A linha dos quadrados mínimos da diferença pode ser encontrada minimizando a soma

$$d_1^2 + d_2^2 + ... + d_n^2 = \sum_{i=1}^n d_i^2$$

Estas são as diferenças.

Dada a equação da linha do modelo $\hat{y} = b x + a$, em que b é o slope e a o deslocamento vertical.

Os valores na linha do modelo são denotados \hat{y} .

Cada distância vertical é a diferença entre \hat{y} e y.

Substituindo \hat{y} em

$$d_i = \hat{y}_i - y_i$$

por b x + a, temos

$$d_i = b x_i + a - y_i$$

Com isto, a soma da minimização dos quadrados da diferença fica

$$(bx_1 + a - y_1)^2 + (bx_2 + a - y_2)^2 + \dots + (bx_n + a - y_n)^2 = \sum_{i=1}^{n} (bx_i + a - y_i)^2.$$

Todos os X_i e Y_i na função são conhecidos (são os dados).

O que fica para definir são b e a.

b e a são comuns a todos os termos; é necessário achar um valor único que torne a soma o menor número possível.

O problema é, para cada ponto a função tem um termo.

Por exemplo, para
$$D = \{\{4, 5\}, \{2, 7\}, \{9, 1\}, \{12, 6\}, \{5, 3\}\}, (4b+a-5)^2 + (2b+a-7)^2 + (9b+a-1)^2 + (12b+a-6)^2 + (5b+a-3)^2 = (9b+a-1)^2 + (12b+a-6)^2 + (12b+a-3)^2 = (12b+a-1)^2 + (12b+a-1)^2 + (12b+a-1)^2 + (12b+a-1)^2 = (12b+a-1)^2 + (12b+a-1)^2 + (12b+a-1)^2 + (12b+a-1)^2 = (12b+a-1)^2 + (12b+a-1)^$$

$$\begin{split} & \text{In[a]:= } \left\{ \text{Expand} \left[\, \left(4\,\, b + a - 5 \right)^{\,2} \right] \text{, Expand} \left[\, \left(2\,\, b + a - 7 \right)^{\,2} \right] \text{,} \\ & \text{Expand} \left[\, \left(9\,\, b + a - 1 \right)^{\,2} \right] \text{, Expand} \left[\, \left(12\,\, b + a - 6 \right)^{\,2} \right] \text{, Expand} \left[\, \left(5\,\, b + a - 3 \right)^{\,2} \right] \right\} \\ & \text{Out[a]:= } \left\{ 25 - 10\,\, a + a^2 - 40\,\, b + 8\,\, a\,\, b + 16\,\, b^2 \text{, } 49 - 14\,\, a + a^2 - 28\,\, b + 4\,\, a\,\, b + 4\,\, b^2 \text{,} \\ & 1 - 2\,\, a + a^2 - 18\,\, b + 18\,\, a\,\, b + 81\,\, b^2 \text{, } 36 - 12\,\, a + a^2 - 144\,\, b + 24\,\, a\,\, b + 144\,\, b^2 \text{, } 9 - 6\,\, a + a^2 - 30\,\, b + 10\,\, a\,\, b + 25\,\, b^2 \right\} \end{split}$$

Somando os termos...

$$In[a] = \text{Expand} \left[\left(4 \text{ b} + \text{a} - 5 \right)^2 \right] + \text{Expand} \left[\left(2 \text{ b} + \text{a} - 7 \right)^2 \right] + \text{Expand} \left[\left(9 \text{ b} + \text{a} - 1 \right)^2 \right] + \text{Expand} \left[\left(12 \text{ b} + \text{a} - 6 \right)^2 \right] + \text{Expand} \left[\left(5 \text{ b} + \text{a} - 3 \right)^2 \right]$$

$$Out[a] = 120 - 44 \text{ a} + 5 \text{ a}^2 - 260 \text{ b} + 64 \text{ a} \text{ b} + 270 \text{ b}^2$$

Agora temos termos $a, b, a^2, b^2 e a b$ (e um termo livre).

Para cada um destes termos, temos um coeficiente.

$$ln[a]:=$$
 FullSimplify [120 - 44 a + 5 a² - 260 b + 64 a b + 270 b²]
Out[a]:= 120 + a (-44 + 5 a) - 260 b + 64 a b + 270 b²

Não dá para agrupar só em a e b porque temos um termo a b.

Se não tivéssemos este termo,

$$ln[*] = FullSimplify[120 - 44 a + 5 a^2 - 260 b + 270 b^2]$$

 $Out[*] = 120 + a(-44 + 5 a) + 10 b(-26 + 27 b)$

Mesmo assim temos as potências.

Mas a função geral para minimizar para $oldsymbol{a}$ e $oldsymbol{b}$ é

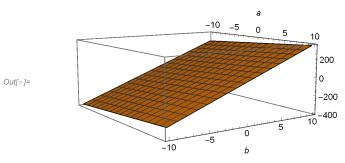
$$120 - 44 a + 5 a^2 - 260 b + 64 a b + 270 b^2$$

Se não fosse a diferença ao quadrado, apenas simples,

Ou seja, é o quadrado da diferença que introduz essa "multiplicidade de variáveis".

