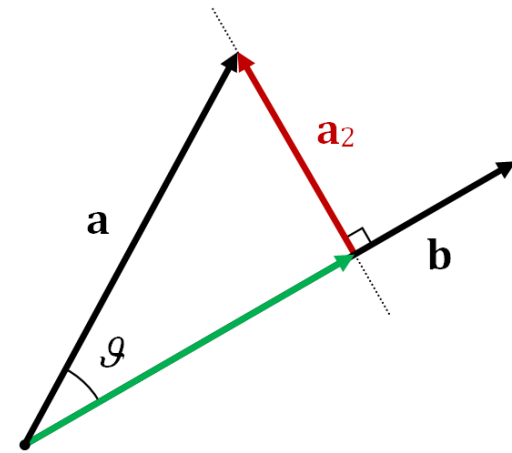
- Computing (using matrix determinant)

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = (a_2 b_3 - a_3 b_2) \mathbf{i} - (a_1 b_3 - a_3 b_1) \mathbf{j} + (a_1 b_2 - a_2 b_1) \mathbf{k}$$

- e.g. $[1, 4, 1] \times [4, 2, 1] = [2, 3, -14]$

- Applications

- Relationship of angular velocity, angular momentum, and torque in a 3D space
- Area of the [parallelogram](#) (평행사변형 in Korean) made by two vectors
- More applications in [computational geometry](#)



Vector

▪ Vector operations (cont'd)

– Vector multiplication

• Cross product

(a.k.a. vector product) is defined only in a 3D space

– Definition: $\mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin \theta \mathbf{n}$

where \mathbf{n} is a unit vector **orthogonal** (수직 in Korean) to a plane containing \mathbf{a} and \mathbf{b}

– Meaning

- Representing angular velocity, angular momentum, and torque
- Calculating the area of the parallelogram (평행사변형 in Korean) made by two vectors
- More applications in computational geometry

– Computing (using matrix multiplication)

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = (a_2 b_3 - a_3 b_2) \mathbf{i} - (a_1 b_3 - a_3 b_1) \mathbf{j} + (a_1 b_2 - a_2 b_1) \mathbf{k}$$

– e.g. $[1, 4, 1] \times [4, 2, 1] = [2, 3, -14]$

▪ Line representation: $ax + by + c = 0$

$$(2x + 3y - 14 = 0)$$

- Area of the parallelogram made by two vectors
- Line from two points
- Intersection point from two lines
- Distance between two *skew* lines
- Volume of the parallelepiped made by three vectors

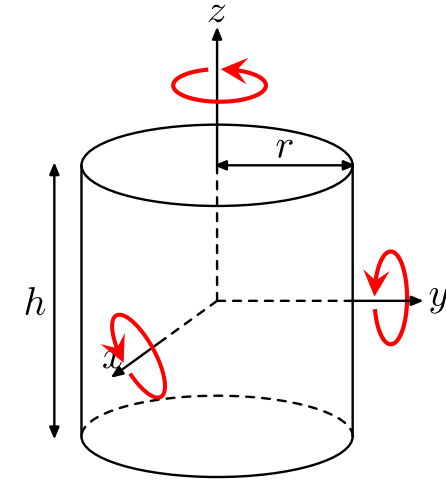
Matrix

▪ Why a matrix?

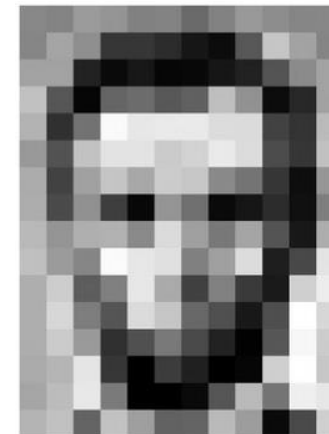
- To represent physical quantities
 - e.g. [Moment of inertia](#) in the 3D space (a.k.a. [inertia tensor](#))
- To represent data and models
 - e.g. Images, multiple sound
 - e.g. [State-space representation](#) (control theory), [camera projection](#)
- To represent geometric transformation
 - e.g. Rotation matrix $R(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix}$
 - e.g. [Rigid transformation](#), [camera projection](#)
- To solve a [system of linear equations](#) (선형연립방정식 in Korean)
 - e.g. A system of equations for a line from (1, 4) and (4, 2)

$$4 = w \cdot 1 + b$$

$$2 = w \cdot 4 + b$$



$$I = \begin{bmatrix} \frac{1}{12}m(3r^2 + h^2) & 0 & 0 \\ 0 & \frac{1}{12}m(3r^2 + h^2) & 0 \\ 0 & 0 & \frac{1}{2}mr^2 \end{bmatrix}$$



187	163	174	168	160	162	129	183	172	163	166	166
156	182	163	74	76	62	33	17	116	210	180	154
180	180	50	14	34	6	10	33	48	106	169	181
206	106	6	124	131	111	120	204	166	15	66	180
194	66	157	281	237	239	239	228	227	87	71	201
172	106	207	233	233	214	220	239	228	96	74	206
188	88	179	209	185	215	211	158	139	75	20	169
189	97	165	84	10	168	134	11	31	62	22	148
199	168	191	182	158	227	178	143	182	106	96	190
205	174	168	282	236	231	148	178	228	43	95	234
190	216	156	149	236	187	86	150	79	38	218	241
190	224	147	106	227	210	127	103	36	101	255	224
190	214	173	66	103	143	91	90	2	106	249	215
187	196	236	75	1	81	47	0	6	217	256	211
183	202	237	148	0	0	12	108	200	136	243	236
196	206	123	207	177	121	123	200	175	13	94	218

