Ejemplos de regresión no lineal (modelo no linealizable)

Prof.: Dr. Juan Ignacio Manassaldi
JTP: Ing. Amalia Rueda

Introducción

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

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

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:

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

Vector Residuo

Residuo:

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

Problema de Mínimos Cuadrados

La norma del residuo al cuadrado corresponde a:

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

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

Podemos resolverlo como un problema de optimización multidimensional no restringido:

$$Min.\ \sum_{i=1}^{n}\left(y_i - k_1 + k_1 exp\left(-k_2 t_i\right)\right)^2$$

$$Min.\ \ f\left(\underline{x}\right) = \sum_{i=1}^{n}\left(y_i - x_1 + x_1 exp\left(-x_2 t_i\right)\right)^2$$

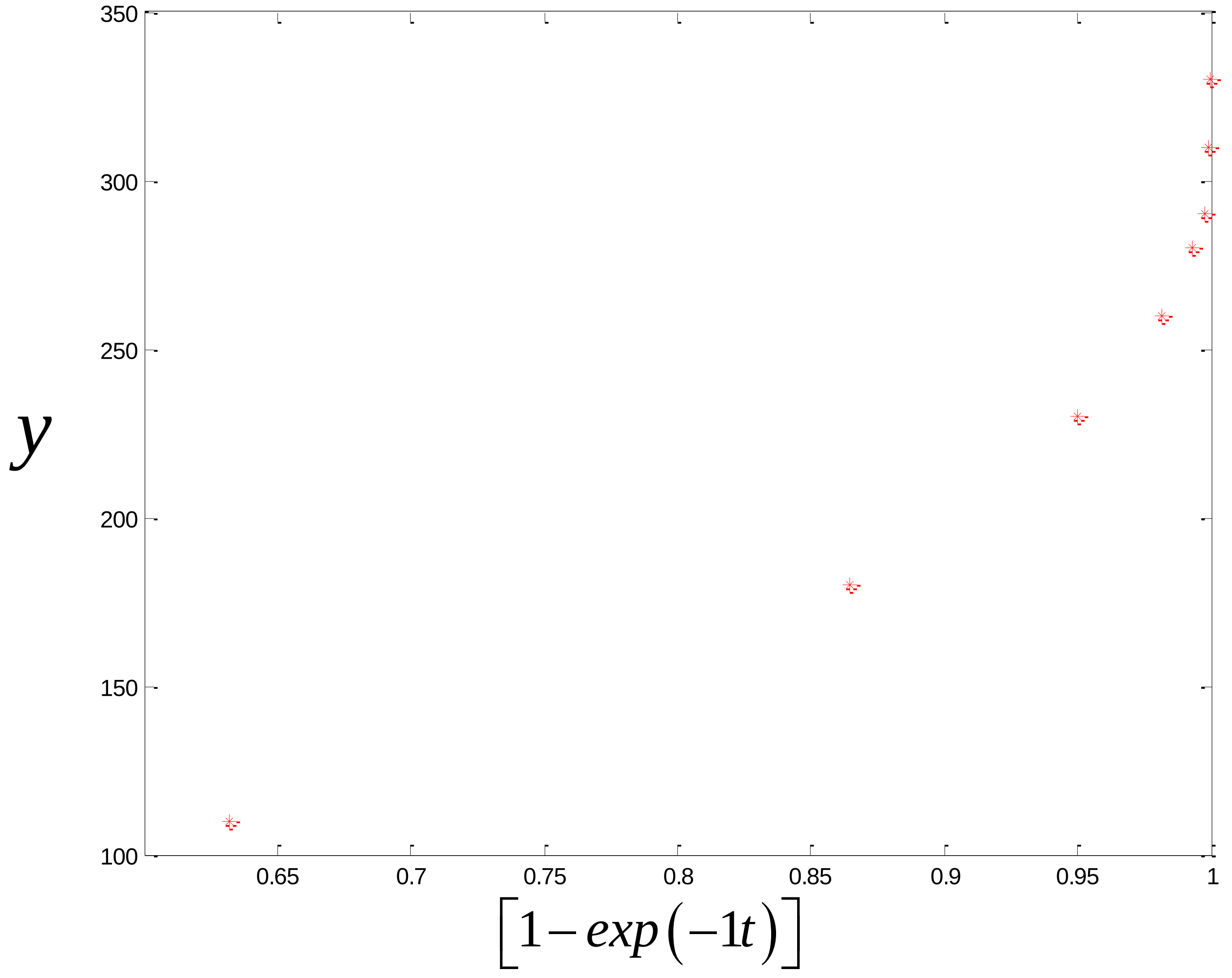
Selección del valor de arranque

¿Valor de arranque?

