Ejemplos de regresión no lineal (modelo no linealizable)

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Introducción

Data on biological oxygen demand versus time are usually modeled by the following equation:

$$y = k_1\left[1 - exp\left(-k_2 t\right)\right]$$

where k_1 is the ultimate carbonaceous oxygen demand (*mg/L*) and k_2 is the BOD reaction rate constant (*days*$^{-1}$). A set of BOD data were obtained by 3rd year Environmental Engineering students at the Technical University of Crete and are given in the next table:

times [days]	BOD [mg/L]
1	110
2	180
3	230
4	260
5	280
6	290
7	310
8	330

Vector Residuo

Residuo:

$$\underline{r} = \begin{bmatrix} y_1 - k_1\left[1 - exp\left(-k_2 t_1\right)\right] \\ y_2 - k_1\left[1 - exp\left(-k_2 t_2\right)\right] \\ y_3 - k_1\left[1 - exp\left(-k_2 t_3\right)\right] \\ y_4 - k_1\left[1 - exp\left(-k_2 t_4\right)\right] \\ y_5 - k_1\left[1 - exp\left(-k_2 t_5\right)\right] \\ y_6 - k_1\left[1 - exp\left(-k_2 t_6\right)\right] \\ y_7 - k_1\left[1 - exp\left(-k_2 t_7\right)\right] \\ y_8 - k_1\left[1 - exp\left(-k_2 t_8\right)\right] \end{bmatrix}$$

Problema de Mínimos Cuadrados

La norma del residuo al cuadrado corresponde a:

$$\left\|\underline{r}\right\|^2 = \sum_{i=1}^{n}\left(y_i - k_1\left[1 - exp\left(-k_2 t_i\right)\right]\right)^2$$

Problema de mínimos cuadrados: $Min\left\|\underline{r}\right\|^2$

Condición de primer orden del mínimo de una función:

$$\nabla\left(\left\|\underline{r}\right\|^2\right) = \underline{0} \rightarrow \nabla\left(\left\|\underline{r}\right\|^2\right) = \begin{bmatrix} \dfrac{\partial\left\|\underline{r}\right\|^2}{\partial k_1} \\ \dfrac{\partial\left\|\underline{r}\right\|^2}{\partial k_2} \end{bmatrix} \rightarrow \begin{cases} \dfrac{\partial\left\|\underline{r}\right\|^2}{\partial k_1} = 0 \\ \dfrac{\partial\left\|\underline{r}\right\|^2}{\partial k_2} = 0 \end{cases}$$

Sistema de ecuaciones correspondiente

$$\left\|\underline{r}\right\|^2 = \sum_{i=1}^{n}\left(y_i - k_1\left[1-exp\left(-k_2 t_i\right)\right]\right)^2$$

El valor de k_1 y k_2 se obtiene resolviendo el siguiente sistema:

$$\begin{cases} \dfrac{\partial\left\|\underline{r}\right\|^2}{\partial k_1} = 0 \\ \dfrac{\partial\left\|\underline{r}\right\|^2}{\partial k_2} = 0 \end{cases} \rightarrow \begin{cases} \sum_{i=1}^{n} 2\left(y_i - k_1\left[1-exp\left(-k_2 t_i\right)\right]\right)\left[-1+exp\left(-k_2 t_i\right)\right] = 0 \\ \sum_{i=1}^{n} 2\left(y_i - k_1\left[1-exp\left(-k_2 t_i\right)\right]\right)\left[k_1\left(-t_i\right)exp\left(-k_2 t_i\right)\right] = 0 \end{cases}$$

$$\underline{f}\left(\underline{x}\right) = \begin{bmatrix} \sum_{i=1}^{n} 2\left(y_i - k_1\left[1-exp\left(-k_2 t_i\right)\right]\right)\left[-1+exp\left(-k_2 t_i\right)\right] \\ \sum_{i=1}^{n} 2\left(y_i - k_1\left[1-exp\left(-k_2 t_i\right)\right]\right)\left[k_1\left(-t_i\right)exp\left(-k_2 t_i\right)\right] \end{bmatrix} \qquad \underline{x} = \begin{bmatrix} k_1 \\ k_2 \end{bmatrix}$$