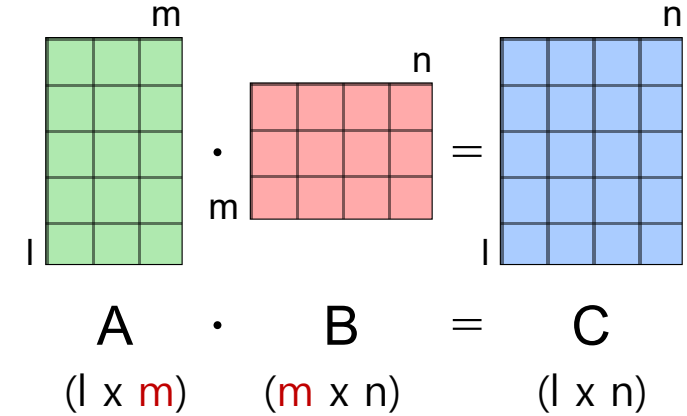
Matrix

▪ Matrix operations

- Matrix addition (subtraction): $A + B$
- Scalar multiplication (division): $a B$
- **Matrix multiplication** (a.k.a. matrix product): AB
 - **Not commutative** (교환법칙 in Korean): $AB \neq BA$
 - Example) ~~Proof~~ Verification using [SymPy](#)
`import sympy as sp`

```
a11, a12, a21, a22 = sp.symbols('a11 a12 a21 a22')
b11, b12, b21, b22 = sp.symbols('b11 b12 b21 b22')
A = sp.Matrix([[a11, a12], [a21, a22]])
B = sp.Matrix([[b11, b12], [b21, b22]])
```

```
print(A+B == B+A) # True
print(A*B == B*A) # False
print(A*B - B*A) # Check their difference
```



Matrix

- **Matrix operations** (cont'd)

- **Matrix inverse** ($AA^{-1} = A^{-1}A = I$; ~ 역수 in Korean)
 - Invertible matrix (a.k.a. non-singular matrix, non-degenerate matrix) if A is
 - Square (A : $n \times n$ matrix)
 - Linearly independent rows/columns
 - Full rank ($\text{rank}(A) = n$)
 - Non-zero determinant ($\det(A) \neq 0$ or $|A| \neq 0$)
- Pseudo-inverse (~ a generalized matrix inverse)
 - **Not necessarily square** (A : $m \times n$ matrix, A^\dagger : $n \times m$ matrix)
 - Left inverse ($A^\dagger A = I_n$): $A^\dagger = (A^T A)^{-1} A^T$
 - If A has linearly independent columns ($\text{rank}(A) = n$)
 - Right inverse ($AA^\dagger = I_m$): $A^\dagger = A^T (AA^T)^{-1}$
 - If A has linearly independent rows ($\text{rank}(A) = m$)

Matrix

- **Matrix operations** (cont'd)

- **Matrix inverse**

- Example) Line fitting from two points, (1, 4) and (4, 2)

- Line representation: $y = wx + b$

- A system of equations: $w \cdot 1 + b = 4$

$$w \cdot 4 + b = 2$$



$$\begin{bmatrix} 1 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} w \\ b \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$$

$$(A\mathbf{x} = \mathbf{b})$$

$$\longrightarrow \mathbf{x} = A^{-1}\mathbf{b}$$

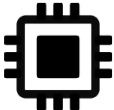













- Pseudo-inverse

- Example) Line fitting from more than two points such as (1, 4), (4, 2), and (7, 1)

- $A = \begin{bmatrix} 1 & 1 \\ 4 & 1 \\ 7 & 1 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix}$

NumPy: A Matrix Library in Python

- [NumPy](#) supports multi-dimensional arrays and matrices with their high-level mathematical functions.
 - It is fundamental for scientific and numerical computing in Python.
- References: [Documentation](#), [Tutorials/Books/Talks](#), and [Cheatsheet](#) (made by DataCamp)

Quantum Computing  QuTiP PyQuil Qiskit	Statistical Computing  Pandas statsmodels Xarray Seaborn	Signal Processing  SciPy PyWavelets python-control	Image Processing  Scikit-image OpenCV Mahotas	Graphs and Networks  NetworkX graph-tool igraph PyGSP	Astronomy Processes  AstroPy SunPy SpacePy	Cognitive Psychology  PsychoPy
Bioinformatics  BioPython Scikit-Bio PyEnsembl ETE	Bayesian Inference  PyStan PyMC3 ArviZ emcee	Mathematical Analysis  SciPy SymPy cvxpy FEniCS	Chemistry  Cantera MDAnalysis RDKit	Geoscience  Pangeo Simpeg ObsPy Fatiando a Terra	Geographic Processing  Shapely GeoPandas Folium	Architecture & Engineering  COMPAS City Energy Analyst Sverchok

NumPy:

- NumPy
 - It is
- Referen

Python For Data Science Cheat Sheet

NumPy Basics

Learn Python for Data Science Interactively at [www.DataCamp.com](https://www.datacamp.com)



NumPy

The NumPy library is the core library for scientific computing in Python. It provides a high-performance multidimensional array object, and tools for working with these arrays.

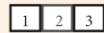
Use the following import convention:

```
>>> import numpy as np
```

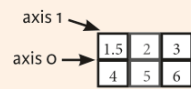


NumPy Arrays

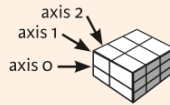
1D array



2D array



3D array



Creating Arrays

```
>>> a = np.array([1,2,3])
>>> b = np.array([(1.5,2,3), (4,5,6)], dtype = float)
>>> c = np.array([(1.5,2,3), (4,5,6)], [(3,2,1), (4,5,6)]),
dtype = float)
```

Initial Placeholders

```
>>> np.zeros((3,4))
>>> np.ones((2,3,4),dtype=np.int16)
>>> d = np.arange(10,25,5)

>>> np.linspace(0,2,9)

>>> e = np.full((2,2),7)
>>> f = np.eye(2)
>>> np.random.random((2,2))
>>> np.empty((3,2))
```