Podemos começar com a simples, -22 + 5a + 32b, para minimizar.

ln[*]:= Plot3D[32 b + 5 a - 22, {a, -10, 10}, {b, -10, 10}, AxesLabel \rightarrow Automatic]



As derivadas parciais.

Mantendo b constante, $\frac{\partial y}{\partial a} = 5$ (pois se b é **uma** constante, 32b é derivado como 0); mantendo a constante, $\frac{\partial y}{\partial b} = 32$ (pois se a é **uma** constante, a é derivado como a0).

$$ln[*]:= \{\partial_a (32b+5a-22), \partial_b (32b+5a-22)\}$$
Out[*]= $\{5, 32\}$

Então as diferenças simples têm parciais constantes.

Mas os extremos são igualar a zero.

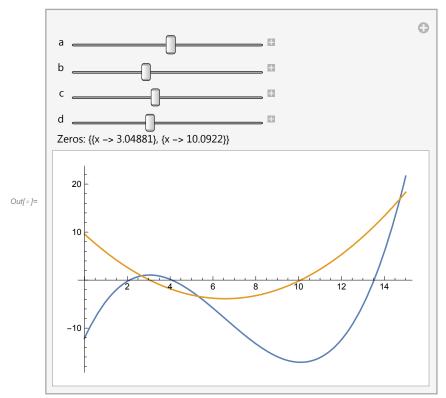
Mas não dá para igualar estas derivadas a zero; elas são os próprios extremos.

Pausando para uma função qualquer arbitrária.

$$ln[-] := \partial_x (0.1 x^3 - 2 x^2 + 10.3 x - 8.1)$$

Out[
$$\circ$$
]= 10.3 - 4 x + 0.3 \times^2

$$\begin{split} & \textit{In[*]} := \mathsf{Module} \Big[\{ \mathsf{f}, \mathsf{df} \}, \mathsf{Manipulate} \Big[\mathsf{f} = \mathsf{a} \, \mathsf{x}^3 + \mathsf{b} \, \mathsf{x}^2 + \mathsf{c} \, \mathsf{x} + \mathsf{d}; \\ & \mathsf{df} = \partial_{\mathsf{x}} \mathsf{f}; \\ & \mathsf{Plot} \big[\{ \mathsf{f}, \mathsf{df} \}, \, \{ \mathsf{x}, \, \mathsf{0}, \, \mathsf{15} \} \, (*, \mathsf{PlotRange} \rightarrow \{ \{ \mathsf{0}, \mathsf{15} \}, \{ -10, 20 \} \} *) \, \big], \\ & \{ \{ \mathsf{a}, \, \mathsf{0}.1 \}, \, \mathsf{0}, \, \mathsf{0}.2, \, \mathsf{0}.001 \}, \, \{ \{ \mathsf{b}, \, -2 \}, \, -2.2, \, -1.8, \, .01 \}, \, \{ \{ \mathsf{c}, \, \mathsf{10}.3 \}, \, \mathsf{5}.3, \, \mathsf{15}.3, \, .1 \}, \\ & \{ \{ \mathsf{d}, \, -8.1 \}, \, -28.1, \, \mathsf{12}.1, \, .1 \}, \, \mathsf{Dynamic} \big["\mathsf{Zeros}: \, " <> \, \mathsf{ToString} \big[\mathsf{Solve} \big[\mathsf{df} = = 0, \, \mathsf{x} \big] \big] \, \big] \, \Big] \, \end{split}$$



Mas estes não são extremos, são pontos de inflexão...

Nestas raízes, y é...

$$\label{eq:local_$$

In[*]:= {f1[x /. First[f1ext]], f1[x /. Last[f1ext]]}

Out[\circ]= {7.73766, -5.12285}

Sem usar os dados, as derivadas parciais da soma da minimização dos quadrados da diferença

$$\partial_a \sum_{i=1}^n (b x_i + a - y_i)^2 e \partial_b \sum_{i=1}^n (b x_i + a - y_i)^2$$
 seriam

$$In[*]:=\sum_{i=1}^{n} \left(b x_i + a - y_i\right)$$

$$\textit{Out[*]} = \sum_{i=1}^{n} \left(a + b \ x_i - y_i \right)$$

$$log_{a} := \left\{ \partial_{a} \sum_{i=1}^{n} \left(b x_{i} + a - y_{i} \right)^{2}, \partial_{b} \sum_{i=1}^{n} \left(b x_{i} + a - y_{i} \right)^{2} \right\}$$

$$\textit{Out[*]} = \Big\{ \sum_{i=1}^{n} \Big(2 \; a \; + \; 2 \; b \; x_i \; - \; 2 \; y_i \Big) \; \text{, } \sum_{i=1}^{n} \Big(2 \; a \; x_i \; + \; 2 \; b \; x_i^2 \; - \; 2 \; x_i \; y_i \Big) \; \Big\}$$

Sem os quadrados...

$$In[*]:= \left\{ \partial_a \sum_{i=1}^n b \ x_i + a - y_i, \ \partial_b \sum_{i=1}^n b \ x_i + a - y_i \right\}$$

$$\textit{Out[s]} = \left\{ a - y_i, \ a - y_i + \sum_{i=1}^{n} x_i \right\}$$

Igualar a zero...

$$lo[a] := Solve \left[\sum_{i=1}^{n} (2a + 2b x_i - 2y_i) == 0, b \right]$$

Solve: This system cannot be solved with the methods available to Solve.

