PROGRAM STUDI INFORMATIKA
FAKULTAS TEKNIK DAN INFORMATIKA
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IF420 – ANALISIS NUMERIK

Pertemuan ke 6 – Least Squares Regression

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Capaian Pembelajaran Mingguan Mata Kuliah (Sub-CPMK):

Sub-CPMK 6: Mahasiswa mampu memahami dan menerapkan regresi kuadrat terkecil – C3

Reviews

- Eigenvalues and Eigenvectors Problem Statement
- The Power Method
- The QR Method
- Eigenvalues and Eigenvectors in Python

Outlines

- Least Squares Regression Problem Statement
- Least Squares Regression Derivation (Linear Algebra)
- Least Squares Regression Derivation (Multivariable Calculus)
- Least Squares Regression in Python
- Least Squares Regression for Nonlinear Functions

Motivation

- Often in science and engineering coursework, we are asked to determine the **state** of a **system** given the **parameters** of the system.
- For example, the relationship between the force exerted by a linear spring, F, and the displacement of the spring from its natural length, x, is usually represented by the model

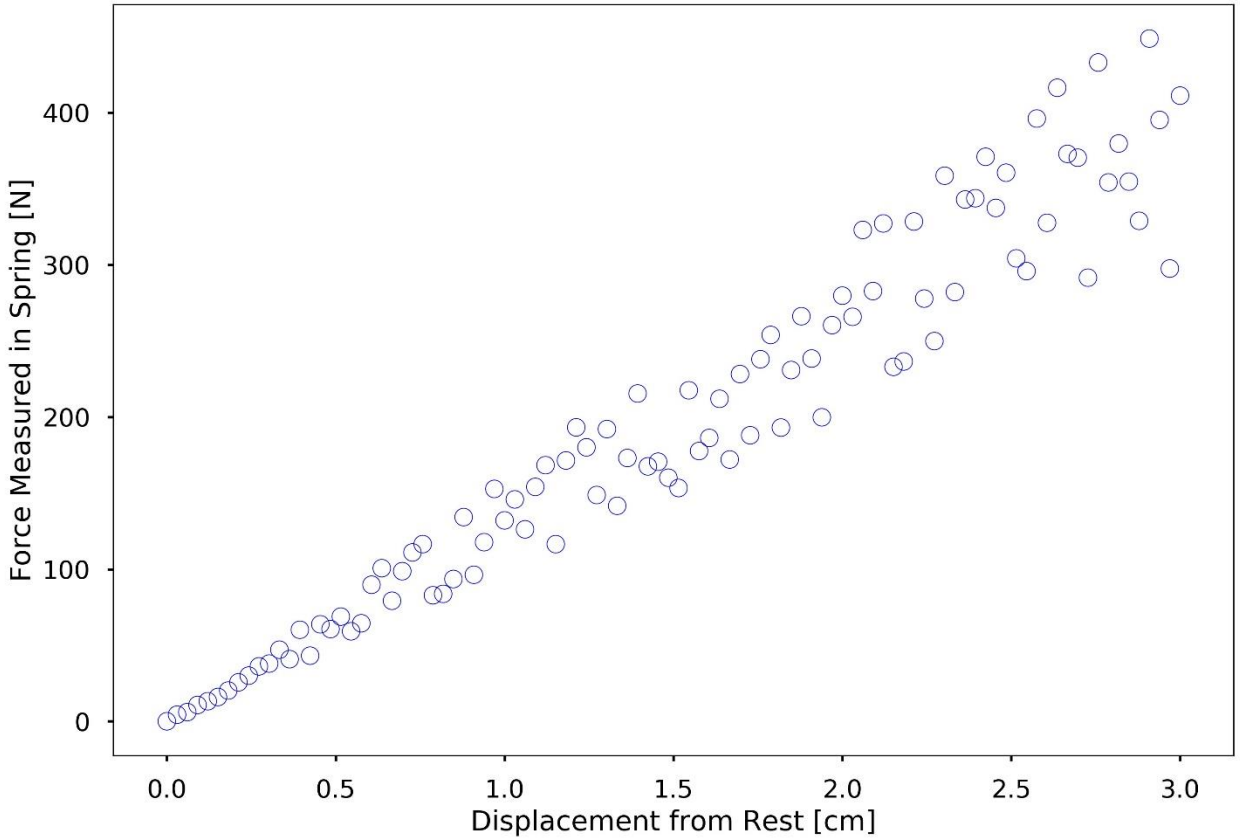
$$F = kx$$

  where k is the spring stiffness. We are then asked to compute the force for a given k and x value.

- However in practice, the stiffness and in general, most of the **parameters** of a system, are **not known** a **priori**.
- Instead, we are usually presented with **data points** about how the system has **behaved** in the past.

- For our spring example, we may be given (x, F) data pairs that have been previously recorded from an experiment. Ideally, all these data points would lie exactly on a line going through the origin (since there is no force at zero displacement). We could then measure the slope of this line and get our **stiffness value** for k. However, practical data usually has some measurement **noise** because of **sensor inaccuracy**, **measurement error**, or a variety of other reasons.