Create an array of zeros
Create an array of ones
Create an array of evenly spaced values (step value)
Create an array of evenly spaced values (number of samples)
Create a constant array
Create a 2X2 identity matrix
Create an array with random values
Create an empty array

I/O

Saving & Loading On Disk

```
>>> np.save('my_array', a)
>>> np savez('array.npz', a, b)
>>> np.load('my_array.npy')
```

Saving & Loading Text Files

```
>>> np.loadtxt("myfile.txt")
>>> np.genfromtxt("my_file.csv", delimiter=',')
>>> np.savetxt("myarray.txt", a, delimiter=" ")
```

Data Types

```
>>> np.int64
>>> np.float32
>>> np.complex
>>> np.bool
>>> np.object
>>> np.string_
>>> np.unicode_
```

Signed 64-bit integer types
Standard double-precision floating point
Complex numbers represented by 128 floats
Boolean type storing TRUE and FALSE values
Python object type
Fixed-length string type
Fixed-length unicode type

Inspecting Your Array

```
>>> a.shape
>>> len(a)
>>> b.ndim
>>> e.size
>>> b.dtype
>>> b.dtype.name
>>> b.astype(int)
```

Array dimensions
Length of array
Number of array dimensions
Number of array elements
Data type of array elements
Name of data type
Convert an array to a different type

Asking For Help

```
>>> np.info(np.ndarray.dtype)
```

Array Mathematics

Arithmetic Operations

```
>>> g = a - b
array([[ -0.5,  0. ,  0. ],
       [-3. , -3. , -3. ]])
>>> np.subtract(a,b)
>>> b + a
array([[ 2.5,  4. ,  6. ],
       [ 5. ,  7. ,  9. ]])
>>> np.add(b,a)
>>> a / b
array([[ 0.66666667,  1. ,  1. ],
       [ 0.25 ,  0.4 ,  0.5 ]])
>>> np.divide(a,b)
>>> a * b
array([[ 1.5,  4. ,  9. ],
       [ 4. , 10. , 18. ]])
>>> np.multiply(a,b)
>>> np.exp(b)
>>> np.sqrt(b)
>>> np.sin(a)
>>> np.cos(b)
>>> np.log(a)
>>> e.dot(f)
array([[ 7. ,  7.]])
```

Subtraction
Subtraction
Addition
Addition
Division
Division
Multiplication
Multiplication
Exponentiation
Square root
Print sines of an array
Element-wise cosine
Element-wise natural logarithm
Dot product

Comparison

```
>>> a == b
array([[False,  True,  True],
       [False, False, False]], dtype=bool)
>>> a < 2
array([[True, False, False], dtype=bool)
>>> np.array_equal(a, b)
```

Element-wise comparison
Element-wise comparison
Array-wise comparison

Aggregate Functions

```
>>> a.sum()
>>> a.min()
>>> b.max(axis=0)
>>> b.cumsum(axis=1)
>>> a.mean()
>>> b.median()
>>> a.corrcoef()
>>> np.std(b)
```

Array-wise sum
Array-wise minimum value
Maximum value of an array row
Cumulative sum of the elements
Mean
Median
Correlation coefficient
Standard deviation

Copying Arrays

```
>>> h = a.view()
>>> np.copy(a)
>>> h = a.copy()
```

Create a view of the array with the same data
Create a copy of the array
Create a deep copy of the array

Sorting Arrays

```
>>> a.sort()
>>> c.sort(axis=0)
```

Sort an array
Sort the elements of an array's axis

Subsetting, Slicing, Indexing

Also see Lists

Subsetting

```
>>> a[2]
3
```



Select the element at the 2nd index

```
>>> b[1,2]
6.0
```

Select the element at row 1 column 2 (equivalent to b[1][2])

Slicing

```
>>> a[0:2]
array([1, 2])
```



Select items at index 0 and 1

```
>>> b[0:2,1]
array([ 2.,  5.])
```



Select items at rows 0 and 1 in column 1

```
>>> b[:1]
array([[1.5, 2., 3.]])
```



Select all items at row 0 (equivalent to b[0:1, :])
Same as [1, :, :]

```
>>> c[1,...]
array([[ 3.,  2.,  1.],
       [ 4.,  5.,  6.]])
```



Reversed array a

```
>>> a[: :-1]
array([3, 2, 1])
```



Boolean Indexing

```
>>> a[a<2]
array([1])
```



Select elements from a less than 2

Fancy Indexing

```
>>> b[[1, 0, 1, 0], [0, 1, 2, 0]]
array([ 4. ,  2. ,  6. ,  1.5])
>>> b[[1, 0, 1, 0]][:, [0,1,2,0]]
array([[ 4.,  5.,  6.,  4. ],
       [ 1.5,  2.,  3.,  1.5],
       [ 4.,  5.,  6.,  4. ],
       [ 1.5,  2.,  3.,  1.5]])
```

Select elements (1,0), (0,1), (1,2) and (0,0)
Select a subset of the matrix's rows and columns

Array Manipulation

Transposing Array

```
>>> i = np.transpose(b)
>>> i.T
```

Permute array dimensions
Permute array dimensions

Changing Array Shape

```
>>> b.ravel()
>>> g.reshape(3,-2)
```

Flatten the array
Reshape, but don't change data

Adding/Removing Elements

```
>>> h.resize((2,6))
>>> np.append(h,g)
>>> np.insert(a, 1, 5)
>>> np.delete(a, [1])
```

Return a new array with shape (2,6)
Append items to an array
Insert items in an array
Delete items from an array

Combining Arrays

```
>>> np.concatenate((a,d),axis=0)
array([ 1,  2,  3, 10, 15, 20])
>>> np.vstack((a,b))
array([[ 1. ,  2. ,  3. ],
       [ 1.5,  2. ,  3. ],
       [ 4. ,  5. ,  6. ]])
>>> np.r_[e,f]
>>> np.hstack((e,f))
array([[ 7. ,  7. ,  1. ,  0. ],
       [ 7. ,  7. ,  0. ,  1.]])
>>> np.column_stack((a,d))
array([[ 1, 10],
       [ 2, 15],
       [ 3, 20]])
>>> np.c_[a,d]
```