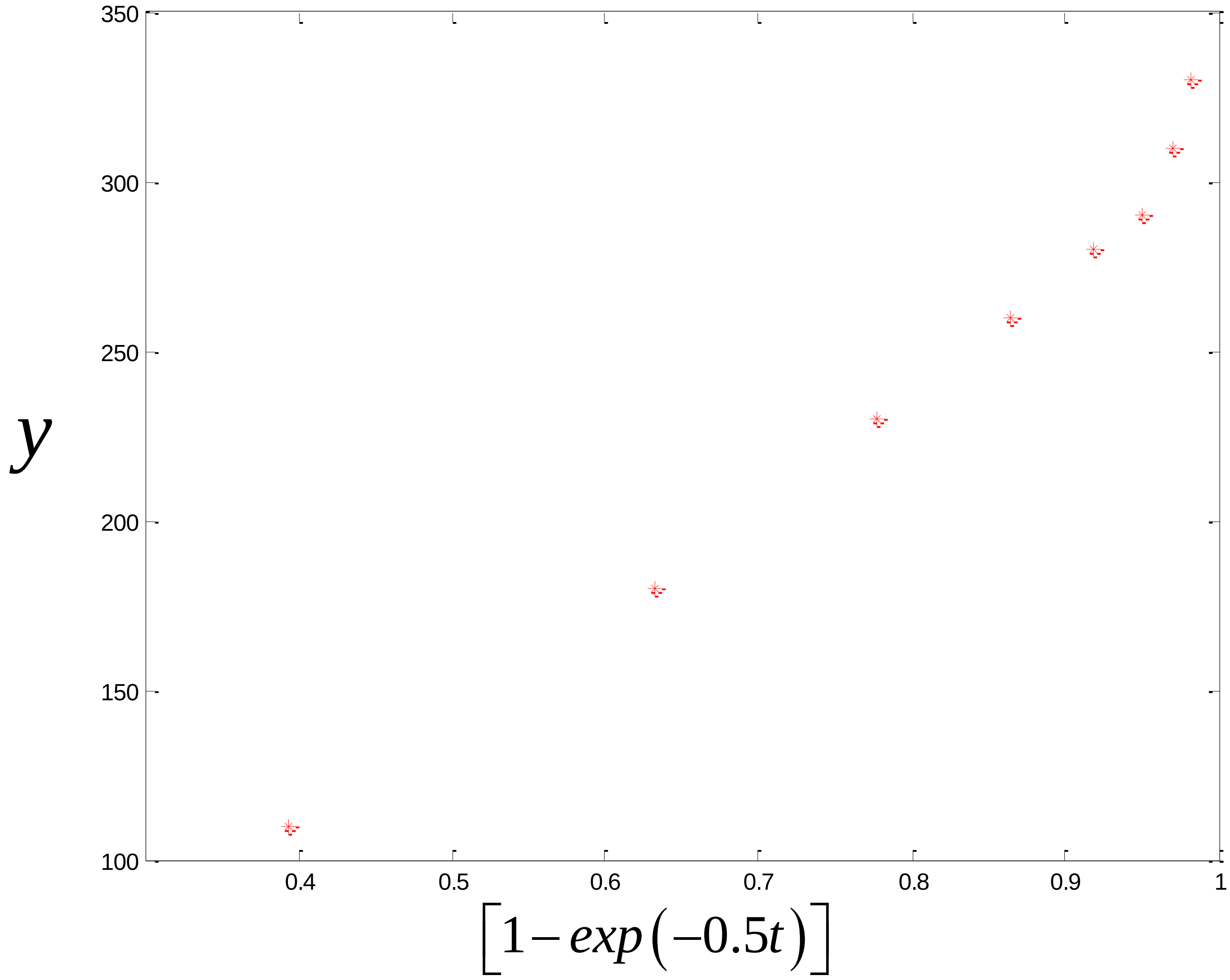
- Una buena estrategia es fijar un valor de k_2 y encontrar k_1 por regresión lineal.
- Variando el valor de k_2 gráficamente se puede visualizar un adecuado ajuste lineal.
- Una vez definido el valor de k_2, a partir de una regresión lineal, se obtiene k_1.
- Estos valores resultan un buen punto de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