- The following figure shows an example of what data might look like for a simple spring experiment.
- Today lesson teaches **methods** of finding the "**most likely**" **model parameters given a set of data**, e.g., how to find the **spring stiffness** in our mock experiment.



The Problem Statement

- Given a set of **independent** data points x_i and **dependent** data points $y_i, i = 1, \dots, m$, we would like to find an **estimation function**, $\hat{y}(x)$, that describes the data **as well as** possible. Note that $\hat{y}$ can be a **function** of **several variables**, but for the sake of this discussion, we **restrict** the domain of $\hat{y}$ to be a **single variable**.
- In **least squares regression**, the **estimation function** must be a **linear combination** of **basis functions**, $f_i(x)$. That is, the estimation function must be of the form

$$\hat{y}(x) = \sum_{i=1}^{n} \alpha_i f_i(x)$$

- The **scalars** α_i are referred to as the **parameters** of the estimation function, and each **basis function** must be **linearly independent** from the others. In other words, in the proper "**functional space**" no basis function should be expressible as a linear combination of the other functions. **Note**: In general, there are significantly **more data points**, m, **than basis functions**, n (i.e., $m >> n$).

The Problem Statement

- **Example**: Create an estimation function for the force-displacement relationship of a linear spring. Identify the **basis function(s)** and **model parameters**.
- The **relationship** between the force, F, and the displacement, x, can be described by the function $F(x) = kx$ where k is the spring stiffness. The only basis function is the function $f_1(x) = x$ and the model parameter to find is $\alpha_1 = k$.
- The **goal** of **least squares regression** is to find the **parameters** of the **estimation function** that **minimize the total squared error**, E, defined by $E = \sum_{i=1}^{m} (\hat{y} - y_i)^2$.
- The **individual errors** or **residuals** are defined as $e_i = (\hat{y} - y_i)$. If e is the vector containing **all the individual errors**, then we are also trying to minimize $E = \|e\|_2^2$, which is the $\boldsymbol{L_2}$ **norm** defined in the previous lesson.
- Next, we will derive the **least squares method** of finding the **desired parameters**.

LSR Derivation (Linear Algebra)

- First, we enumerate the estimation of the data at each data point x_i

$$\hat{y}(x_1) = \alpha_1 f_1(x_1) + \alpha_2 f_2(x_1) + \cdots + \alpha_n f_n(x_1),$$
$$\hat{y}(x_2) = \alpha_1 f_1(x_2) + \alpha_2 f_2(x_2) + \cdots + \alpha_n f_n(x_2),$$
$$\ldots$$
$$\hat{y}(x_m) = \alpha_1 f_1(x_m) + \alpha_2 f_2(x_m) + \cdots + \alpha_n f_n(x_m).$$

- Let $X \in \mathbb{R}^n$ be a **column vector** such that the i-th element of X contains the value of the i-th x-data point, x_i, $\hat{Y}$ be a **column vector** with elements, $\hat{Y} = \hat{y}(x_i)$, β be a **column vector** such that $\beta_i = \alpha_i$, $F_i(x)$ be a **function** that returns a column vector of $f_i(x)$ computed on every element of x, and A be an $m \times n$ **matrix** such that the i-th column of A is $F_i(x)$.
- Given this notation, the previous **system of equations** becomes $\hat{Y} = A\beta$.

- Now if Y is a column vector such that $Y_i = y_i$, the **total squared error** is given by $E = \left\|\hat{Y} - Y\right\|_2^2$. You can verify this by substituting the definition of the L_2 **norm**.
- Since we want to make E as **small** as possible and norms are a **measure of distance**, this previous expression is equivalent to saying that we want $\hat{Y}$ and Y to be a "close as possible." Note that in general Y will not be in the range of A and therefore $E > 0$.
- The vector in the range of A, $\hat{Y}$, that is closest to Y is the one that can point **perpendicularly** to Y. Therefore, we want a vector $Y - \hat{Y}$ that is perpendicular to the vector $\hat{Y}$.
- Recall from Linear Algebra that two vectors are **perpendicular**, or **orthogonal**, if their **dot product** is 0. Noting that the dot product between two vectors, v and w, can be written as $dot(v, w) = v^T w$, we can state that $\hat{Y}$ and $Y - \hat{Y}$ are **perpendicular** if $dot(\hat{Y}, Y - \hat{Y}) = 0$.
- Therefore, $\hat{Y}^T\left(Y - \hat{Y}\right) = 0$, which is **equivalent** to $(A\beta)^T(Y - A\beta) = 0$.

LSR Derivation (Linear Algebra)

- Noting that for two matrices A and B, $(AB)^T = B^T A^T$ and using **distributive** properties of **vector multiplication**, this is equivalent to

$$\beta^T A^T Y - \beta^T A^T A\beta = \beta^T (A^T Y - A^T A\beta) = 0.$$

- The solution, $\beta = 0$, is a **trivial solution**, so we use $A^T Y - A^T A\beta = 0$ to find a more **interesting solution**.
- Solving this equation for β gives the **least squares regression** formula:

$$\beta = (A^T A)^{-1} A^T Y$$

- Note that $(A^T A)^{-1} A^T$ is called the **pseudo-inverse** of A and exists when $m > n$ and A has **linearly independent** columns.