Concatenate arrays
Stack arrays vertically (row-wise)
Stack arrays vertically (row-wise)
Stack arrays horizontally (column-wise)
Create stacked column-wise arrays
Create stacked column-wise arrays

Splitting Arrays

```
>>> np.hsplit(a,3)
[array([1]),array([2]),array([3])]
>>> np.vsplit(c,2)
[array([[ 1.5,  2. ,  1. ],
       [ 4. ,  5. ,  6. ]]),
array([[ 3.,  2.,  3. ],
       [ 4.,  5.,  6.]])]
```

Split the array horizontally at the 3rd index
Split the array vertically at the 2nd index



NumPy: A Matrix Library in Python

- Usage example) Creating n-dimensional arrays (1/2)
 - `numpy.array` can contain a **homogenous** (~ same) data type. (vs. list and tuple)

```
import numpy as np
```

```
# 1. Create an array from a composite data (list or tuple, not set and dictionary)
```

```
A = np.array([3, 29, 82])
```

```
B = np.array(((3., 29, 82), (10, 18, 84)))
```

```
C = np.array([[3, 29, 82], [10, 18, 84]], dtype=float)
```

```
D = np.array([3, 29, 'Choi'])
```

```
E = np.array([[3], [29], [82]])
```

```
print(A.ndim, A.size, A.shape, A.dtype) # 1 3 (3,) int32
```

```
# Note) np.array_equal(A, A.T) == True
```

```
print(B.ndim, B.size, B.shape, B.dtype) # 2 6 (2, 3) float64
```

```
print(C.ndim, C.size, C.shape, C.dtype) # 2 6 (2, 3) float64
```

```
print(D.ndim, D.size, D.shape, D.dtype) # 1 3 (3,) <U11 (Unicode)
```

```
# Note) array(['3', '29', 'Choi'])
```

```
print(E.ndim, E.size, E.shape, E.dtype) # 2 3 (3,1) int32
```

```
# Note) np.array_equal(E, E.T) == False
```

```
# because E.T == array([[3, 29, 82]])
```

NumPy: A Matrix Library in Python

- Usage example) Creating n-dimensional arrays (2/2)
 - `numpy.array` can contain a **homogenous** (~ same) data type. (vs. list and tuple)

```
import numpy as np
```

```
# 2. Create an array using initializers
```

```
F = np.zeros((3, 2))          # Create a 3x2 array filled with 0 (default: float64)
G = np.ones((3, 2))           # Create a 2x3 array filled with 1
H = np.eye(3, dtype=np.float32) # Create a 3x3 identity matrix (single-precision)
I = np.empty((3, 2))          # == np.zeros((3, 2))
J = np.empty((0, 9))           # [ ] with size of (0, 9)
K = np.arange(0, 1, 0.2)       # Step 0.2: array([0., 0.2, 0.4, 0.6, 0.8])
L = np.linspace(0, 1, 5)       # Number 5: array([0., 0.25, 0.50, 0.75, 1.])
M = np.random.random((3, 2))   # == np.random.uniform(size=(3, 2))
                                # Note) np.random.normal()
```

NumPy: A Matrix Library in Python

- Usage example) Indexing and slicing
 - numpy.array can access elements of a n-dim array not only with `[r][c]` but also with `[r,c]`.
 - numpy.array can access elements with a Boolean array (called **logical indexing**).

```
import numpy as np
A = np.array(((3., 29, 82), (10, 18, 84)))
```

	0	1	2
0	3	29	82
1	10	18	84

```
# 1. Indexing and slicing
```

```
A[1][1]                # 18.0
A[1, 1]                # 18.0 Note) list[1, 1] does not work!
A[1,1:2]               # array([18.])
A[1,:]                # Get a row:      array([10., 18., 84.])
A[:,2]                # Get a column:   array([82., 84.])
A[0:2,0:2]            # Get a submatrix: array([[3., 29.], [10., 18.]])
```

```
# 2. Logical indexing
```

```
A > 80                 # array([[False, False, True], [False, False, True]])
A[A > 80]              # array([82., 84.])
A[A > 80] = 80         # Masked operations are possible!
```

```
# 3. Fancy indexing
```

```
A[(1, 0, 0), (1, 0, 2)] # array([18., 3., 82.])
                        # Get items at (1, 1), (0, 0), (0, 2)
```

