

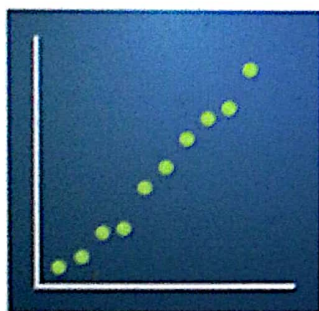
Fitting a non-linear function

TOTAL POINTS 5

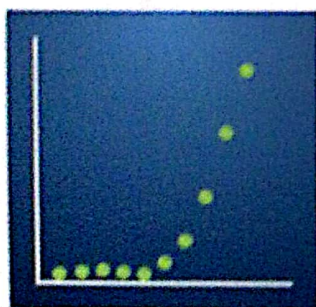
1. The previous quiz tested our knowledge of linear regression, and how we can begin to model sets of data. In the last video, we developed on this idea further, looking at the case for data that cannot be effectively modelled by linear approximations. As such, we were introduced to the nonlinear least squares method, as a way of fitting nonlinear curves to data.

In this question, we have a set of graphs highlighting different distributions of data. Select the appropriate graphs where the nonlinear least squares method can be adapted to provide an effective fit to this data.

☐ Option A



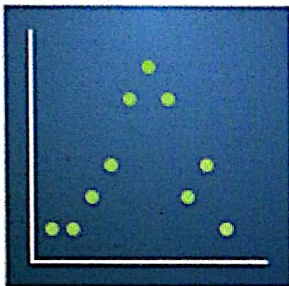
☒ Option B



✓ **Correct**

This data looks similar to an exponential function and should be able to be fitted through the nonlinear regression technique.

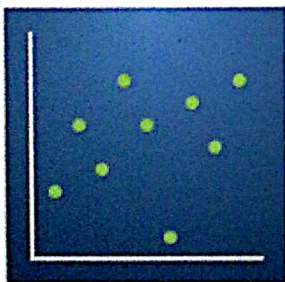
✓ **Option C**



✓ **Correct**

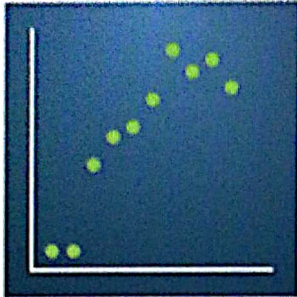
This data looks similar to a Gaussian and should be able to be fitted through the **nonlinear** regression technique.

☐ **Option D**



☐ **Option E**

☐ Option E



You didn't select all the correct answers

2. In the previous lecture, you were taken through the example of χ^2 and how it is important in utilising the sum of the differences and the least squares method. We were also introduced to the expression $\chi^2 = \sum_{i=1}^n \frac{[y_i - y(x_i; a_k)]^2}{\sigma^2}$. For the parameter χ^2 , select all the statements below that are true.

- ☐ When χ^2 is large, we have a good fit to our data.
- ☒ Taking the gradient of χ^2 and setting this to zero allows us to determine effective fitting parameters.

✓ **Correct**

By finding the gradient, we are finding the minimum of χ^2 . This should allow us to build a set of simultaneous equations which can then be analysed to effectively fit the parameters through the steepest descent.

☒ The parameter χ is squared so that the effect of bad uncertainties are minimised.

✓ **Correct**

When calculating χ , we divide by the uncertainty value σ . As a result, χ is squared in order to minimise the effect of dividing by a highly uncertain result.

☐ The parameter χ^2 is the uncertainty value of our variables.

3. In the previous lecture, we took the derivative of χ^2 with respect to our fitting parameters, the form of which is shown below.

$$\frac{\partial \chi^2}{\partial a_j} = -2 \sum_{i=1}^n \frac{y_i - f(x_i, a)}{\sigma_i^2} \frac{\partial f(x_i, a)}{\partial a_j} \text{ for } j = 1, \dots, n$$

Here we will define the matrix $[Z_j] = \frac{\partial f(x_i, a)}{\partial a_j}$

Assuming $f(x_i, a) = a_1 x^3 - a_2 x^2 + e^{-a_3 x}$, select the option that correctly shows the partial differentiation for this function.