Resolución mediante Newton

$$\underline{f}\left(\underline{x}\right)=\begin{bmatrix}\sum_{i=1}^{n}2\left(y_i-k_1\left[1-exp\left(-k_2t_i\right)\right]\right)\left[-1+exp\left(-k_2t_i\right)\right]\\ \sum_{i=1}^{n}2\left(y_i-k_1\left[1-exp\left(-k_2t_i\right)\right]\right)\left[k_1\left(-t_i\right)exp\left(-k_2t_i\right)\right]\end{bmatrix}\qquad \underline{x}=\begin{bmatrix}k_1\\ k_2\end{bmatrix}$$

$$\frac{\partial f_1}{\partial x_1}=\sum_{i=1}^{n}2\left[-1+exp\left(-k_2t_i\right)\right]^2$$

$$\frac{\partial f_1}{\partial x_2}=\sum_{i=1}^{n}2\left[k_1\left(-t_i\right)exp\left(-k_2t_i\right)\right]\left[-1+exp\left(-k_2t_i\right)\right]+2\left(y_i-k_1\left[1-exp\left(-k_2t_i\right)\right]\right)\left[\left(-t_i\right)exp\left(-k_2t_i\right)\right]$$

$$\frac{\partial f_2}{\partial x_1}=\sum_{i=1}^{n}2\left[-1+exp\left(-k_2t_i\right)\right]\left[k_1\left(-t_i\right)exp\left(-k_2t_i\right)\right]+2\left(y_i-k_1\left[1-exp\left(-k_2t_i\right)\right]\right)\left[\left(-t_i\right)exp\left(-k_2t_i\right)\right]$$

$$\frac{\partial f_2}{\partial x_2}=\sum_{i=1}^{n}2\left[k_1\left(-t_i\right)exp\left(-k_2t_i\right)\right]^2+2\left(y_i-k_1\left[1-exp\left(-k_2t_i\right)\right]\right)\left[k_1t_i^{\,2}exp\left(-k_2t_i\right)\right]$$