NumPy: A Matrix Library in Python

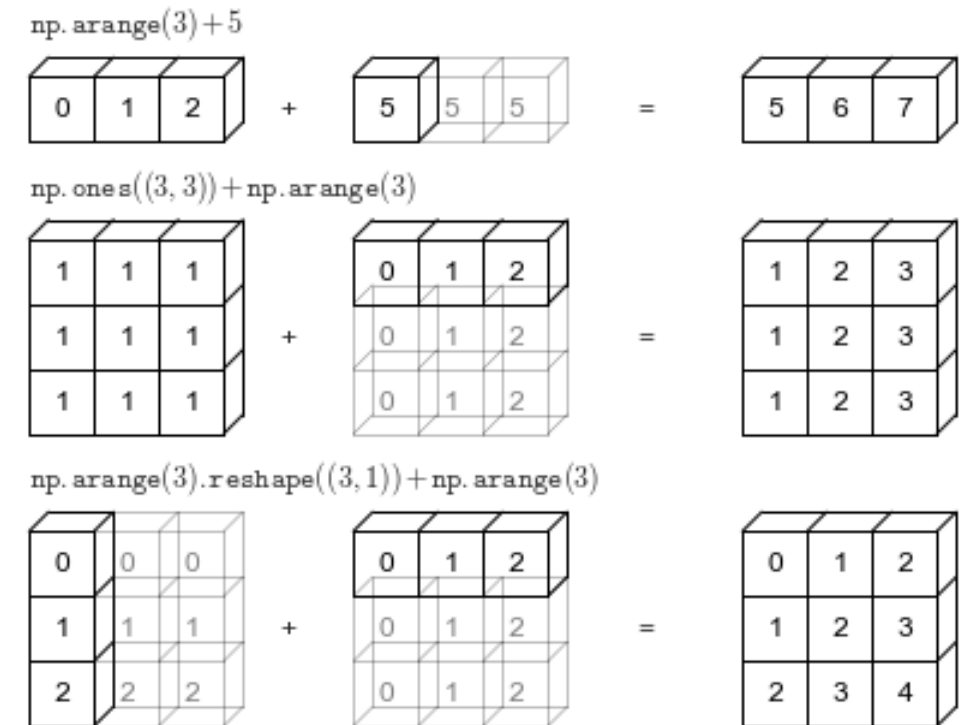
- Usage example) Arithmetic operations (vs. list and tuple)

```
import numpy as np
A = np.array([[1, 2], [3, 4]])
B = np.array([[5, 6], [7, 8]])

# 1. Element-wise arithmetic operations
print(A + B)           # np.add(A, B)
print(A - B)           # np.subtract(A, B)
print(A * B)           # np.multiply(A, B)
print(A / B)           # np.divide(A, B)

# 2. Matrix operations
print(A.T)              # A.transpose()
print(A @ B)            # np.matmul(A, B)
print(np.linalg.norm(A)) # 5.48 (default: L2-norm)
print(np.linalg.matrix_rank(A)) # 2, full rank
print(np.linalg.det(A))   # -2, non-zero determinant
print(np.linalg.inv(A))   # Matrix inverse
print(np.linalg.pinv(A))  # Matrix pseudo-inverse

# 3. Broadcasting
print(A + 1)            # [[2, 3], [4, 5]]
print(A + [0, -1])      # [[1, 1], [3, 3]]
print(A + [[1], [-1]])  # [[2, 3], [2, 3]]
```



Matrix

- Example) Line fitting from two points, (1, 4) and (4, 2)

- Line representation: $y = ax + b$
- A system of equations: $a \cdot 1 + b = 4$

$$a \cdot 4 + b = 2$$



$$\begin{bmatrix} 1 & 1 \\ 4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$$

$$(A\mathbf{x} = \mathbf{b})$$

$$\longrightarrow \mathbf{x} = A^{-1}\mathbf{b}$$

- Example) Line fitting from two points, (1, 4) and (4, 2), using [NumPy](#)

```
import numpy as np
```

```
A = np.array([[1., 1.], [4., 1.]])
```

```
b = np.array([[4.], [2.]])
```

```
A_inv = np.linalg.inv(A)
```

```
print(A_inv * b) # [[-1.33333333  1.33333333]
```

```
                # [ 2.66666667 -0.66666667]] Note) broadcast
```

```
print(A_inv @ b) # [[-0.66666667]
```

```
                # [ 4.66666667]]
```

Matrix

- Example) Line fitting from two points, (1,4) and (4,2), using [NumPy](#)

```
import numpy as np
```

```
A = np.array([[1., 1.], [4., 1.]])
```

```
b = np.array([[4.], [2.]])
```

```
A_inv = np.linalg.inv(A)
```

```
print(A_inv @ b) # [[-0.6666667]  
# [ 4.6666667]]
```

- Example) Line fitting from more than two points such as (1,4), (4,2), and (7,1) using [NumPy](#)

– $A = \begin{bmatrix} 1 & 1 \\ 4 & 1 \\ 7 & 1 \end{bmatrix}$ and $\mathbf{b} = \begin{bmatrix} 4 \\ 2 \\ 1 \end{bmatrix}$

```
import numpy as np
```

```
A = np.array([[1., 1.], [4., 1.], [7., 1.]])
```

```
b = np.array([[4.], [2.], [1.]])
```

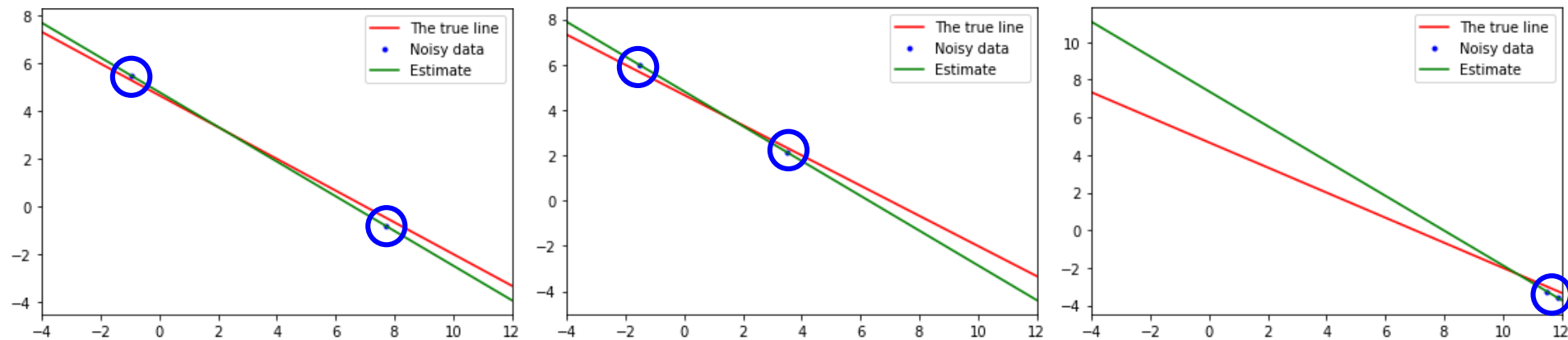
```
A_inv = np.linalg.pinv(A) # Left inverse
```

```
print(A_inv @ b) # [[-0.5]  
# [ 4.33333333]]
```