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

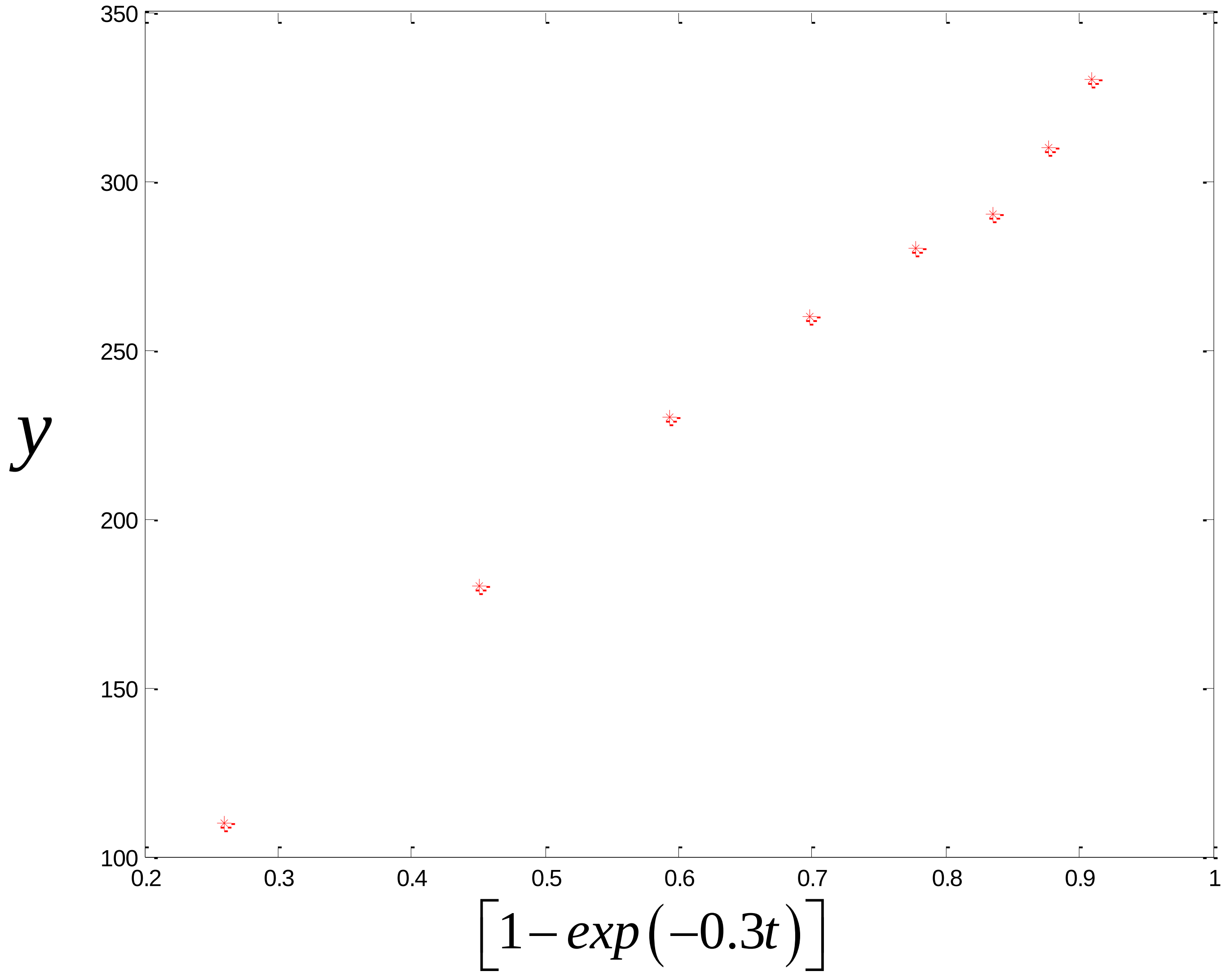
Grafica de datos para k_2=1



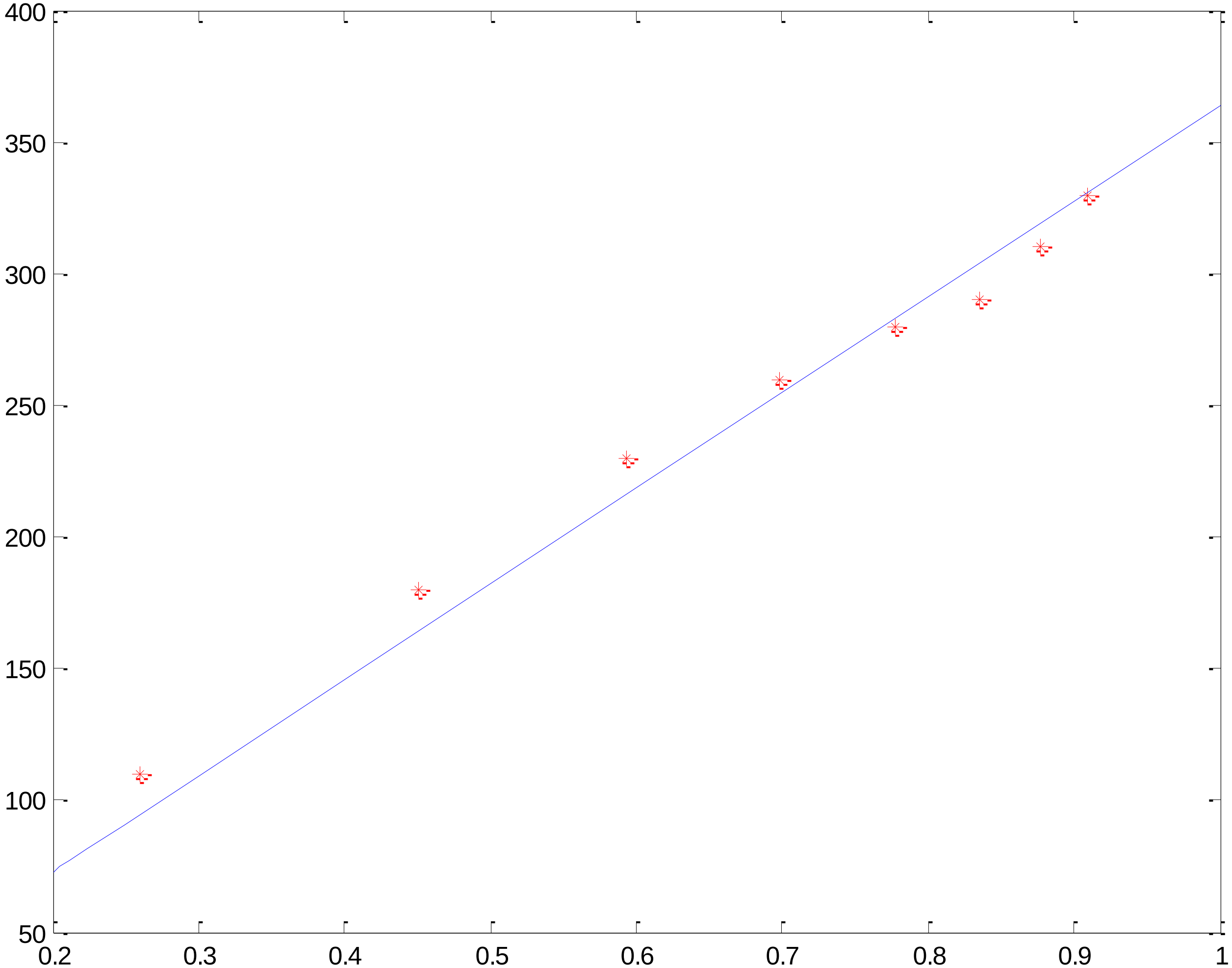
Grafica de datos para k_2=0.5



Grafica de datos para k_2=0.3



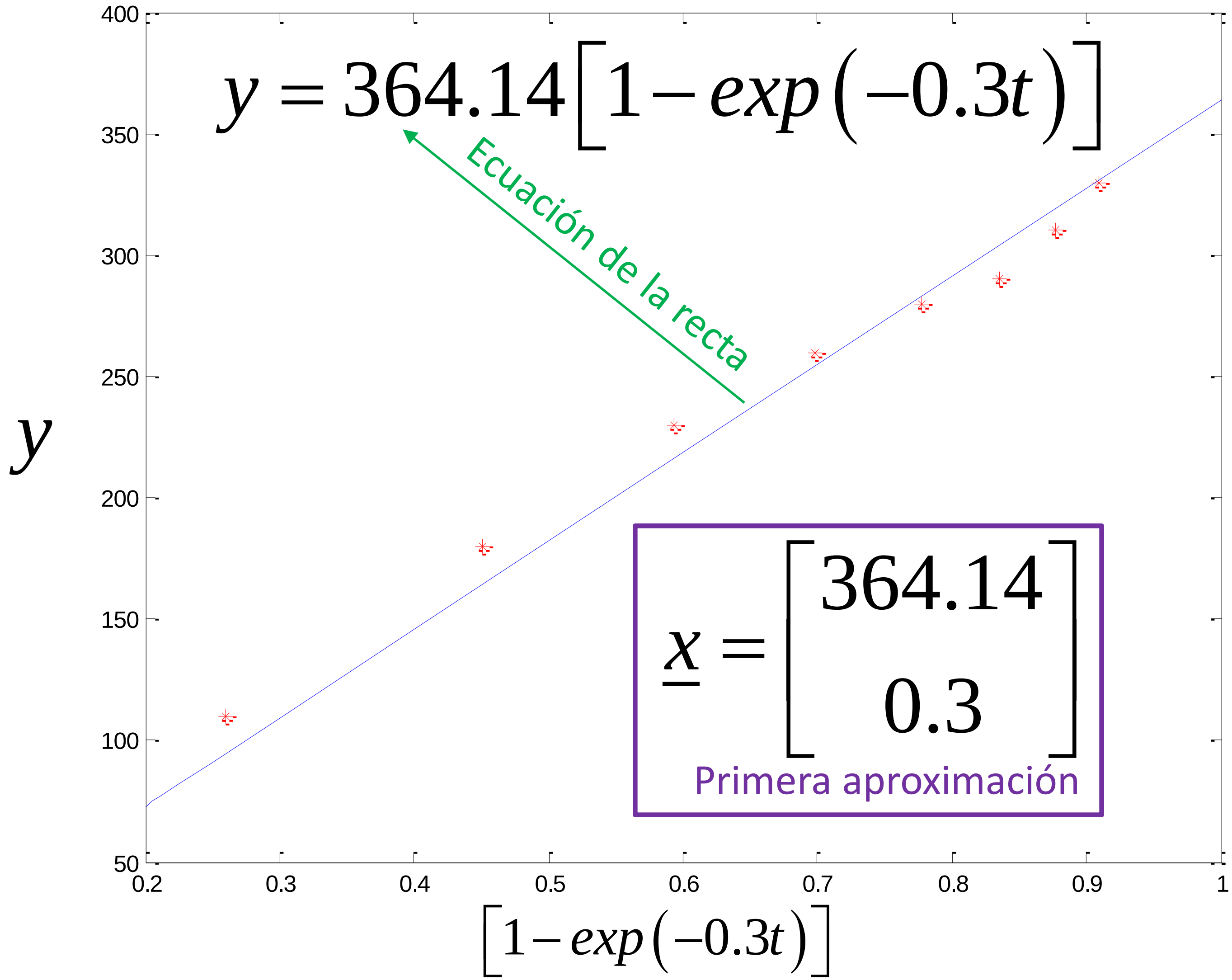
Ajuste lineal para k_2=0.3



$$y$$

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

Ajuste lineal para $k_2=0.3$



Regresión no linealizable

```
function alfa=linesearchMIPS(fun, xk, d, a_0)
  x1 = a_0*0.98;
  x2 = a_0;
  x3 = a_0*1.02;
  for i= 1:100
    A=[x1^2 x1 1
    x2^2 x2 1
    x3^2 x3 1 ];
    b=[fun(xk + x1*d)
    fun(xk + x2*d)
    fun(xk + x3*d)];
    xx=A\b;
    x4=-xx(2)/(2*xx(1));
    if norm(x4-x3) < 1e-6
      alfa=x4;
      break
    end
    x1=x2; x2=x3; x3=x4;
  end
  if i==100
    alfa=[];
  end