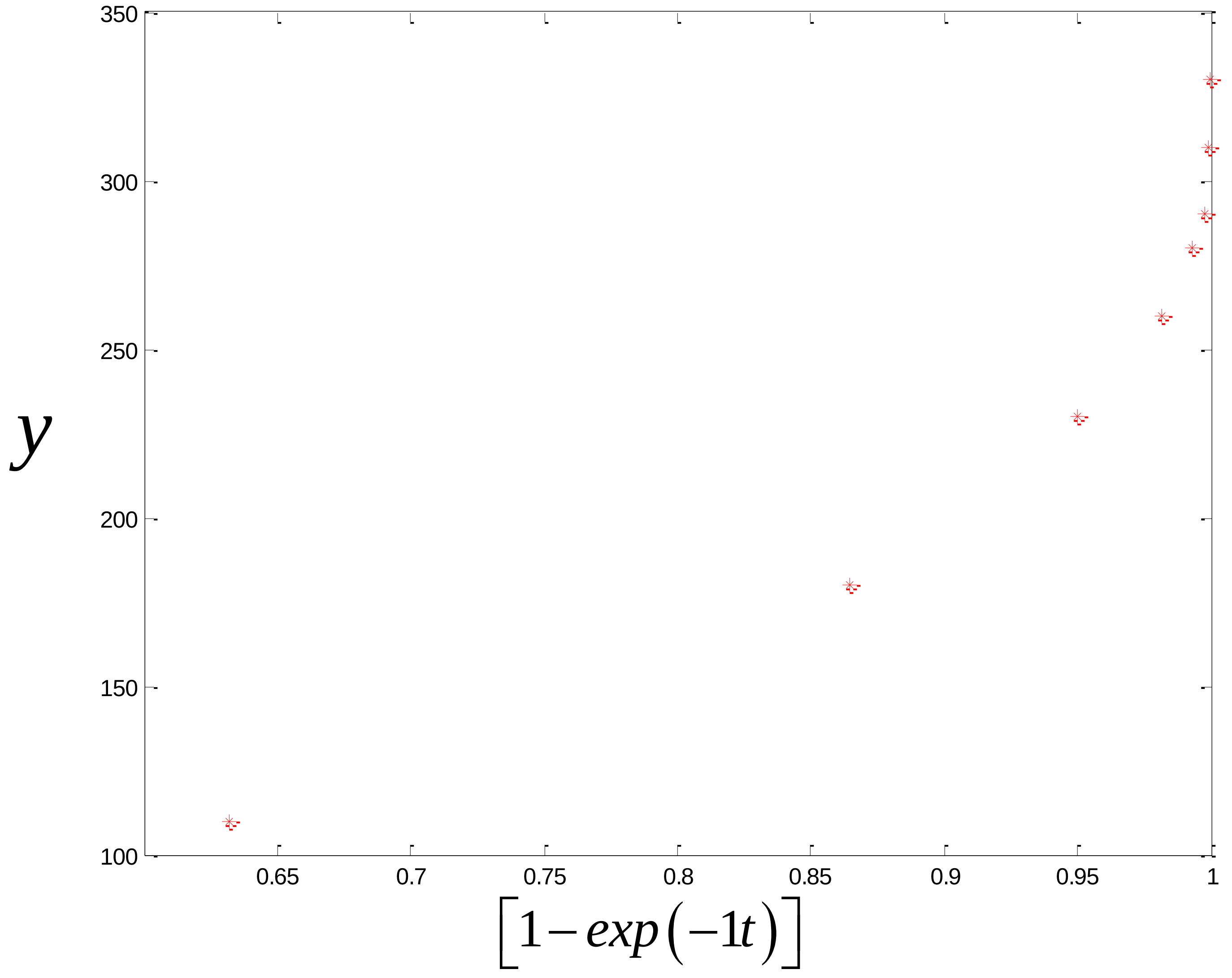
Selección del valor de arranque

¿Valor de arranque?