LSR Derivation (Multivariable Calculus)

- Recall that the **total error** for m data points and n basis functions is:

$$E = \sum_{i=1}^{m} e_i^2 = \sum_{i=1}^{m} (\hat{y}(x_i) - y_i)^2 = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} \alpha_j f_j (x_i) - y_i \right)^2 .$$

  which is an ***n*-dimensional paraboloid** in α_k.

- From Calculus, we know that the **minimum** of a **paraboloid** is where all the **partial derivatives equal zero**. So taking partial derivative of E with respect to the variable α_k (remember that in this case the parameters are our variables), setting the system of equations equal to 0 and solving for the α_k's should give the correct results.

LSR Derivation (Multivariable Calculus)

- The **partial derivative** with respect to α_k and setting equal to 0 yields:

$$\frac{\partial E}{\partial \alpha_k} = \sum_{i=1}^{m} 2\left(\sum_{j=1}^{n} \alpha_j f_j(x_i) - y_i\right) f_k(x_i) = 0$$

- With some rearrangement, the previous expression can be manipulated to the following:

$$\sum_{i=1}^{m}\sum_{j=1}^{n} \alpha_j f_j(x_i) f_k(x_i) - \sum_{i=1}^{m} y_i f_k(x_i) = 0$$

and further rearrangement taking advantage of the fact that addition **commutes** results in

$$\sum_{j=1}^{n} \alpha_j \sum_{i=1}^{m} f_j(x_i) f_k(x_i) = \sum_{i=1}^{m} y_i f_k(x_i)$$

LSR Derivation (Multivariable Calculus)

- Now let X be a column vector such that the $i-$th element of X is x_i and Y similarly constructed, and let $F_j(X)$ be a column vector such that the $i-$th element of $F_j(X)$ is $f_j(x_i)$.
- Using this notation, the previous expression can be rewritten in **vector notation** as:

$$\left[F_k^T(X)F_1(X), F_k^T(X)F_2(X), \dots, F_k^T(X)F_j(X), \dots, F_k^T(X)F_n(X)\right]\begin{bmatrix}\alpha_1\\ \alpha_2\\ \cdots\\ \alpha_j\\ \cdots\\ \alpha_n\end{bmatrix} = F_k^T(X)Y$$

LSR Derivation (Multivariable Calculus)

- If we repeat this equation for every k, we get the following **system of linear equations** in **matrix form**:

$$\begin{bmatrix} F_1^T(X)F_1(X), F_1^T(X)F_2(X), \ldots, F_1^T(X)F_j(X), \ldots, F_1^T(X)F_n(X) \\ F_2^T(X)F_1(X), F_2^T(X)F_2(X), \ldots, F_2^T(X)F_j(X), \ldots, F_2^T(X)F_n(X) \\ \\ F_n^T(X)F_1(X), F_n^T(X)F_2(X), \ldots, F_n^T(X)F_j(X), \ldots, F_n^T(X)F_n(X) \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \ldots \\ \alpha_j \\ \ldots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} F_1^T(X)Y \\ F_2^T(X)Y \\ \ldots \\ F_n^T(X)Y \end{bmatrix}.$$

- If we let $A = \left[F_1(X), F_2(X), \ldots, F_j(X), \ldots, F_n(X)\right]$ and β be a column vector such that j-th element of β is α_j, then the previous system of equations becomes $A^T A\beta = A^T Y$, and solving this matrix equation for β gives $\beta = (A^T A)^{-1} A^T Y$, which is exactly the same formula as the previous derivation.

LSR in Python

- Recall that if we enumerate the estimation of the data at each data point, x_i, this gives us the following system of equations:

$$\begin{aligned}
\hat{y}(x_1) &= \alpha_1 f_1(x_1) + \alpha_2 f_2(x_1) + \cdots + \alpha_n f_n(x_1),\\
\hat{y}(x_2) &= \alpha_1 f_1(x_2) + \alpha_2 f_2(x_2) + \cdots + \alpha_n f_n(x_2),\\
&\cdots\\
\hat{y}(x_m) &= \alpha_1 f_1(x_m) + \alpha_2 f_2(x_m) + \cdots + \alpha_n f_n(x_m).
\end{aligned}$$

- If the data was absolutely **perfect** (i.e., **no noise**), then the estimation function would go through all the data points, resulting in the following system of equations:

$$\begin{aligned}
y_1 &= \alpha_1 f_1(x_1) + \alpha_2 f_2(x_1) + \cdots + \alpha_n f_n(x_1),\\
y_2 &= \alpha_1 f_1(x_2) + \alpha_2 f_2(x_2) + \cdots + \alpha_n f_n(x_2),\\
&\cdots\\
y_m &= \alpha_1 f_1(x_m) + \alpha_2 f_2(x_m) + \cdots + \alpha_n f_n(x_m).
\end{aligned}$$

- If we take A to be as defined previously, this would result in the matrix equation $Y = A\beta$.