☐ $\frac{\partial f}{\partial a_1} = x^3 - a_2 x^2 + e^{-a_3 x}, \frac{\partial f}{\partial a_2} = a_1 x^3 - x^2 + e^{-a_3 x}, \frac{\partial f}{\partial a_3} = a_1 x^3 - a_2 x^2 - x e^{-a_3 x}$

☐ $\frac{\partial f}{\partial a_1} = x^3, \frac{\partial f}{\partial a_2} = 2x^2, \frac{\partial f}{\partial a_3} = x e^{a_3 x}$

☒ $\frac{\partial f}{\partial a_1} = x^3, \frac{\partial f}{\partial a_2} = -x^2, \frac{\partial f}{\partial a_3} = -x e^{-a_3 x}$

☐ $\frac{\partial f}{\partial a_1} = 3a_0 x^2, \frac{\partial f}{\partial a_2} = -2a_2 x, \frac{\partial f}{\partial a_3} = -a_3 e^{-a_3 x}$

4. In this question, we want to put our working knowledge of the partial differentiation of our functions and arrange this into the Jacobian. As a reminder, the Jacobian for the nonlinear least squares method will take the form: $\mathbf{J} = \left[\frac{\partial(\chi^2)}{\partial a_k} \right] = \left[\frac{\partial(\chi^2)}{\partial a_1}, \quad \frac{\partial(\chi^2)}{\partial a_2} \right]$.

For the equation $y(x_i; \mathbf{a}) = a_1(1 - e^{-a_2 x_i^2})$ and assuming $\sigma^2 = 1$, select the correct Jacobian that should be evaluated for our fit function.



$$\begin{aligned} \frac{\partial(\chi^2)}{\partial a_1} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](1 - e^{-a_2 x_i^2}) \\ \frac{\partial(\chi^2)}{\partial a_2} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](a_1 x_i^2 e^{-a_2 x_i^2}) \end{aligned}$$



$$\begin{aligned} \frac{\partial(\chi^2)}{\partial a_1} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](1 + e^{-a_2 x_i^2}) \\ \frac{\partial(\chi^2)}{\partial a_2} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](a_1 x_i e^{-a_2 x_i^2}) \end{aligned}$$



$$\begin{aligned} \frac{\partial(\chi^2)}{\partial a_1} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](1 - e^{-a_2 x_i^2}) \\ \frac{\partial(\chi^2)}{\partial a_2} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](-x_i^2 e^{-a_2 x_i^2}) \end{aligned}$$



$$\begin{aligned} \frac{\partial(\chi^2)}{\partial a_1} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](e^{-a_2 x_i^2}) \\ \frac{\partial(\chi^2)}{\partial a_2} &= -2 \sum_{i=1}^n [y_i - a_1(1 - e^{-a_2 x_i^2})](a_1 x_i^2 e^{-a_2 x_i^2}) \end{aligned}$$



Correct

With the Jacobian, we can effectively perform our steepest descent method. Its form also allows for ease of use in using computational methods to evaluate this.

5. In this question, we will develop our idea of building the Jacobian further by looking at a function with more fitting parameters. The function below is of a Gaussian distribution with 4 fitting parameters (σ, x_p, I, b) which are to be used in the nonlinear least squares method.

$$y(x; \sigma, x_p, I, b) = b + \frac{I}{\sigma\sqrt{2\pi}} \exp \left\{ -\frac{(x - x_p)^2}{2\sigma^2} \right\}$$

In the lectures, we also showed how to find χ^2 and how this forms the Jacobian shown below: $\mathbf{J} = \left[\frac{\partial(\chi^2)}{\partial a_k} \right] = \left[\frac{\partial(\chi^2)}{\partial \sigma}, \frac{\partial(\chi^2)}{\partial x_p}, \frac{\partial(\chi^2)}{\partial I}, \frac{\partial(\chi^2)}{\partial b} \right]$.

where

$$\frac{\partial \chi^2}{\partial a_j} = -2 \sum_{i=1}^n \frac{y_i - y(x_i; \mathbf{a})}{\sigma_i^2} \frac{\partial y(x_i; \mathbf{a})}{\partial a_j} \text{ for } j = 1, \dots, n$$

For the Gaussian function above, determine the partial differential

$$\frac{\partial y}{\partial x_p}$$



$$\frac{\partial y}{\partial x_p} = \frac{I}{\sqrt{2\pi}} \frac{2(x - x_p)}{\sigma} \exp \left\{ -\frac{(x - x_p)^2}{2\sigma^2} \right\}$$



$$\frac{\partial y}{\partial x_p} = \frac{I}{\sqrt{2\pi}} \frac{(x - x_p)}{\sigma^3} \exp \left\{ -\frac{(x - x_p)^2}{2\sigma^2} \right\}$$



$$\frac{\partial y}{\partial x_p} = -\frac{I}{\sqrt{2\pi}} \frac{(x - x_p)}{2\sigma^3} \exp \left\{ -\frac{(x - x_p)^2}{2\sigma^2} \right\}$$



$$\frac{\partial y}{\partial x_p} = \frac{I}{\sqrt{2\pi}} \frac{2x}{\sigma} \exp \left\{ -\frac{(x - x_p)^2}{2\sigma^2} \right\}$$

✓ **Correct**

Here we are only evaluating one partial derivative that forms part of the Jacobian. In order to correctly fit the Gaussian to a specific set of data, we will need to evaluate all the partial