$$Out[*]= Solve \Big[\sum_{i=1}^{n} (2 a + 2 b x_i - 2 y_i) == 0, b \Big]$$

Usando os dados D na diferença sem quadrados, as diferenças simples têm parciais constantes. Nestas derivadas (números), V é

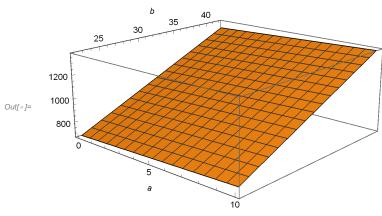
In[*]:= Clear[f2,f2ext]
f2=Function[{a,b},32b+5a-22];
f2ext=<|"a"
$$\rightarrow \partial_a$$
f2[a,b],"b" $\rightarrow \partial_b$ f2[a,b]|>

Out[
$$\bullet$$
]= $\langle \mid a \rightarrow 5$, $b \rightarrow 32 \mid \rangle$

A função é bidimensional e tem os extremos para cada variável/dimensão. Logo devemos plugar estes extremos na função bidimensional?

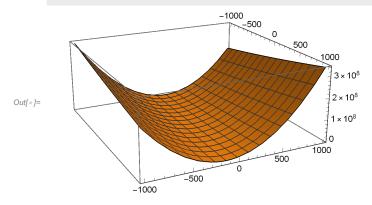
Out[•]= 1027

 $log_{[a]} = Plot3D[32b + 5a - 22, \{a, 0, 10\}, \{b, 22, 42\}, AxesLabel \rightarrow Automatic(*,Epilog \rightarrow Line[\{5,32\}]*)]$



Acho que é por isso que a diferença é ao quadrado... Função linear não tem extremo. Visualizar a diferença ao quadrado.

Hide steps 🕀



$$ln[\bullet]:= \{\partial_a f3[a, b], \partial_b f3[a, b]\}$$

$$\textit{Out[*]} = \; \left\{ \, -\, 44 \, +\, 10 \; a \, +\, 64 \; b \, , \; -\, 260 \, +\, 64 \; a \, +\, 540 \; b \, \right\}$$

$$log[a] := \{ Solve[\partial_a f3[a, b] == 0, a], Solve[\partial_b f3[a, b] == 0, b] \}$$

$$\textit{Out[*]} = \; \left\{ \, \left\{ \, \left\{ \, a \, \rightarrow \, -\, \frac{2}{5} \, \, \left(\, -\, 11 \, +\, 16 \, \, b \, \right) \, \right\} \, \right\} \, , \; \left\{ \, \left\{ \, b \, \rightarrow \, \frac{1}{135} \, \, \left(65 \, -\, 16 \, \, a \, \right) \, \right\} \, \right\} \, \right\}$$

Invertido? (Não sei o significado.)

$$ln[\cdot]:= \{Solve[\partial_a f3[a, b] == 0, b], Solve[\partial_b f3[a, b] == 0, a]\}$$

$$\text{Out[*]= } \left\{ \left. \left\{ \left\{ b \to \frac{1}{32} \, \left(22 - 5 \, a \right) \right\} \right\} \text{, } \left\{ \left\{ a \to -\frac{5}{16} \, \left(-13 + 27 \, b \right) \right\} \right\} \right\} \right.$$

As derivadas parciais das bidimensionais ainda são bidimensionais, mas como achar seus extremos (números)? Parece que é encontrar a solução comum das equações parciais... Exatamente o que monta a matriz.

$$log(a) = Solve[(\partial_a f3[a, b] == 0) && (\partial_b f3[a, b] == 0), a]$$

Out[•]= { }

$$lo(a) = Solve[(-44 + 10 a + 64 b = 0) & (-260 + 64 a + 540 b = 0), a]$$

Out[•]= { }

In[
$$\circ$$
]:= Solve $\left[\left(\partial_b f3[a, b] == 0 \right) \&\& \left(\partial_a f3[a, b] == 0 \right), b \right]$

Out[•]= { }

$$ln[*]:=$$
 Solve $[(-44 + 10 a + 64 b == 0) & (-260 + 64 a + 540 b == 0), b]$

 $Out[\, \circ \,]= \quad \left\{ \ \right\}$

Talvez não tenha solução por causa destes dados.

o 2 antes das derivadas parciais é por causa da diferenciação do quadrado 1 . E o X_1 multiplicado extra na b?

$$ln[*]:= \{\partial_b (b x_1 + a - y_1)^2, \partial_a (b x_1 + a - y_1)^2\}$$

$$\textit{Out[=]} = \; \left\{ \; 2 \; x_1 \; \left(\; a \; + \; b \; x_1 \; - \; y_1 \right) \; \text{, 2} \; \left(\; a \; + \; b \; x_1 \; - \; y_1 \right) \; \right\}$$

In[•]:= Partial derivative for b of (b*x+a-y)^2

Derivative:

$$\frac{\partial}{\partial b} ((bx + a - y)^2) = 2x(a + bx - y)$$

Possible intermediate steps:

Possible derivation:

$$\frac{\partial}{\partial b} \left((a + b \, x - y)^2 \right)$$

Using the chain rule, $\frac{\partial}{\partial b}((a+bx-y)^2) = \frac{\partial u^2}{\partial u} \frac{\partial u}{\partial b}$, where u = a+bx-y and $\frac{\partial}{\partial u}(u^2) = 2u$: = $2(a+bx-y)\left(\frac{\partial}{\partial b}(a+bx-y)\right)$

Differentiate the sum term by term and factor out constants:

$$= \frac{\partial}{\partial b}(a) + x \frac{\partial}{\partial b}(b) + \frac{\partial}{\partial b}(-y) 2(a + bx - y)$$

The derivative of *a* is zero:

$$= 2(a+bx-y)\left(x\left(\frac{\partial}{\partial b}(b)\right) + \frac{\partial}{\partial b}(-y) + \boxed{0}\right)$$

Simplify the expression:

$$= 2(a+bx-y)\left(x\left(\frac{\partial}{\partial b}(b)\right) + \frac{\partial}{\partial b}(-y)\right)$$

The derivative of b is 1:

$$= 2 (a + b x - y) \left(\frac{\partial}{\partial b} (-y) + 1 x \right)$$

The derivative of -y is zero:

$$= 2(a+bx-y)(x+0)$$

Simplify the expression:

Answer:

$$= 2x(a+bx-y)$$

Geometric figure:

hyperbolic paraboloid

Alternate forms:

$$\frac{(a+2\,b\,x-y)^2}{2\,b} - \frac{a^2-2\,a\,y+y^2}{2\,b}$$

$$2 a x + 2 b x^2 - 2 x y$$

$$x(2a+2bx-2y)$$

Real root:

$$x = 0$$

Root:

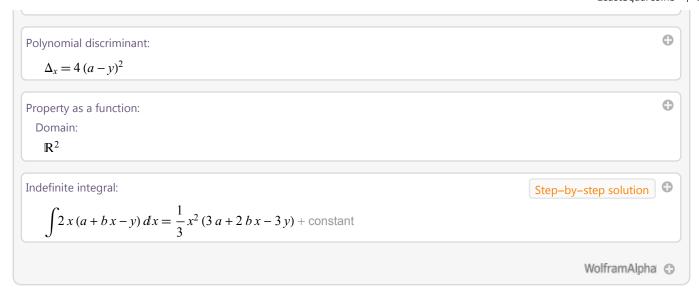
$$y = a + bx$$

Step-by-step solution

•

0

More •



É a chain rule.

A somatória de uma soma pode ser a soma das somatórias.2

$$\partial_{a} \sum_{i=1}^{n} (b x_{i} + a - y_{i})^{2} =$$

$$\sum_{i=1}^{n} (2 a + 2 b x_{i} - 2 y_{i}) =$$

$$2 n a + 2 \sum_{i=1}^{n} b x_{i} - 2 \sum_{i=1}^{n} y_{i} =$$

$$2 a n + 2 b \sum_{i=1}^{n} x_{i} - 2 \sum_{i=1}^{n} y_{i}$$
e

$$\partial_{b} \sum_{i=1}^{n} (b x_{i} + a - y_{i})^{2} =$$

$$\sum_{i=1}^{n} (2 a x_{i} + 2 b x_{i}^{2} - 2 x_{i} y_{i}) =$$

$$2 \sum_{i=1}^{n} a x_{i} + 2 \sum_{i=1}^{n} b x_{i}^{2} - 2 \sum_{i=1}^{n} y_{i} x_{i} =$$

$$2 a \sum_{i=1}^{n} x_{i} + 2 b \sum_{i=1}^{n} x_{i}^{2} - 2 \sum_{i=1}^{n} y_{i} x_{i}.$$

Em ∂_a , por algum motivo, $\sum_{i=1}^n a$ vira n a.

Mas este não é o principal; mesmo na forma básica, as parciais já contam com uma separação das variáveis. Igualando a zero,

$$2an + 2b \sum_{i=1}^{n} x_i - 2 \sum_{i=1}^{n} y_i = 0 \Rightarrow$$

$$2an + 2b \sum_{i=1}^{n} x_i = 2 \sum_{i=1}^{n} y_i$$
e
$$2a \sum_{i=1}^{n} x_i + 2b \sum_{i=1}^{n} x_i^2 - 2 \sum_{i=1}^{n} v_i x_i = 0$$

$$2 a \sum_{i=1}^{n} x_i + 2 b \sum_{i=1}^{n} x_i^2 - 2 \sum_{i=1}^{n} y_i x_i = 0 \Rightarrow$$

$$2 a \sum_{i=1}^{n} x_i + 2 b \sum_{i=1}^{n} x_i^2 = 2 \sum_{i=1}^{n} y_i x_i.$$

Dividindo ambos por 2,

$$a n + b \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i e$$

$$a \sum_{i=1}^{n} x_i + b \sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} y_i x_i.$$

Este sistema é na forma

$$an + br = se$$

$$ar + bt = u$$
, onde

$$r = \sum_{i=1}^{n} x_i,$$

$$s = \sum_{i=1}^{n} y_i,$$

$$t = \sum_{i=1}^{n} x_i^2,$$

$$u = \sum_{i=1}^n y_i x_i.$$

Somando,

$$an+br+ar+bt=s+u$$

Para isolar b.