  if fun(xk + alfa*d)>=fun(xk)
    alfa=[];
  end
endfunction
```

```
function alfa=linesearchMN(Fun, Grad, Hess, xk, d, a_0)
  a=a_0;
  for i=1:100
    fp = Grad(xk + a*d)'*d;
    fpp= d'*Hess(xk + a*d)*d;
    a=a-fp/fpp;
    if norm(fp/fpp) < 1e-5
      alfa=a;
      break
    end
  end
  if i==100
    alfa=[];
  end
  if Fun(xk + alfa*d) >= Fun(xk)
    alfa=[];
  end
endfunction
```

Regresión no linealizable

$$f\left(\underline{x}\right)=\sum_{i=1}^{n}\left(y_i-x_1+x_1exp\left(-x_2t_i\right)\right)^2$$

```
function r=Fun(x)
t=[1,2,3,4,5,6,7,8];
BOD=[110,180,230,260,280,290,310,330];
r=sum( (BOD - x(1) + x(1)*exp(-x(2)*t)).^2);
endfunction
```

Resolución un variable a la vez

$$\underline{x}^{(0)} = \begin{bmatrix} 364.14 \\ 0.3 \end{bmatrix}$$

$$f\left(\underline{x}^{(0)}\right) = 1010.05$$

$$\underline{d}_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

```
--> alfa = linesearchMIPS(Fun,x0,d1,1)
 alfa  =

  -0.0037421
```

$$\underline{x}^{(0)} = \begin{bmatrix} 364.13626 \\ 0.3 \end{bmatrix}$$

$$\underline{d}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

```
-->alfa = linesearchMIPS(Fun,x0,d2,1)
alfa  =

    []
--> alfa = linesearchMIPS(Fun,x0,d2,1e-1)
 alfa  =

    0.0095396
```

$$\underline{x}^{(1)} = \begin{bmatrix} 364.13626 \\ 0.3095396 \end{bmatrix}$$

$$f\left(\underline{x}^{(1)}\right) = 920.13$$

Resolución un variable a la vez

$$\underline{x}^{(0)} = \begin{bmatrix} 364.14 \\ 0.3 \end{bmatrix}$$

$$f\left(\underline{x}^{(0)}\right) = 1010.05$$

$$\underline{x}^{(1)} = \begin{bmatrix} 364.13626 \\ 0.3095396 \end{bmatrix}$$

$$f\left(\underline{x}^{(1)}\right) = 920.13$$