LSR in Python

- However, since the data is **not perfect**, there will not be an **estimation function** that can go through all the data points, and this system will have **no solution**.
- Therefore, we need to use the **least square regression** that we derived in the previous two sections to get a solution.

$$\beta = (A^T A)^{-1} A^T Y$$

- **Example**: Consider the artificial data created by $x = np.linspace(0, 1, 101)$ and $y = 1 + x + x * np.random.random(len(x))$. Do a least squares regression with an estimation function defined by $\hat{y} = \alpha_1 x + \alpha_2$. Plot the data points along with the least squares regression. Note that we expect $\alpha_1 = 1.5$ and $\alpha_2 = 1.0$ based on this data. Due to the random noise we added into the data, your results maybe slightly different.

Use Direct Inverse Method

In [1]:
```
import numpy as np
from scipy import optimize
import matplotlib.pyplot as plt

plt.style.use('seaborn-poster')
```

In [2]:
```
# generate x and y
x = np.linspace(0, 1, 101)
y = 1 + x + x * np.random.random(len(x))
```

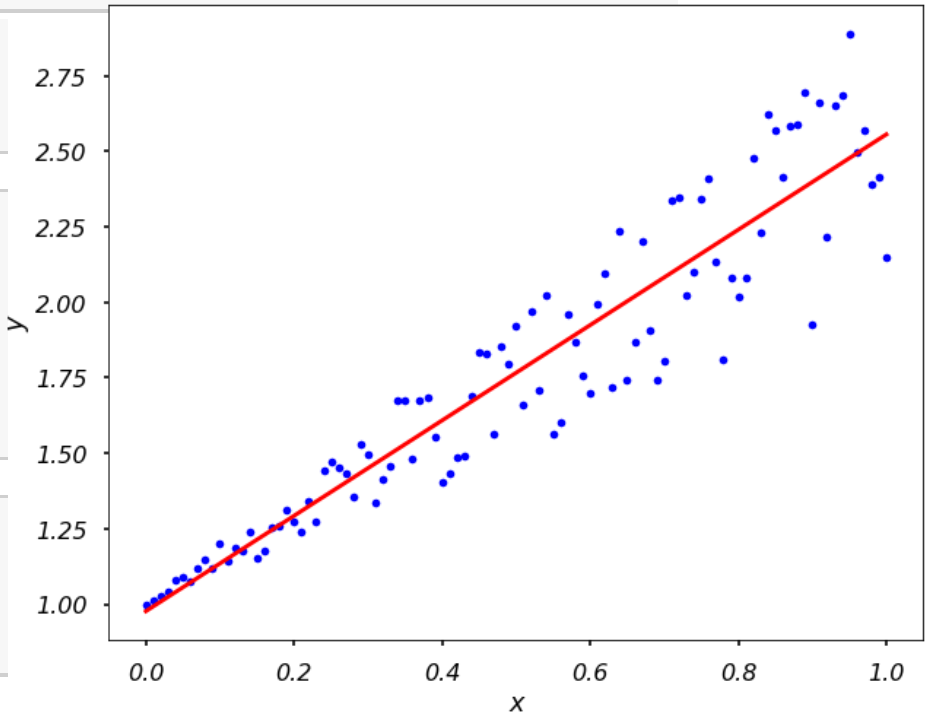
In [3]:
```
# assemble matrix A
A = np.vstack([x, np.ones(len(x))]).T

# turn y into a column vector
y = y[:, np.newaxis]
```

In [4]:
```
# Direct least square regression
alpha = np.dot((np.dot(np.linalg.inv(np.dot(A.T,A)),A.T)),y)
print(alpha)
```

```
[[1.57877489]
 [0.976713  ]]
```

In [5]:
```
# plot the results
plt.figure(figsize = (10,8))
plt.plot(x, y, 'b.')
plt.plot(x, alpha[0]*x + alpha[1], 'r')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



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Use the Pseudoinverse

- We talked before that the $(A^T A)^{-1} A^T$ is called the **pseudo-inverse**, therefore, we could use the **pinv** function in **numpy** to directly calculate it.

```
In [6]: pinv = np.linalg.pinv(A)
        alpha = pinv.dot(y)
        print(alpha)
```

```
[[1.57877489]
 [0.976713  ]]
```

Use numpy.linalg.lstsq

- Actually, **numpy** has already implemented the **least square methods** that we can just call the function to get a solution.
- The function will return more things than the solution itself, please check the documentation for details.