$$b(r+t) = s + u - a(n-r) \Rightarrow$$

$$b = \frac{s+u-a(n-r)}{r+t}$$

e **a**.

$$a(r+t) = s + u - b(r+t) \Rightarrow$$

$$a = \frac{s+u-b(r+t)}{r+t}.$$

Para resolver o sistema, antes de somar,

$$r(an+br) = rse$$

$$-n(ar+bt) = -nu,$$

$$arn+br^{2}-anr-bnt = rs-nu \Rightarrow$$

$$b(r^{2}-nt) = rs-nu \Rightarrow$$

$$b = \frac{rs-nu}{r^{2}-nt}.$$

Reescrevendo a primeira equação por $\mathbf{0}$,

$$an + br = s \Rightarrow$$

$$an = s - br \Rightarrow$$

$$a = \frac{s - br}{n}.$$

O paper pára aqui (sem substituir $\frac{rs-nu}{r^2-nt}$ como b).

As equações normais são as equações das variáveis em função de x_i e $y_i - \hat{y}_i$, ou seja, a diferença entre o modelo e os dados.

(As variáveis compõem os coeficientes do modelo.)

Estas equações são o mínimo de cada variável em função da função diferença dados/modelo.

(Ou seja, igualar a derivada parcial de cada variável a zero.)

A função da diferença dados/modelo "como um todo" só tem mínimo se todas as variáveis ou derivadas

parciais têm mínimo simultaneamente. Por isso o mínimo de cada variável é inputado em um sistema que deve ter resolução simultânea para todas as variáveis.

A função da diferença dados/modelo é a soma ou somatória de n instâncias da função diferença dado/modelo com X_i e Y_i substituídos na função, vindos dos dados, e Y_i substituído na função vindo do modelo, com n a quantidade de pontos nos dados.

(Ou seja, a soma de todas as funções diferença modelo/dado determina os coeficientes desta função, que são os valores que compõem o sistema para solução.)

Na prática, como as variáveis são as incógnitas, são as somas dos X e $y-\hat{y}$ dos dados e modelo que definem os coeficientes do sistema.

Ao resolver o sistema, temos os valores do mínimo de cada variável para a função modelo + diferença dados/modelo, o que são os coeficientes que compõem o modelo que minimiza estes números.

Prática

O seguinte dado com fit cosseno manual em eta e V resulta nos seguintes coeficientes:

 $\beta = 0.4$

y = 0.7

 $\tau = 35.4$

M = -0.6.

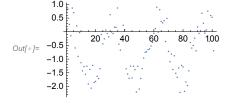
Com erro ao quadrado 39.0437.

(*isso deve sempre ser verdadeiro*) In[•]:= Clear[M,τ,β,γ]

(*Modeling.nb points2b2*) In[•]:= Clear[points1,vpar1]

points1={0.8284486071053614`,0.2673766376785629`,-0.14587103848031902`,0.8659704680415028`,0.69910541120 ListPlot[points1,ImageSize→Small]

vpar1=<| $"\beta"\to0.4$, $"\gamma"\to0.7$, $"\tau"\to35.4$, $"M"\to-0.6$ |>;



A função do modelo é

$$\hat{Y}(t) = M + A \cos(\frac{2\pi t}{\tau} + \phi)$$
, com a identidade trigonométrica,

$$\hat{Y}(t) = M + A\cos(\phi)\cos(\frac{2\pi t}{\tau}) - A\sin(\phi)\sin(\frac{2\pi t}{\tau})$$
, com os parâmetros,

$$\hat{Y}(t) = M + \beta \cos(\frac{2\pi t}{\tau}) - \gamma \sin(\frac{2\pi t}{\tau}).$$

Tomando em alguns pontos

```
Clear[testt1,fmodelparam1] testt1={11,30,50,65}; (*fmodelparam1 dá o modelo em um ponto*) (*t na função modelo é baseado em 0, e não 1*) fmodelparam1=Function[\{t,M,\tau,\beta,\gamma\},M+\beta Cos[\frac{2\pi t}{\tau}]-\gamma Sin[\frac{2\pi t}{\tau}]]
```

```
Out[*]= \mbox{Function} \left[ \{ \mbox{t, M, $\tau$, $\beta$, $\gamma$} \}, \mbox{M} + \beta \mbox{Cos} \left[ \frac{2 \mbox{$\pi$t}}{\tau} \right] - \gamma \mbox{Sin} \left[ \frac{2 \mbox{$\pi$t}}{\tau} \right] \right] \\ In[*]:= \mbox{Table} \left[ \mbox{fmodelparam1}[\mbox{t, vpar1}["M"], vpar1["\tau"], vpar1["\beta"], vpar1["\beta"]], {t, testt1} \right] \\ Out[*]:= \mbox{fmodelparam1}[\mbox{10, vpar1}["M"], vpar1["\tau"], $\beta$, $\gamma$} \\ In[*]:= \mbox{fmodelparam1}[\mbox{10, vpar1}["M"], vpar1["\tau"], $\beta$, $\gamma$} \\ Out[*]:= -0.6 - 0.2027 \mbox{$\beta$ - 0.979241 $\gamma$} \right]
```

Simulando dados nestes pontos

```
ln[*]:= Clear[testdata1]
testdata1={{11,-1},{30,0.5},{50,-1.4},{65,0.1}};
```