$$\underline{x}^{(2)} = \begin{bmatrix} 359.70875 \\ 0.3185861 \end{bmatrix}$$

$$f\left(\underline{x}^{(2)}\right) = 766.27$$

Continuar….

$$\underline{x}^{(59)} = \begin{bmatrix} 334.26777 \\ 0.3807448 \end{bmatrix}$$

$$f\left(\underline{x}^{(2)}\right) = 288.96732$$

Resolución por descenso mas pronunciado

$$\nabla f\left(\underline{x}\right)=\begin{bmatrix}\sum_{i=1}^{n}2\left(y_i-x_1+x_1 exp\left(-x_2t_i\right)\right)\left(-1+exp\left(-x_2t_i\right)\right)\\ \sum_{i=1}^{n}2\left(y_i-x_1+x_1 exp\left(-x_2t_i\right)\right)\left(-t_ix_1 exp\left(-x_2t_i\right)\right)\end{bmatrix}$$

```
function G=Grad(x)
t=[1,2,3,4,5,6,7,8];
BOD=[110,180,230,260,280,290,310,330];
G(1,1)=sum( 2*(BOD - x(1) + x(1)*exp(-x(2)*t)).*(-1 + exp(-x(2)*t)) );
G(2,1)=sum( 2*(BOD - x(1) + x(1)*exp(-x(2)*t)).*((-t).*x(1).*exp(-x(2)*t)) );
endfunction
```