```
In [7]: alpha = np.linalg.lstsq(A, y, rcond=None)[0]
        print(alpha)
```

```
[[1.57877489]
 [0.976713  ]]
```

Use optimize.curve_fit from Scipy

- This **scipy** function is actually very powerful, that it can fit not only **linear** functions, but many different function forms, such as **non-linear** function. Here we will show the linear example from above.
- Note that, using this function, we don't need to turn y into a column vector.

In [8]:
```
# generate x and y
x = np.linspace(0, 1, 101)
y = 1 + x + x * np.random.random(len(x))
```

In [9]:
```
def func(x, a, b):
    y = a*x + b
    return y

alpha = optimize.curve_fit(func, xdata = x, ydata = y)[0]
print(alpha)
```

```
[1.61564576 0.96182858]
```

LSR for Nonlinear Functions

- A **least squares regression** requires that the **estimation function** be a **linear combination** of **basis** **functions**.
- There are some functions that cannot be put in this form, but where a least squares regression is **still appropriate**.
- Introduced later are several ways to deal with **nonlinear** **functions**.
  - We can accomplish this by taking advantage of the properties of **logarithms**, and **transform** the **non-linear** function into a **linear** function.
  - We can use the **curve_fit** function from **scipy** to estimate directly the parameters for the **non-linear** function using least square.

Log Tricks for Exponential Functions

- Assume you have a function in the form $\hat{y}(x) = \alpha e^{\beta x}$ and data for x and y, and that you want to perform **least squares regression** to find α and β.
- Clearly, the previous set of basis functions (**linear**) would be inappropriate to describe $\hat{y}(x)$; however, if we take the **log** of both sides, we get $\log(\hat{y}(x)) = \log(\alpha) + \beta x$.
- Now, say that $\tilde{y}(x) = \log(\hat{y}(x))$ and $\tilde{\alpha} = \log(\alpha)$, then $\tilde{y}(x) = \tilde{\alpha} + \beta x$.
- Now, we can perform a **least squares regression** on the **linearized** expression to find $\tilde{y}(x)$, $\tilde{\alpha}$, and β, and then recover α by using the expression $\alpha = e^{\tilde{\alpha}}$.

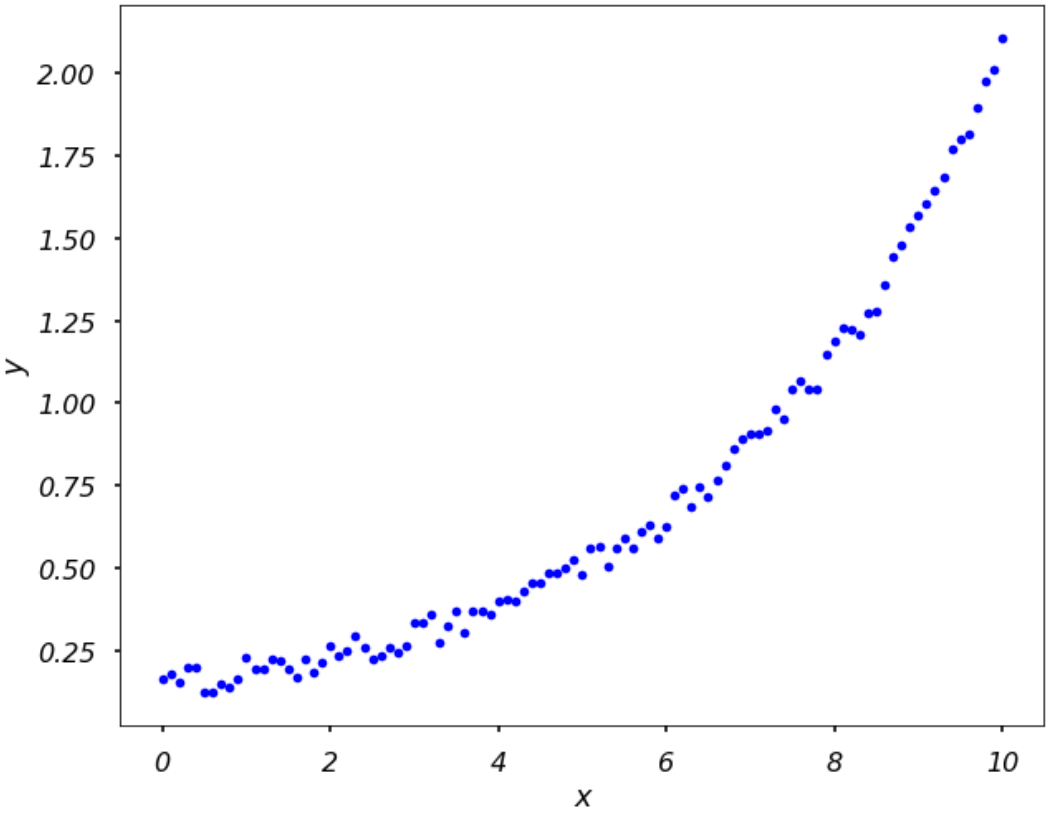
Log Tricks for Exponential Functions

- For the example below, we will generate data using $\alpha = 0.1$ and $\beta = 0.3$.

In [13]:
```
import numpy as np
from scipy import optimize
import matplotlib.pyplot as plt

plt.style.use('seaborn-poster')
```

In [14]:
```
# Let's generate x and y, and add some noise into y
x = np.linspace(0, 10, 101)
y = 0.1*np.exp(0.3*x) + 0.1*np.random.random(len(x))
```

In [15]:
```
# Let's have a look of the data
plt.figure(figsize = (10,8))
plt.plot(x, y, 'b.')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