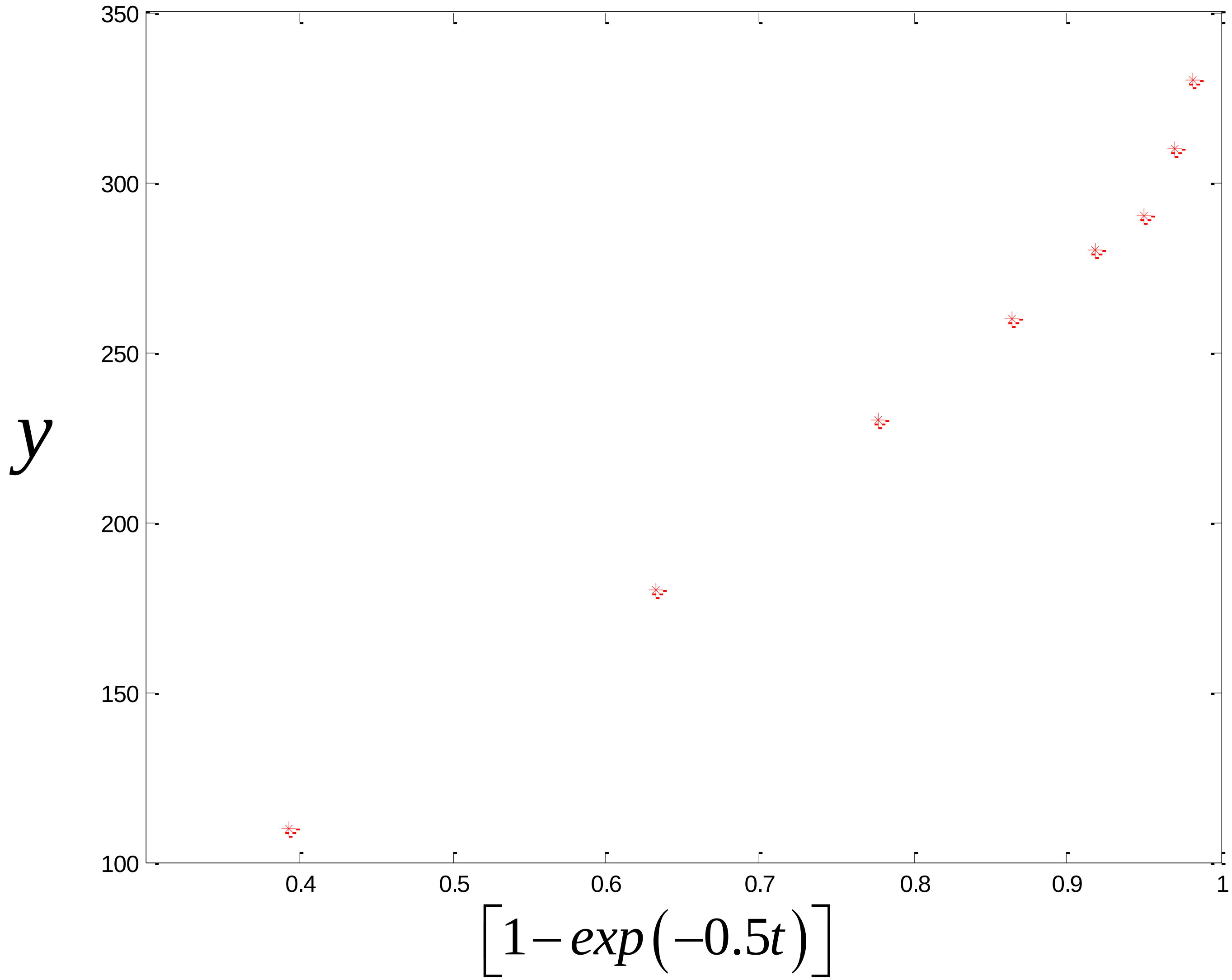
- Una buena estrategia es fijar un valor de k_2 y encontrar k_1 por regresión lineal.
- Variando el valor de k_2 gráficamente se puede visualizar un adecuado ajuste lineal.
- Una vez definido el valor de k_2, a partir de una regresión lineal, se obtiene k_1.
- Estos valores resultan un buen punto de arranque para la búsqueda de la solución del sistema.