Resolución gradiente

$$\underline{x}^{(0)} = \begin{bmatrix} 364.14 \\ 0.3 \end{bmatrix}$$

$$f\left(\underline{x}^{(0)}\right) = 1010.05$$

$$\nabla f\left(\underline{x}^{(0)}\right) = \begin{bmatrix} 0.0299997 \\ -19226.542 \end{bmatrix}$$

$$\underline{d} = \begin{bmatrix} -0.0299997 \\ 19226.542 \end{bmatrix}$$

$$Min\ \ f\left(\underline{x}^{(0)} + \alpha \underline{d}\right)$$

```
--> alfa=linesearchMN(Fun,Grad,Hess,x0,d,1)
 alfa  =

    []

--> alfa = linesearchMN(Fun,Grad,Hess,x0,d,1e-2)
 alfa  =

    []
```

⋮

```
--> alfa = linesearchMN(Fun,Grad,Hess,x0,d,1e-6)
 alfa  =

   0.0000005
```

$$\underline{x}^{(1000)} = \begin{bmatrix} 363.93013 \\ 0.3099337 \end{bmatrix}$$

$$f\left(\underline{x}^{(1000)}\right) = 912.64412$$

Muuuy lento….

Resolución por Newton

$$H_{f(\underline{x})}=\begin{bmatrix} \sum_{i=1}^{n} 2\left(-1+exp\left(-x_2t_i\right)\right)\left(-1+exp\left(-x_2t_i\right)\right) & \sum_{i=1}^{n} 2\left(-t_ix_1exp\left(-x_2t_i\right)\right)\left(-1+exp\left(-x_2t_i\right)\right)+2\left(y_i-x_1+x_1exp\left(-x_2t_i\right)\right)\left(-t_iexp\left(-x_2t_i\right)\right) \\ \sum_{i=1}^{n} 2\left(-t_ix_1exp\left(-x_2t_i\right)\right)\left(-1+exp\left(-x_2t_i\right)\right)+2\left(y_i-x_1+x_1exp\left(-x_2t_i\right)\right)\left(-t_iexp\left(-x_2t_i\right)\right) & \sum_{i=1}^{n} 2\left(-t_ix_1exp\left(-x_2t_i\right)\right)\left(-t_ix_1exp\left(-x_2t_i\right)\right)+2\left(y_i-x_1+x_1exp\left(-x_2t_i\right)\right)\left(t_it_ix_1exp\left(-x_2t_i\right)\right) \end{bmatrix}$$

```
function H=Hess(x)
t=[1,2,3,4,5,6,7,8];
BOD=[110,180,230,260,280,290,310,330];
H(1,1)=sum( 2*(- 1 + exp(-x(2)*t)).*(-1 + exp(-x(2)*t)) );
H(1,2)=sum( 2*((-t).*x(1).*exp(-x(2)*t)).*(-1 + exp(-x(2)*t))  + 2*(BOD - x(1) + x(1)*exp(-x(2)*t)).*((-t).*exp(-x(2)*t)));
H(2,1)=sum( 2*((-t).*x(1).*exp(-x(2)*t)).*(-1 + exp(-x(2)*t))  + 2*(BOD - x(1) + x(1)*exp(-x(2)*t)).*((-t).*exp(-x(2)*t)));
H(2,2)=sum( 2*((-t).*x(1).*exp(-x(2)*t)).*((-t).*x(1).*exp(-x(2)*t))  + 2*(BOD - x(1) + x(1)*exp(-x(2)*t)).*((-t).*(-t).*x(1).*exp(-x(2)*t)));
endfunction
```

Resolución por Newton

$$\underline{x}^{(0)} = \begin{bmatrix} 364.14 \\ 0.3 \end{bmatrix}$$

$$f\left(\underline{x}^{(0)}\right) = 1010.05$$

$$\nabla f\left(\underline{x}^{(0)}\right) = \begin{bmatrix} 0.0299997 \\ -19226.542 \end{bmatrix}$$

$$H_{f\left(\underline{x}^{(0)}\right)} = \begin{bmatrix} 8.016729 & 3850.531 \\ 3850.531 & 2141428.7 \end{bmatrix}$$