A função diferença dados/modelo é

$$\Delta Y(t) = \sum_{i=1}^{n} y_i - \left[M + \beta \cos\left(\frac{2\pi t_i}{\tau}\right) - \gamma \sin\left(\frac{2\pi t_i}{\tau}\right) \right]$$

```
Clear [fmodeldif1part1, fmodeldif1part2, fmodeldif1indiv, fmodeldifsq1indiv,
fmodeldif1,fmodeldifsq1]
(*testando a somatória*)
fmodeldif1part1=Function \Big[ \{t,data\}, \sum_{i=1}^{Length [data]} data \Big[ \Big[ i \Big] \Big] \big[ [2] \big] \Big];
fmodeldif1part2=Function {t,data},
\sum_{i=1}^{\mathsf{Length}[\mathsf{data}]} \mathsf{fmodelparam1}\big[\mathsf{t}\big[\big[i\big]\big], \mathsf{vpar1}[\mathsf{"M"}], \mathsf{vpar1}[\mathsf{"\tau"}], \beta, \gamma\big]\Big];
(*teste de diferença em um ponto*)
 (*fmodeldif1indiv dá a diferença entre um dado e o modelo em um ponto*)
fmodeldif1indiv=Function [\{M, \tau, \beta, \gamma, t, y\}, y-fmodelparam1[t, M, \tau, \beta, \gamma]];
fmodeldifsq1indiv=Function [\{M, \tau, \beta, \gamma, t, y\}, (y-fmodelparam1[t, M, \tau, \beta, \gamma])^2];
(*a(s) função(ões)*)
(*estas funções, sem os parâmetros definidos, dão as funções a minimizar
(igualar as parciais a zero) -- ainda separadas por termo -- usar
Simplify[] --, e com os parâmetros, as somas dos resíduos.*)
(*t é uma lista de posições (x também chamado t), com início em 0, que
também deve constar em data, que são pontos (x,y)*)
fmodeldif1=Function \{M, \tau, \beta, \gamma, t, data\},
\sum_{i=1}^{\mathsf{Length}[\mathsf{data}]} \left(\mathsf{data}\big[\big[\mathtt{i}\big]\big]\,[\,[\mathtt{2}]\,]\,\mathsf{-fmodelparam1}\big[\mathsf{t}\big[\big[\mathtt{i}\big]\big]\,\mathsf{,M},\tau,\beta,\gamma\big]\big)\,\big];
fmodeldifsq1=Function \{M, \tau, \beta, \gamma, t, data\},
\sum_{i=1}^{Length[data]} \left( \text{data} \left[ \left[ i \right] \right] \left[ \left[ 2 \right] \right] - \text{fmodelparam1} \left[ \text{t} \left[ \left[ i \right] \right], M, \tau, \beta, \gamma \right] \right)^2 \right];
```

Testes da somatória...

```
log[a]:= {fmodeldif1part1[testt1, testdata1], fmodeldif1part2[testt1, testdata1]} Out[a]:= {-1.8, -2.4 - 0.134741 \beta + 0.224373 \gamma}
```

Testando as diferenças para os pontos...

São tantas diferenças quanto pontos.

Aqui estou passando índice baseado em 1 para testt1 (ao invés de baseado 0) porque ele não é um ts, é uma lista contendo as posições. (?)

```
| Print[Column[Table[fmodeldif1indiv[vpar1["M"], vpar1["τ"], β,
              γ, testt1[[i+1]], testdata1[[i+1]][[2]]], {i, 0, Length[testt1] - 1}]]]
        -0.4 + 0.372411 \beta + 0.928068 \gamma
        1.1 – 0.574787 \beta – 0.818303 \gamma
        -0.8 + 0.852408 \beta + 0.522877 \gamma
        0.7 – 0.515292 \beta – 0.857015 \gamma
        Soma das diferenças...
 ln[a] := -0.4 + 0.372411 \beta + 0.928068 \gamma + 1.1 - 0.574787 \beta -
         0.818303 \, \gamma + -0.8 + 0.852408 \, \beta + 0.522877 \, \gamma + 0.7 - 0.515292 \, \beta - 0.857015 \, \gamma
Out[\circ]= 0.6 + 0.13474 \beta - 0.224373 \gamma
        Soma das diferenças via somatória.
 In[*]:= Clear[residual1]
        residual1 = fmodeldif1[vpar1["M"], vpar1["\tau"], \beta, \gamma, testt1, testdata1];
        Simplify[residual1]
Out[\circ]= 0.6 + 0.134741 \beta - 0.224373 \gamma
        Bateu. Minimizar em oldsymbol{\mathcal{B}}e oldsymbol{V}.
 ln[\bullet]:= \{\partial_{\beta} \text{ residual1}, \partial_{\gamma} \text{ residual1}\}
Out[\bullet]= {0.134741, -0.224373}
        Estou tendo as derivadas constantes porque estou fazendo erro linear e não quadrático...
         Clear[residualsq1];
In[ • ]:=
         residualsq1=fmodeldifsq1[vpar1["M"],vpar1["\tau"],\beta,\gamma,testt1,testdata1];
         Print[residualsq1];
         Simplify[residualsq1]
        (0.7 - 0.515292 \beta - 0.857015 \gamma)^2 + (1.1 - 0.574787 \beta - 0.818303 \gamma)^2 +
         (-0.8 + 0.852408 \beta + 0.522877 \gamma)^2 + (-0.4 + 0.372411 \beta + 0.928068 \gamma)^2
Out[*]= 2.5 + 1.4612 \beta^2 - 4.57914 \gamma + 2.5388 \gamma^2 + \beta \left( -3.64772 + 3.40658 \gamma \right)
        A somatória veio sem somar.
        Minimizar em \betae \gamma.
 ln[a]:= Print[Column[{\partial_{\beta} residualsq1, "\n", \partial_{\gamma} residualsq1}]]
        -1.03058 (0.7 - 0.515292 \beta - 0.857015 \gamma) - 1.14957 (1.1 - 0.574787 \beta - 0.818303 \gamma) +
         \textbf{1.70482} \  \, (\textbf{-0.8} + \textbf{0.852408} \  \, \beta + \textbf{0.522877} \  \, \gamma) \  \, + \textbf{0.744823} \  \, (\textbf{-0.4} + \textbf{0.372411} \  \, \beta + \textbf{0.928068} \  \, \gamma)
        -1.71403 (0.7 - 0.515292 \beta - 0.857015 \gamma) - 1.63661 (1.1 - 0.574787 \beta - 0.818303 \gamma) +
         1.04575 (-0.8 + 0.852408 \beta + 0.522877 \gamma) + 1.85614 (-0.4 + 0.372411 \beta + 0.928068 \gamma)
        Vem sem somar, somando...
         Clear[partials1]
         partials1=\{Simplify[\partial_{\beta}residualsq1],Simplify[\partial_{\gamma}residualsq1]\};
         Print[Column[{partials1[[1]],"\n",partials1[[2]]}]]
```

```
In[ • ]:=
```

```
-3.64772 + 2.92239 \beta + 3.40658 \gamma
-4.57914 + 3.40658 \beta + 5.07761 \gamma
```