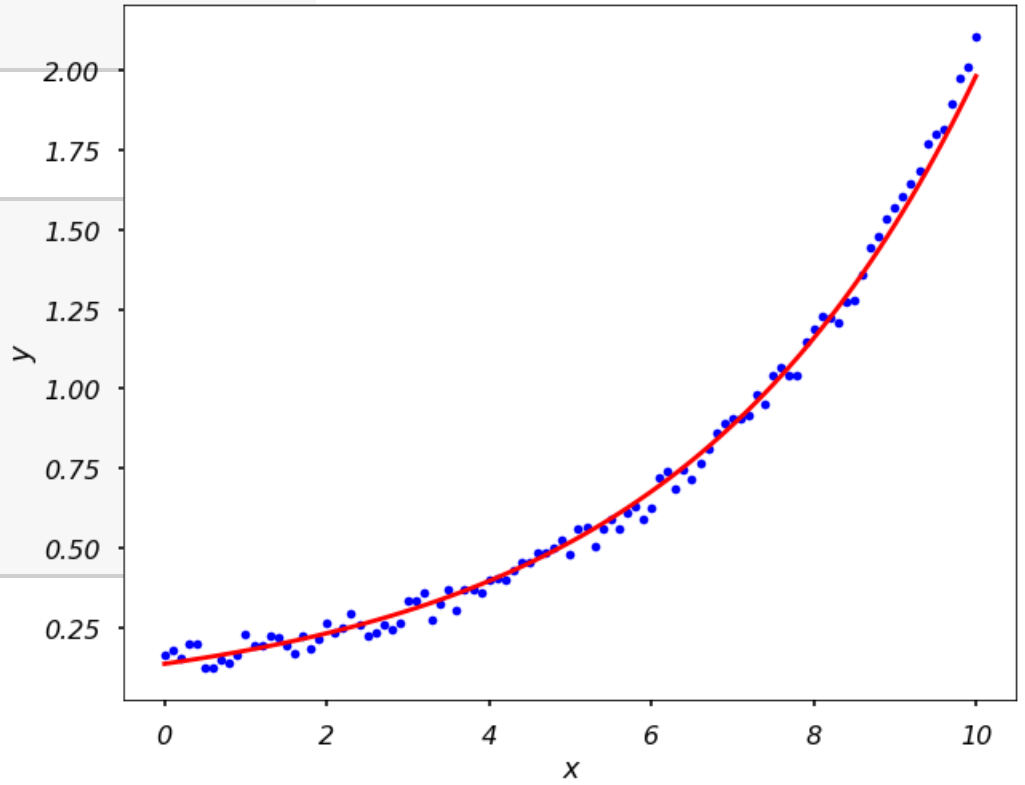
Log Tricks for Exponential Functions

- Let's fit the data after we applied the **log trick**.

In [16]:
```
A = np.vstack([x, np.ones(len(x))]).T
beta, log_alpha = np.linalg.lstsq(A, np.log(y), rcond = None)[0]
alpha = np.exp(log_alpha)
print(f'alpha={alpha}, beta={beta}')
```

```
alpha=0.13504743256802007, beta=0.2686771402218146
```