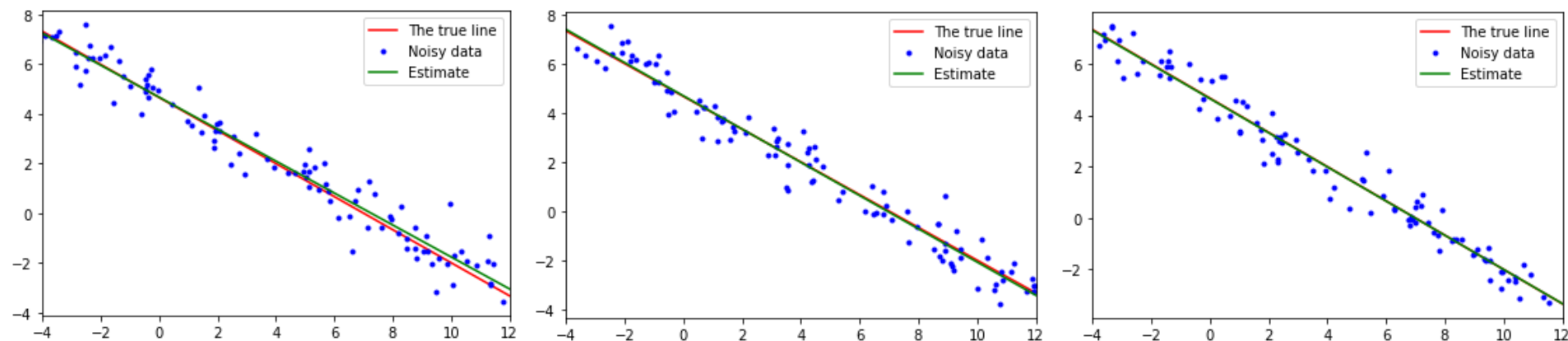
Matrix

- Example) Line fitting with noisy but more data (1/2)

- data_num = 2



- data_num = 100



Matrix

- Example) Line fitting with noisy but more data (2/2)

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

true_line = lambda x: -2/3*x + 14/3
data_range = np.array([-4, 12])
data_num = 100
noise_std = 0.5

# Generate the true data
x = np.random.uniform(data_range[0], data_range[1], size=data_num)
y = true_line(x) # y = -2/3*x + 10/3

# Add Gaussian noise
xn = x + np.random.normal(scale=noise_std, size=x.shape)
yn = y + np.random.normal(scale=noise_std, size=y.shape)

# Solve the system of equations
A = np.vstack((xn, np.ones(xn.shape))).T
b = yn
line = np.linalg.pinv(A) @ b

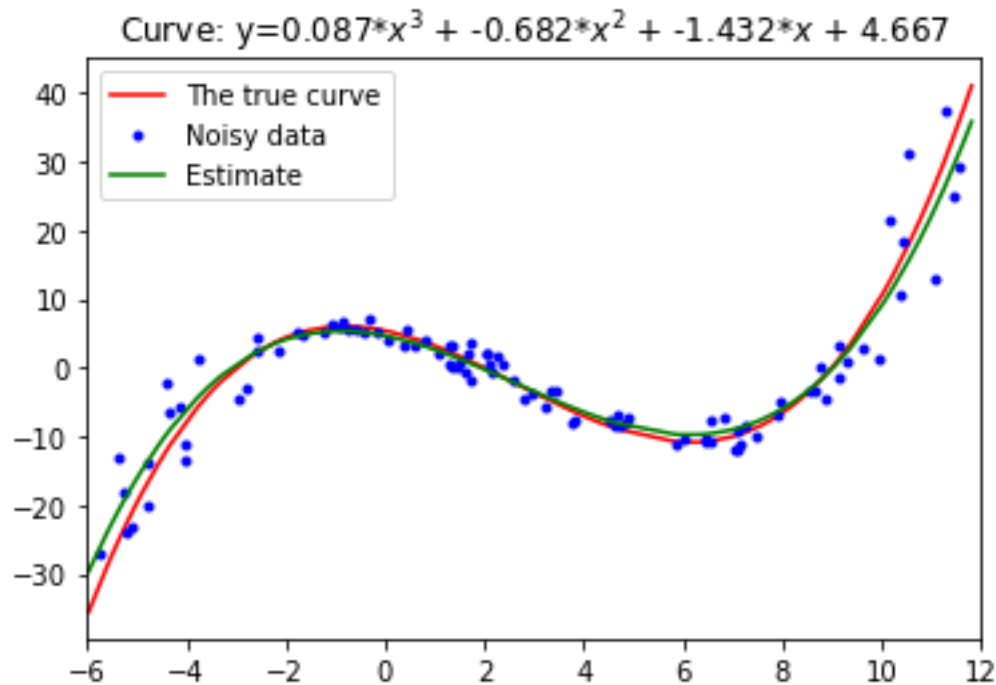
# Plot the data and result
plt.title(f'Line: y={line[0]:.3f}*x + {line[1]:.3f} ')
plt.plot(data_range, true_line(data_range), 'r-', label='The true line')
plt.plot(xn, yn, 'b.', label='Noisy data')
plt.plot(data_range, line[0]*data_range + line[1], 'g-', label='Estimate')
plt.xlim(data_range)
plt.legend()
plt.show()
```

$$\begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix} \xrightarrow{\text{transpose}} \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

(Ax = b)

Matrix

- Example) Curve fitting (1/2)
 - Curve representation: $y = ax^3 + bx^2 + cx + d$ (a 3rd-order polynomial equation)
 - e.g. $y = 0.1x^3 - 0.8x^2 - 1.5x + 5.4$



$$\begin{bmatrix} x_1^3 & x_1^2 & x_1 & 1 \\ x_2^3 & x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_n^3 & x_n^2 & x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

($A\mathbf{x} = \mathbf{b}$)

Matrix

- Example) Curve fitting (2/2)

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

true_curve = lambda x: 0.1*x**3 - 0.8*x**2 - 1.5*x + 5.4
data_range = (-6, 12)
data_num = 100
noise_std = 0.5

# Generate the true data
x = np.random.uniform(data_range[0], data_range[1], size=data_num)
y = true_curve(x)

# Add Gaussian noise
xn = x + np.random.normal(scale=noise_std, size=x.shape)
yn = y + np.random.normal(scale=noise_std, size=y.shape)

# Solve the system of equations
A = np.vstack((xn**3, xn**2, xn, np.ones(xn.shape))).T
b = yn
curve = np.linalg.pinv(A) @ b

# Plot the data and result
plt.title(f'Curve: y={curve[0]:.3f}*x^3 + {curve[1]:.3f}*x^2 + {curve[2]:.3f}*x + {curve[3]:.3f}')
xc = np.linspace(data_range[0], data_range[1], 100)
plt.plot(xc, true_curve(xc), 'r-', label='The true curve')
plt.plot(xn, yn, 'b.', label='Noisy data')
plt.plot(xc, curve[0]*xc**3 + curve[1]*xc**2 + curve[2]*xc + curve[3], 'g-', label='Estimate')
plt.xlim(data_range)
plt.legend()
plt.show()
```