Estas são as duas parciais, uma em cada variável.

As duas têm que ser igualadas a zero simultaneamente.

```
Clear[minpars1]
Inf = 1:=
                 minpars1=Solve[partials1[[1]]==0&&partials1[[2]]==0]
 Out[\circ]= { {\beta \rightarrow 0.903683, \gamma \rightarrow 0.295548}
              Estes parâmetros substituem o oldsymbol{eta} e oldsymbol{\gamma} definidos visualmente, mas mantendo o M e 	au.
              O erro ao quadrado para os parâmetros definidos visualmente é
                 Clear[residual1v]
                 residual1v = fmodeldifsq1[vpar1["M"], vpar1["\tau"], vpar1["\beta"], vpar1["\gamma"], testt1, testdata1]; \\
                 residual1v
 Out[ • ]= 0.267158
  In[*]:= Clear[difindivs1v]
              difindivs1v = Table[fmodeldifsq1indiv[vpar1["M"], vpar1["τ"],
                      vpar1["β"], vpar1["γ"], testt1[[i]], testdata1[[i]][[2]]], {i, Length[testt1]}]
 Outf = \{0.158892, 0.0883713, 0.00865326, 0.0112417\}
 In[*]:= Total[difindivs1v]
 Out[*]= 0.267158
              Batendo as diferenças manualmente...
  ln[*]:= \{(-1+1.3986119758301152)^2, (0.5-0.20272690722148112)^2, (0.5-0.20272690722148112)^2\}
                  (-1.4 + 1.3069770906904363)^2, (0.1 - 0.2060270811124157)^2
 Out[\circ] = \{0.158892, 0.0883713, 0.00865326, 0.0112417\}
              Estar diferente da diferença no modelo original (39.0437) é por causa dos dados.
              As diferenças com os parâmetros minimizados...
  In[*]:= difindivs1 =
                 Table[fmodeldifsq1indiv[vpar1["M"], vpar1["t"], \beta, \gamma, testt1[[i]], testdata1[[i]][[2]]] /.
                      First[minpars1], {i, Length[testt1]}]
 Out[\circ] = \{0.0444494, 0.114736, 0.0155855, 0.000359067\}
 In[*]:= Total[difindivs1]
 Out[ • ]= 0.17513
              Diminuiu!
  In[*]:= Clear[residual1]
              residual1 = fmodeldifsq1[vpar1["M"], vpar1["τ"], β, γ, testt1, testdata1] /. First[minpars1];
              residual1
 Out[*]= 0.17513
              Agora, usando os dados.
              Minimizar oldsymbol{eta} e oldsymbol{V}. Pegar a somatória do resíduo sem estas variáveis.
  /// Inf | Image |
Out[*]= Function \left[ \{t, M, \tau, \beta, \gamma\}, M + \beta Cos \left[ \frac{2\pi t}{\tau} \right] - \gamma Sin \left[ \frac{2\pi t}{\tau} \right] \right]
  log[\cdot]:= fmodelparam1[0, vpar1["M"], vpar1["\tau"], vpar1["\beta"], vpar1["\gamma"]]
 Out[\circ] = -0.2
```

```
In[ • ]:= fmodeldif1indiv
Out[\[\circ\]] = Function[\{M, \tau, \beta, \gamma, t, y\}, y - fmodelparam1[t, M, \tau, \beta, \gamma]]
In[*]:= fmodeldif1
Out[*] = Function [\{M, \tau, \beta, \gamma, t, data\}, \sum_{i=1}^{Length[data]} (data[i][2] - fmodelparam1[t[i], M, \tau, \beta, \gamma])]
     Nas chamadas ao fmodelparam1, passar t baseado em 0.
     Como uso o tS para passar, montar o tS a partir de 0.
In[*]:= Module [{dta, dtapoints, mdl, mdlpoints, ts, difsq, rss,
        minrssf, minrsspar, minrsssol, minrss, Ahat, K, \phihat},
       (*definir o dado, criar o ts, "discretizar" ou samplear o modelo*)
       dta = points1;
       (*Print[dta];*)
       ts = Range[0, Length[dta] - 1]; (*já gerar o ts baseado no dta*)
       (*gerar o dtapoints baseado no ts (base 0) e dta (base 1)*)