In [17]:
```
# Let's have a look of the data
plt.figure(figsize = (10,8))
plt.plot(x, y, 'b.')
plt.plot(x, alpha*np.exp(beta*x), 'r')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



Log Tricks for Power Functions

- The **power function** case is very similar.
- Assume we have a function in the form $\hat{y}(x) = bx^m$ and data for x and y.
- Then we can turn this function into a **linear** form by taking **log** to both sides

$$\log(\hat{y}(x)) = m\log(x) + \log b\,.$$

- Therefore, we can solve this function as a **linear regression**.
- Since it is very similar to the previous example, we will not spend more time on this.

Polynomial Regression

- We can also use **polynomial** and **least squares** to fit a **nonlinear** function.
- Previously, we have our functions all in **linear** form, that is, $y = ax + b$.
- But **polynomials** are functions with the following form:

$$f(x) = a_n x^n + a_{n-1} x^{n-1} + \cdots + a_2 x^2 + a_1 x^1 + a_0$$

  where $a_n, a_{n-1}, \ldots, a_2, a_1, a_0$ are the **real number coefficients**, and n, a nonnegative integer, is the **order** or **degree** of the polynomial.

- If we have a set of data points, we can use **different order of polynomials** to fit it.
- The coefficients of the polynomials can be estimated using the least squares method as before, that is, **minimizing the error** between the real data and the polynomial fitting results.

Polynomial Regression

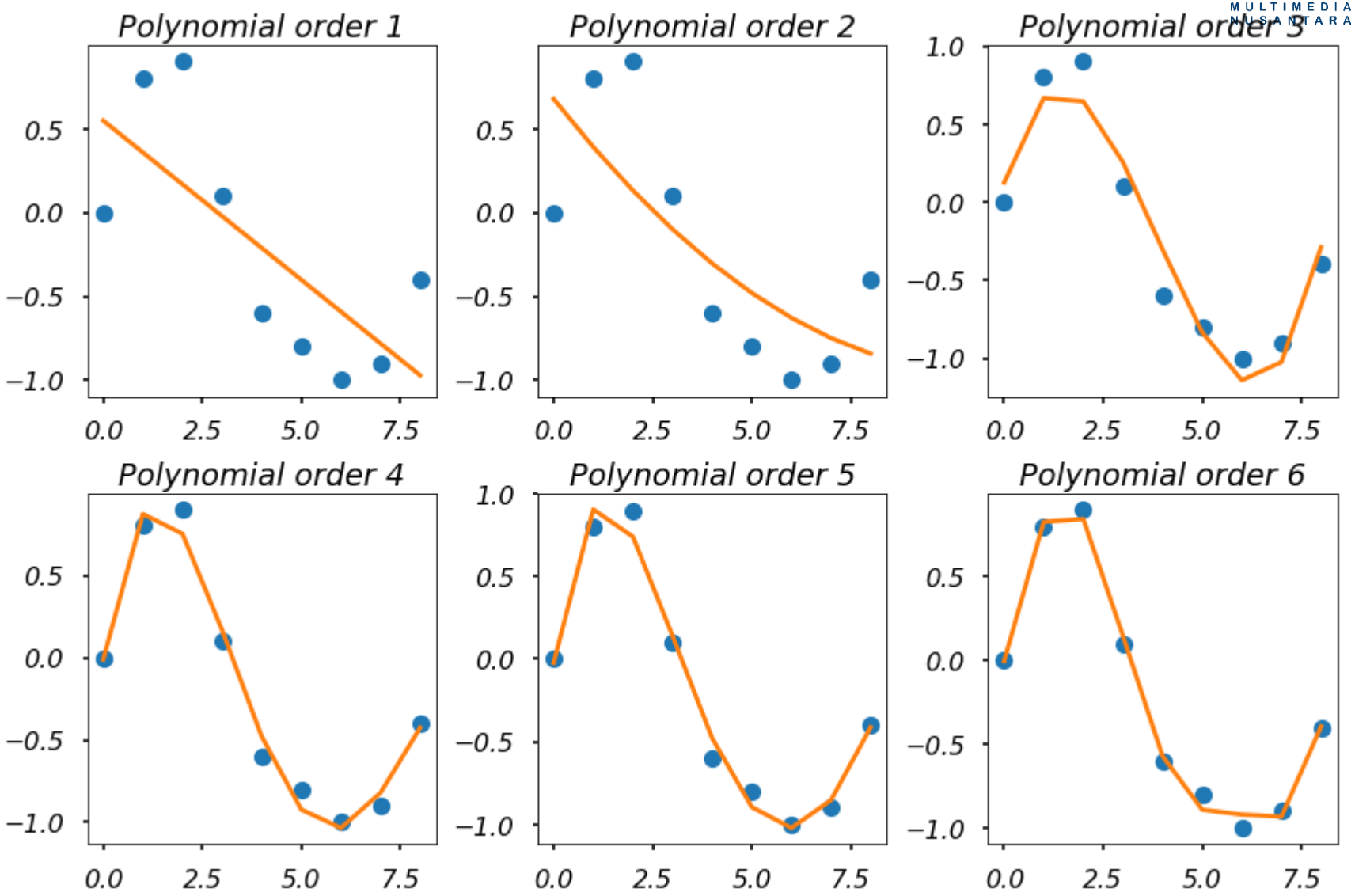
- In Python, we can use **numpy.polyfit** to obtain the **coefficients** of different order polynomials with the least squares.
- With the coefficients, we then can use **numpy.polyval** to get **specific values** for the given **coefficients**.
- Let us see an example how to perform this in Python.

In [18]:

```
x_d = np.array([0, 1, 2, 3, 4, 5, 6, 7, 8])
y_d = np.array([0, 0.8, 0.9, 0.1, -0.6, -0.8, -1, -0.9, -0.4])

plt.figure(figsize = (12, 8))
for i in range(1, 7):

    # get the polynomial coefficients
    y_est = np.polyfit(x_d, y_d, i)
    plt.subplot(2,3,i)
    plt.plot(x_d, y_d, 'o')
    # evaluate the values for a polynomial
    plt.plot(x_d, np.polyval(y_est, x_d))
    plt.title(f'Polynomial order {i}')

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

Polynomial Regression

- The figure shows that we can use different order of polynomials to fit the same data.
- The **higher** the **order**, the curve we used to fit the data will be **more flexible to fit** the data. But what order to use is not a simple question, it depends on the specific problems in science and engineering.