$$\begin{bmatrix} x_1^3 & x_1^2 & x_1 & 1 \\ x_2^3 & x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ x_n^3 & x_n^2 & x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

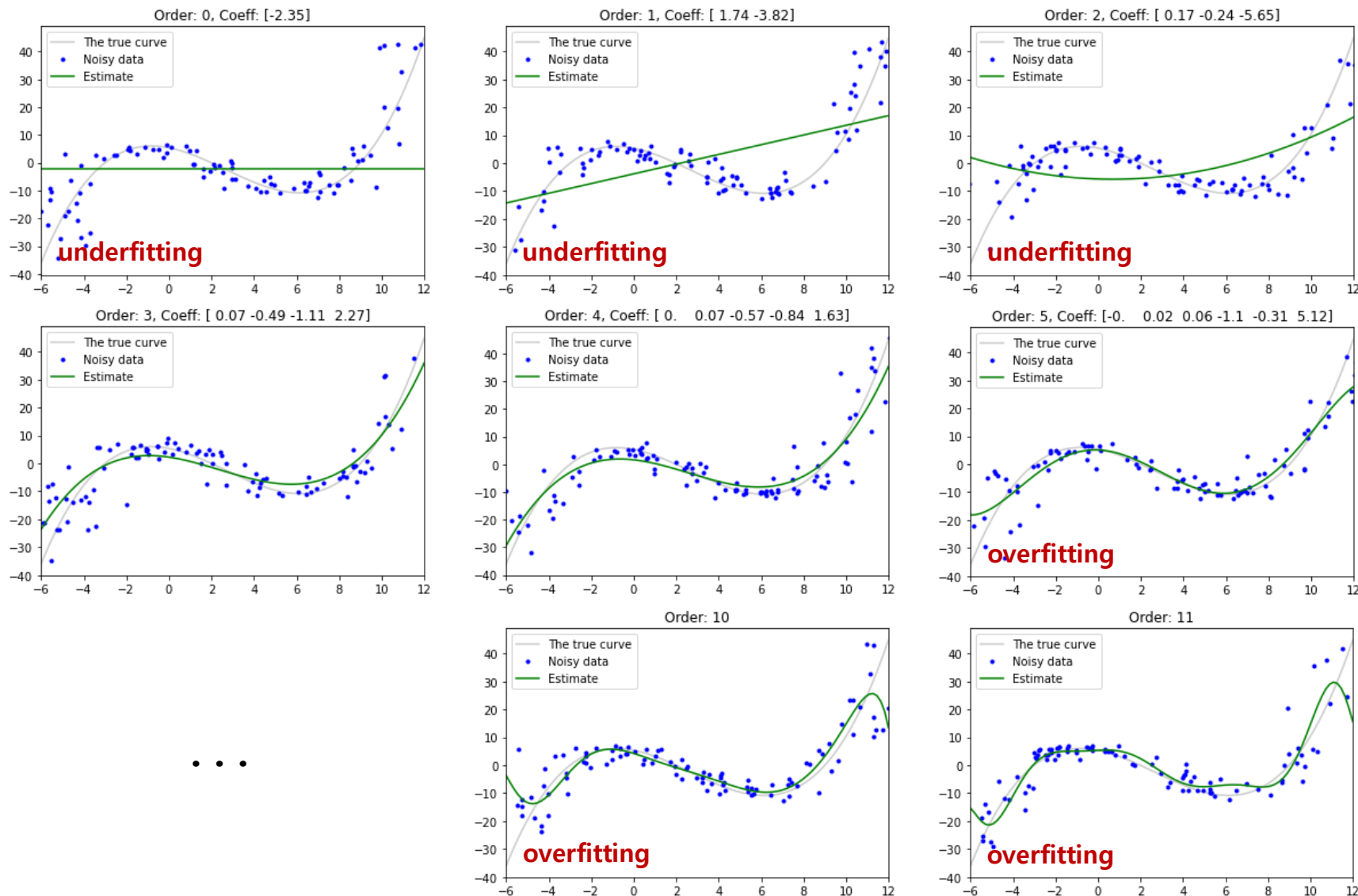
$(A\mathbf{x} = \mathbf{b})$

Matrix

- Example) Curve fitting with model selection (1/2)

$$\begin{bmatrix} x_1^r & x_1^{r-1} & \cdots & x_1^2 & x_1 & 1 \\ x_2^r & x_2^{r-1} & \cdots & x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^r & x_n^{r-1} & \cdots & x_n^2 & x_n & 1 \end{bmatrix} \begin{bmatrix} c_r \\ c_{r-1} \\ \vdots \\ c_2 \\ c_1 \\ c_0 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