$$\underline{\underline{H}}\,\underline{d} = -\underline{\nabla f}$$

$$\underline{d} = \begin{bmatrix} -31.656239 \\ 0.0658999 \end{bmatrix}$$

$$\underline{x}^{(1)} = \begin{bmatrix} 338.58988 \\ 0.3531886 \end{bmatrix}$$

$$f\left(\underline{x}^{(1)}\right) = 444.05982$$

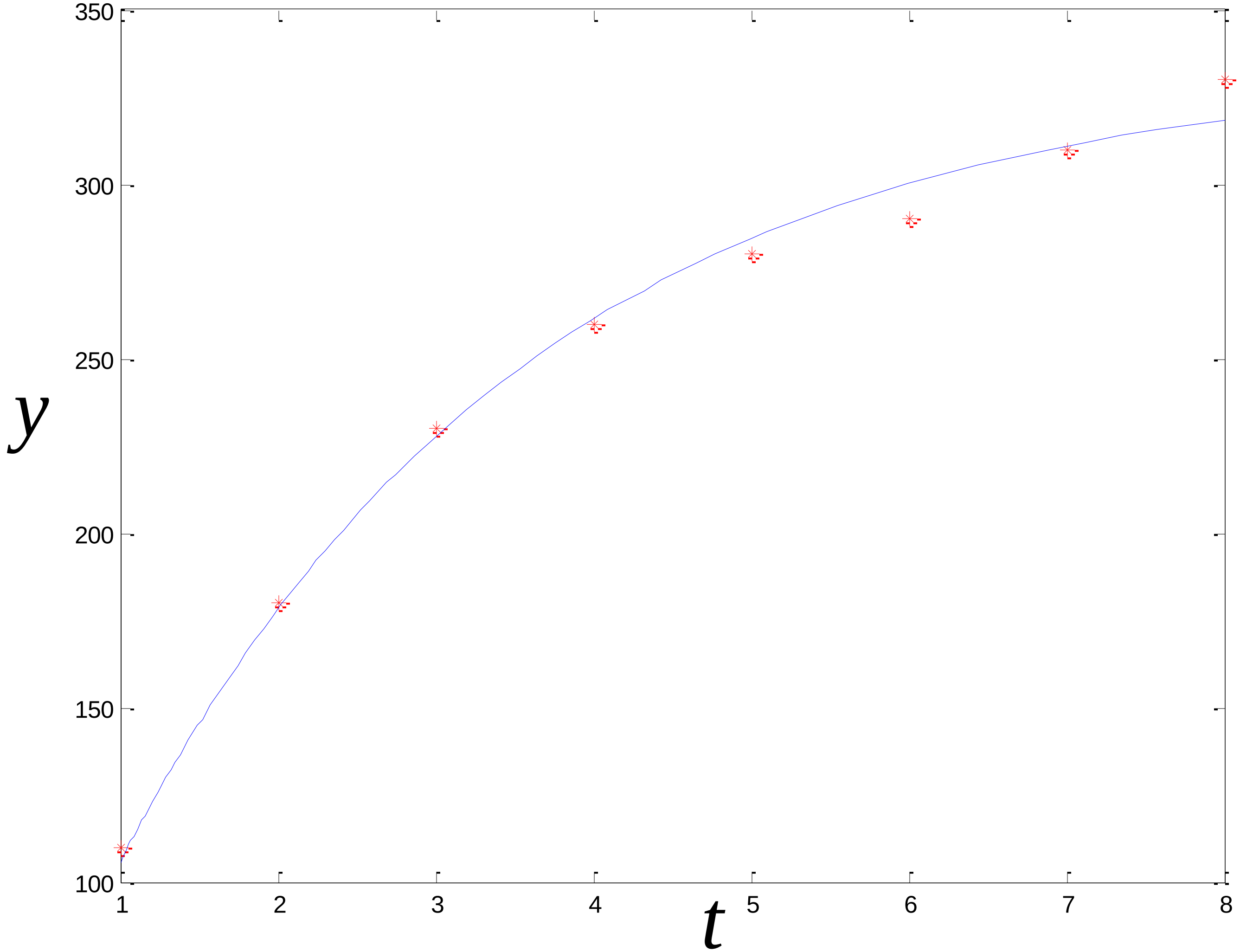
$$\vdots$$

$$\underline{x}^{(6)} = \begin{bmatrix} 334.26764 \\ 0.3807452 \end{bmatrix}$$

$$f\left(\underline{x}^{(6)}\right) = 288.96732$$

Grafica

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



Propuesta