Use optimize.curve_fit from Scipy

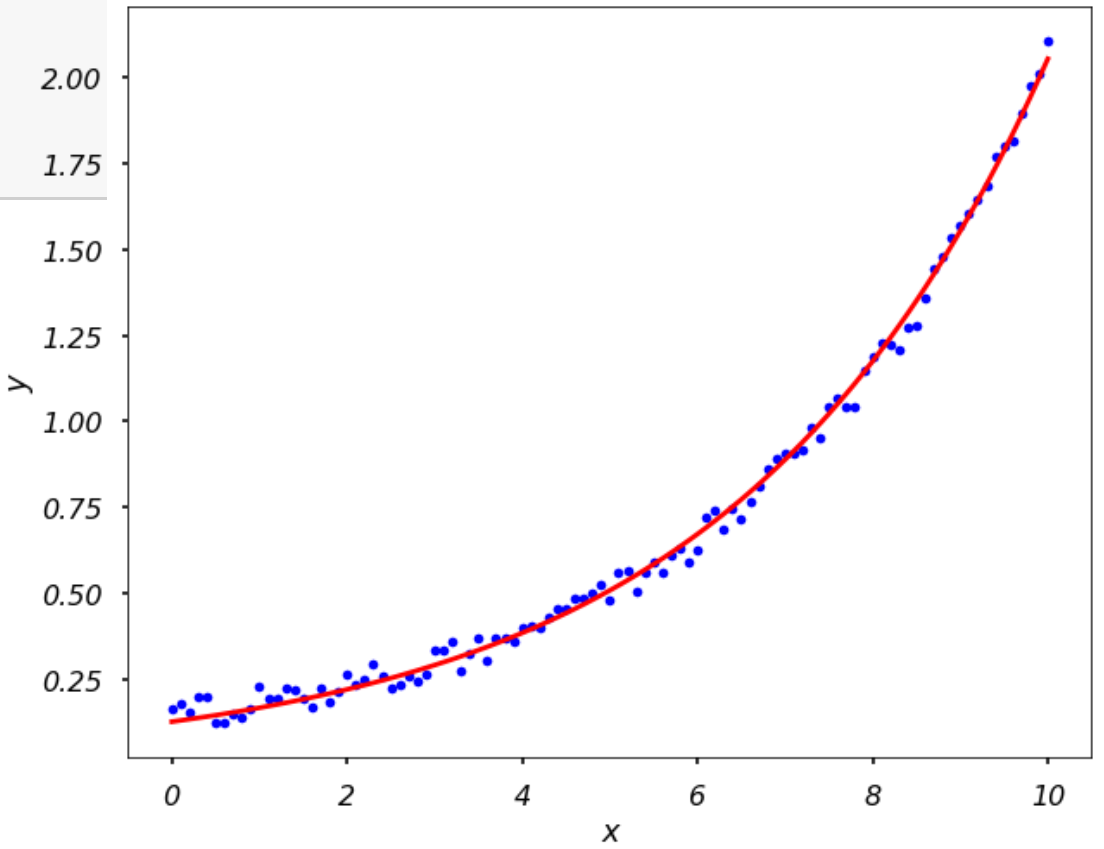
- We can use the **curve_fit** function to fit any form function and estimate the parameters of it.
- Here is how we solve the above problem in the **log** tricks section using the **curve_fit** function.

```
In [19]:
# Let's define the function form
def func(x, a, b):
    y = a*np.exp(b*x)
    return y

alpha, beta = optimize.curve_fit(func, xdata = x, ydata = y)[0]
print(f'alpha={alpha}, beta={beta}')
```

```
alpha=0.1254246477296184, beta=0.2796455030268306
```

Use optimize.curve_fit from Scipy

In [20]:
```
# Let's have a look of the data
plt.figure(figsize = (10,8))
plt.plot(x, y, 'b.')
plt.plot(x, alpha*np.exp(beta*x), 'r')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```



Practice

1. Write a function **my_ls_params(f, x, y)**, where **x** and **y** are arrays of the same size containing experimental data, and **f** is a list with each element a function object to a basis vector of the estimation function. The output argument, **beta**, should be an array of the parameters of the least squares regression for **x**, **y**, and **f**.

```
# Test case
x = np.linspace(0, 1, 101)
y = 1 + x + x * np.random.random(len(x))
```

```
beta = my_ls_params(func, x, y)
print(beta)
```

```
[[1.31459484]
 [1.05853804]]
```

Next Week's Outline

- Interpolation Problem Statement
- Linear Interpolation
- Cubic Spline Interpolation
- Lagrange Polynomial Interpolation
- Newton's Polynomial Interpolation

References

- Kong, Qingkai; Siauw, Timmy, and Bayen, Alexandre. 2020. Python Programming and Numerical Methods: A Guide for Engineers and Scientists. Academic Press. https://www.elsevier.com/books/python-programming-and-numerical-methods/kong/978-0-12-819549-9
- Other online and offline references

Visi

Menjadi Program Studi Strata Satu Informatika **unggulan** yang menghasilkan lulusan **berwawasan internasional** yang **kompeten** di bidang Ilmu Komputer (*Computer Science*), **berjiwa wirausaha** dan **berbudi pekerti luhur**.

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Misi

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2. Melaksanakan kegiatan penelitian di bidang Informatika untuk memajukan ilmu dan teknologi Informatika.
3. Melaksanakan kegiatan pengabdian kepada masyarakat berbasis ilmu dan teknologi Informatika dalam rangka mengamalkan ilmu dan teknologi Informatika.