($Ax = b$)



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

```
def buildA(order, xs):
    A = np.empty((0, len(xs)))
    for i in range(order + 1):
        A = np.vstack((xs**i, A))
    return A.T
```

```
true_coeff = [0.1, -0.8, -1.5, 5.4]
poly_order = 3 # Try other integer (>= 0)
data_range = (-6, 12)
data_num = 100
noise_std = 1
```

```
# Generate the true data
x = np.random.uniform(data_range[0], data_range[1], size=data_num)
y = buildA(len(true_coeff) - 1, x) @ true_coeff
```

```
# Add Gaussian noise
xn = x + np.random.normal(scale=noise_std, size=x.shape)
yn = y + np.random.normal(scale=noise_std, size=y.shape)
```

```
# Solve the system of equations
A = buildA(poly_order, xn)
b = yn
coeff = np.linalg.pinv(A) @ b
```

```
# Plot the data and result
plt.title(f'Order: {poly_order}, Coeff: ' + np.array2string(coeff, precision=2, suppress_small=True))
xc = np.linspace(*data_range, 100)
plt.plot(xc, np.matmul(buildA(len(true_coeff) - 1, xc), true_coeff), 'k-', label='The true curve', alpha=0.2)
plt.plot(xn, yn, 'b.', label='Noisy data')
plt.plot(xc, np.matmul(buildA(poly_order, xc), coeff), 'g-', label='Estimate')
plt.xlim(data_range)
plt.legend()
plt.show()
```

$$\begin{bmatrix} x_1^r & x_1^{r-1} & \cdots & x_1^2 & x_1 & 1 \\ x_2^r & x_2^{r-1} & \cdots & x_2^2 & x_2 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_n^r & x_n^{r-1} & \cdots & x_n^2 & x_n & 1 \end{bmatrix} \begin{bmatrix} c_r \\ c_{r-1} \\ \vdots \\ c_2 \\ c_1 \\ c_0 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

($\mathbf{Ax} = \mathbf{b}$)

Matrix

- Example) Line fitting from two points, (1, 4) and (1, 2)

- Line representation: $y = ax + b$
- A system of equations: $a \cdot 1 + b = 4$

$$a \cdot 1 + b = 2$$



$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 4 \\ 2 \end{bmatrix}$$

$$(A\mathbf{x} = \mathbf{b})$$

$$\longrightarrow \mathbf{x} = A^{-1}\mathbf{b}$$

- Example) Line fitting from two points, (1, 4) and (1, 2), using [NumPy](#)

```
import numpy as np
```

```
A = np.array([[1., 1.], [1., 1.]])
```

```
b = np.array([[4.], [2.]])
```

```
A_inv = np.linalg.inv(A) # Error! (singular matrix)
```

```
print(A_inv @ b)
```

Matrix

- **Null space** (a.k.a. [kernel](#))

- A set of vectors which map A (m -by- n matrix) to the zero vector

$$N(A) = \{ \mathbf{v} \in K^n \mid A\mathbf{v} = \mathbf{0} \}$$

- [Rank-nullity theorem](#): $\text{rank}(A) + \text{nullity}(A) = n$
- Application) Solving a **homogenous** system of linear equations, $A\mathbf{x} = \mathbf{0}$

- Practice) Line fitting from two points, $(1, 4)$ and $(1, 2)$, using [NumPy](#)

- Line representation: $ax + by + c = 0$

How about $(1, 4)$ and $(4, 2)$?

- In a matrix form, $\begin{bmatrix} 1 & 4 & 1 \\ 1 & 2 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

```
import numpy as np
from scipy import linalg
```

```
A = np.array([[1., 4., 1.], [1., 2., 1.]])
x = linalg.null_space(A)
print(x / x[0]) # [[1.], [0.], [-1.]] Note) Line:  $x - 1 = 0$ 
```

Summary

- [NumPy](#): N-dimensional array representation and [numerical analysis](#) (수치해석 in Korean)

- `numpy.array` vs. `list/tuple`
 - Homogeneous data type
 - + Indexing/slicing and arithmetic operations

~~▪ Linear algebra~~ [Vector](#)

- Why? 1) To represent physical quantities / 2) To represent data and models
- Vector operations
 - Note) [Norm](#) (~ the distance from the origin, magnitude)
 - [Vector multiplication](#)
 - Dot product: $\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \cos \theta$
 - Applications: [Cosine similarity](#)
 - Cross product: $\mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin \theta \hat{\mathbf{n}}$ ($\hat{\mathbf{n}}$: the unit orthogonal vector of \mathbf{a} and \mathbf{b}) defined in 3D spaces
 - Applications: Physics in a 3D space, ..., [computational geometry](#)

Summary

~~Linear algebra~~ Matrix

- Why? + 3) To represent geometric transformation / 4) **To solve a system of linear equations**
- Matrix operations
 - Matrix multiplication (not commutative)
 - Matrix inverse (square + full rank), pseudo-inverse
- Examples) **Line and curve fitting** (regression analysis; 회귀분석 in Korean)
 - What is a model and its parameters?
 - e.g. Line: $y = ax + b$ (or $ax + by + c = 0$)
 - e.g. Curve: n th-order polynomial equations (e.g. $y = ax^3 + bx^2 + cx + d$)
 - How to formulate the problem using matrices: $A\mathbf{x} = \mathbf{b}$ (or $A\mathbf{x} = \mathbf{0}$)
 - How to solve the equations using matrix operations: Pseudo-inverse (or finding null vectors)
 - Lesson #1) **Benefit of more (over-constrained) data**
 - The estimation result becomes *robust* (\sim strong) to noise!
 - Lesson #2) Underfitting and overfitting in model selection
 - More complex (flexible) models may have little error but may not be desired.