$$y = k_1 \left[1 - exp\left(-k_2 t \right) \right]$$

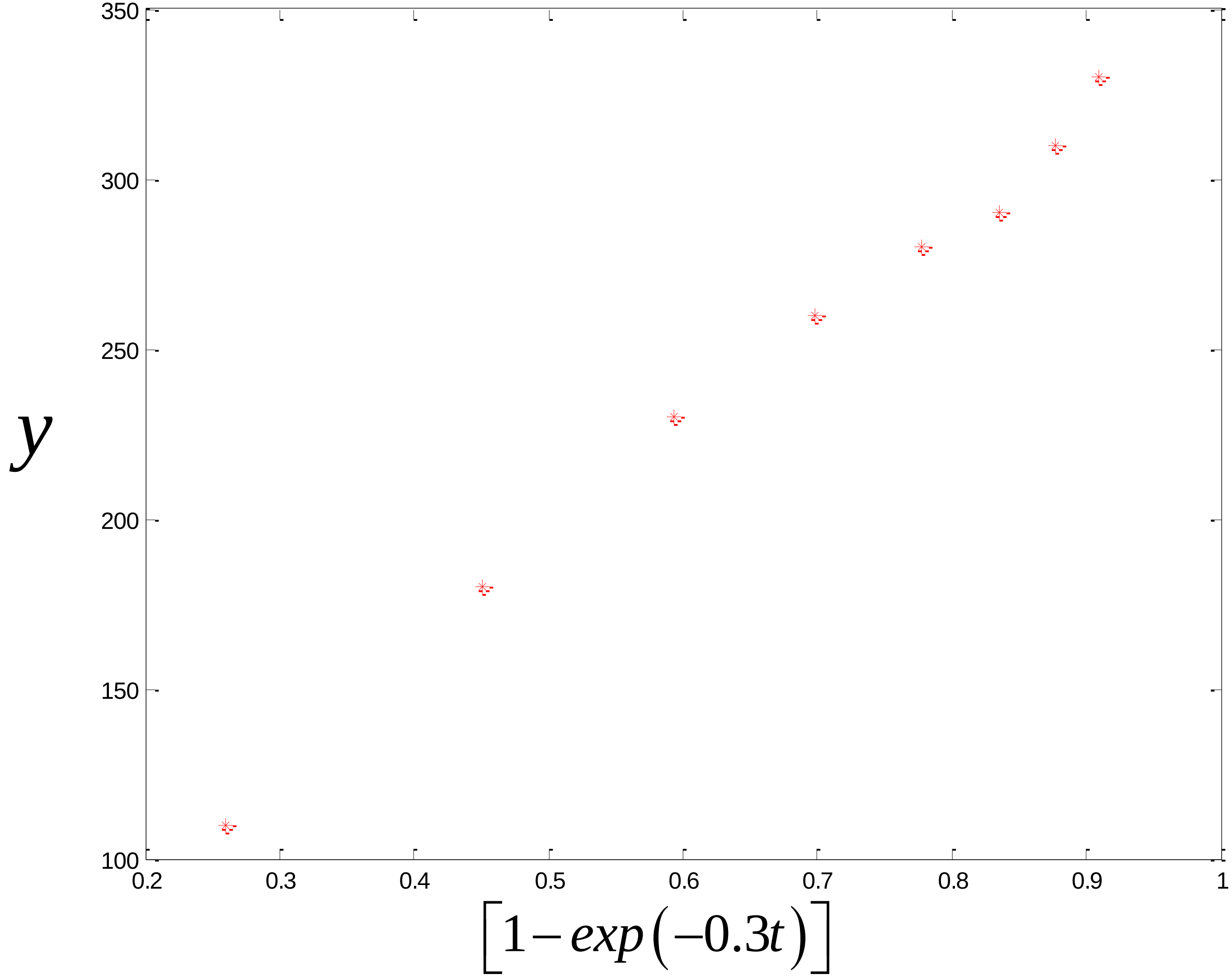
Grafica de datos para k_2=1



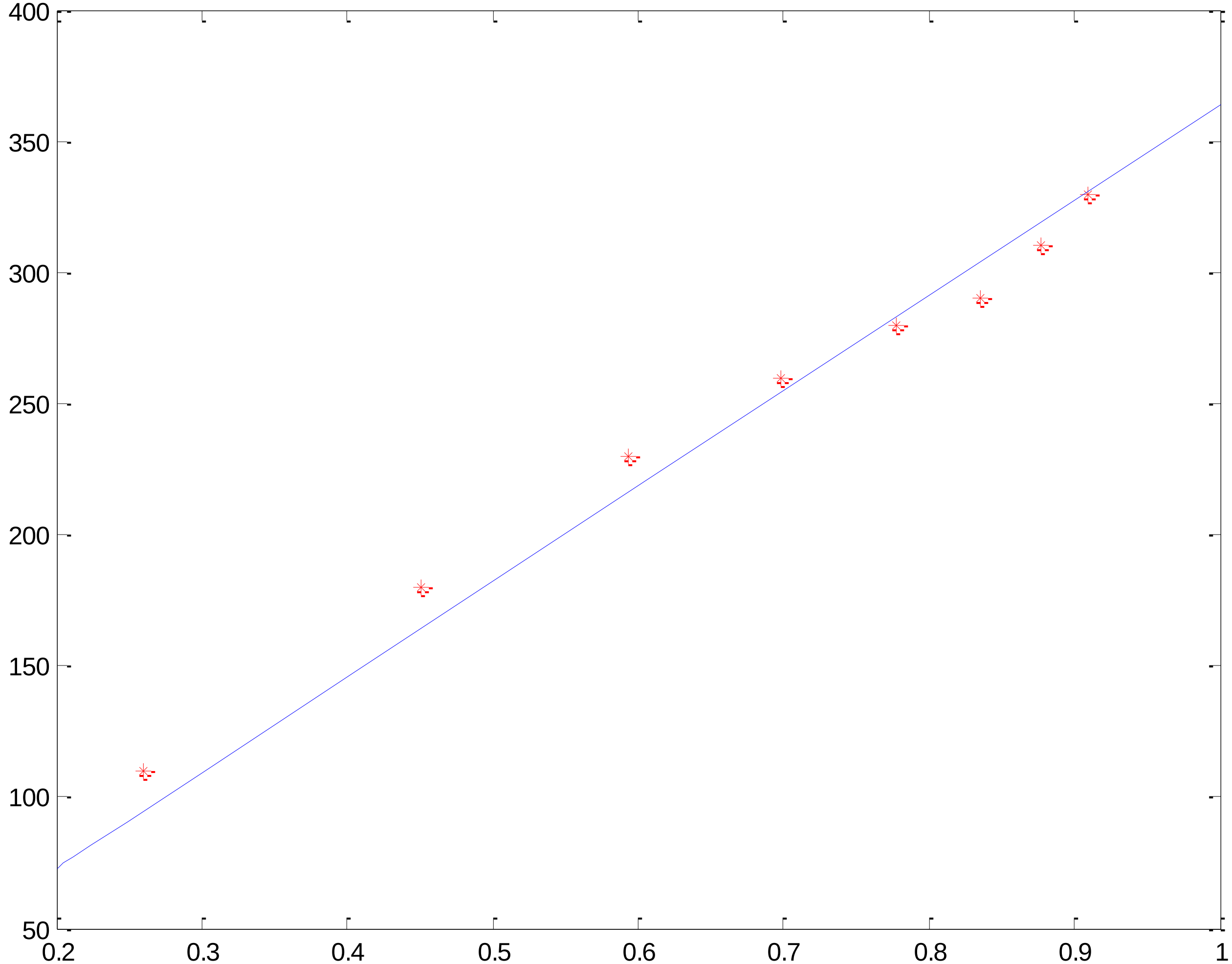
Grafica de datos para k_2=0.5



Grafica de datos para k_2=0.3



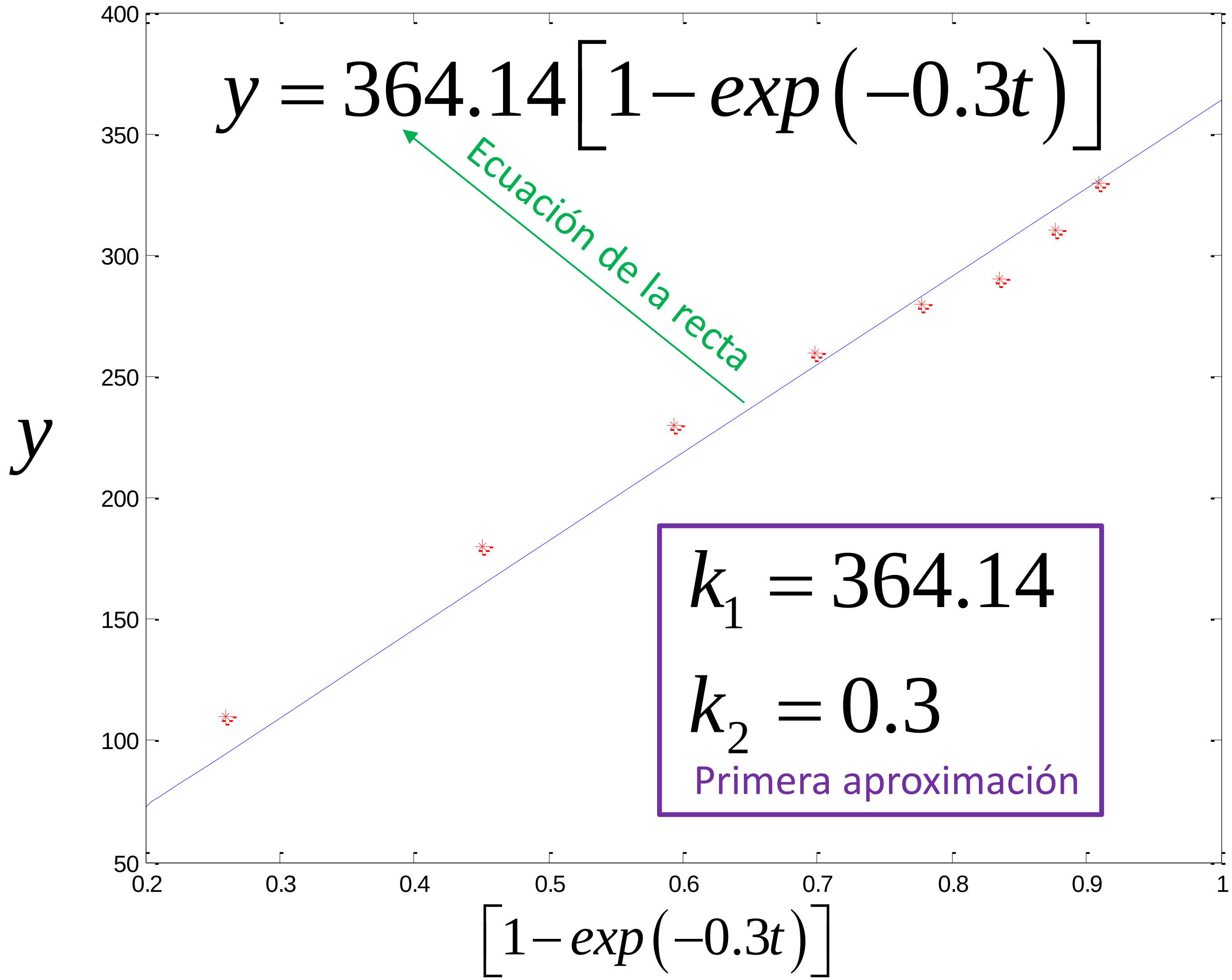
Ajuste lineal para k_2=1



$$y$$

$$\left[1-exp\left(-0.3t\right)\right]$$

Ajuste lineal para k_2=1



Implementación de la resolución

$$\underline{x}^{(0)} = \begin{bmatrix} 364.14 \\ 0.3 \end{bmatrix} \rightarrow \underline{x}^{(1)} = \underline{x}^{(0)} - \underline{\underline{J}}\left(\underline{x}^{(0)}\right)^{-1} \underline{f}\left(\underline{x}^{(0)}\right) = \begin{bmatrix} 332.4838 \\ 0.3659 \end{bmatrix}$$

$$\underline{x}^{(2)} = \begin{bmatrix} 335.5456 \\ 0.3764 \end{bmatrix} \qquad \rightarrow \underline{x}^{(3)} = \begin{bmatrix} 334.2650 \\ 0.3807 \end{bmatrix}$$

$$\left\| f\left(\underline{x}^{(2)}\right) \right\| = 393.4308 \qquad \left\| f\left(\underline{x}^{(3)}\right) \right\| = 26.1561$$

$$\underline{x}^{(10)} = \begin{bmatrix} 334.2676 \\ 0.3807 \end{bmatrix} \qquad \left\| f\left(\underline{x}^{(10)}\right) \right\| = 1.0459 \times 10^{-11}$$

Grafica

$$y = 334.2676\left[1 - exp\left(-0.3807t\right)\right]$$