       dtapoints = Table[{i, dta[[i+1]]}, {i, ts}];
       (*Print[dtapoints];*)
       (*discretize*)
       mdl = Table[
         fmodelparam1[t, vpar1["M"], vpar1["\tau"], vpar1["\beta"], vpar1["\gamma"]], \{t, 0, Length[dta] - 1\}];
       (*checado*)
       (*Print[mdl];*)
       Print[
        ListLinePlot[\{dta, mdl\}, ImageSize \rightarrow Medium, PlotRange \rightarrow \{\{0, Length[dta] - 1\}, \{-3, 3\}\}\}];
       (*Print[{Length[dta],Length[dtapoints],Length[mdl],Length[ts]}];*)
       (*calcular o resíduo visual*)
       rss = fmodeldifsq1[vpar1["M"], vpar1["\tau"], vpar1["\beta"], vpar1["\gamma"], ts, dtapoints];
       Print["visual rss: ", rss];
       (*testes de debug de rss*)
       (*Print[fmodelparam1[ts[[1]],vpar1["M"],vpar1["τ"],vpar1["β"],vpar1["γ"]]];*)
       (*Print["first data is ",First[dta]];
       Print["first model is ",First[mdl]];
       Print["first res should be ",ToString[0.828449+0.2]];
       Print["first res is ",
        fmodeldif1indiv[vpar1["M"],vpar1["\tau"],vpar1["\beta"],vpar1["\gamma"],First[ts],First[dta]]];
       Print["first res sq2 is ",fmodeldifsq1indiv[vpar1["M"],
         vpar1["τ"], vpar1["β"], vpar1["γ"], First[ts], First[dta]]];*)
       (*calcular o resíduo mínimo*)
       (*paper: τ não tem estimativa.*)
       minrssf = fmodeldifsq1[M, vpar1["\tau"], \beta, \gamma, ts, dtapoints];
       Print["min rss fun: ", Simplify[minrssf]];
       minrsspar = <|
         "M" → Simplify[∂<sub>M</sub>minrssf],
         "\beta" → Simplify [\partial_{\beta} minrssf],
         "\gamma" \rightarrow Simplify[\partial_{\gamma} minrssf]
         |>;
       Print["min rss par: ", minrsspar];
       minrsssol = Solve[
         minrsspar["M"] == 0&&
           minrsspar["\beta"] == 0 \&\&
          minrsspar["\gamma"] == 0
       Print["min rss solution: ", minrsssol];
       minrss = minrssf /. minrsssol;
       Print["min rss: ", minrss];
```

```
(*plotar o minimizado*)
      (*TODO: porquê necessário First? abaixo*)
     minmdlf = First[fmodelparam1[t, M, vpar1["\tau"], \beta, \gamma] /. minrsssol];
     Print["min model fun: ", minmdlf];
      (*Plot[minmdlf, {t,0,100}]*)
     minmdl = Table[minmdlf, {t, 0, Length[dta] - 1}];
          ListLinePlot[{mdl, minmdl}, ImageSize → Medium, PlotRange → {{0, Length[dta] - 1}, {-3, 3}}]];
      (*estimar amplitude e acrofase*)
     Ahat = \sqrt{\beta^2 + \gamma^2} /. minrsssol;
     \phi \text{hat = ArcTan} \left[ \frac{-Y}{\beta} \right] + K \pi /. \text{ minrsssol;}
     Print["Â: ", Ahat];
     Print["\hat{\phi}: ", \phihat];
    3
 -2
_3 L
visual rss: 39.0437
min rss fun: 101. (1.12753 + M^2 + 0.489868 \beta^2 +
               \texttt{M} \; (1.25139 - 0.0848016 \, \beta - 0.0520183 \, \gamma) \; + \beta \; (-0.405116 - 0.0398594 \, \gamma) \; - 0.782083 \, \gamma + 0.510132 \, \gamma^2) 
min rss par: <\mid M \rightarrow 202. (0.625696 + M - 0.0424008 \beta - 0.0260091 \gamma) ,
         \beta \rightarrow -40.9167 - 8.56497 \text{ M} + 98.9532 \ \beta - 4.0258 \ \gamma, \ \gamma \rightarrow -78.9904 - 5.25385 \ \text{M} - 4.0258 \ \beta + 103.047 \ \gamma \mid > 100.047 \ \gamma \mid > 100.
min rss solution: \{ \{M \rightarrow -0.589475, \beta \rightarrow 0.393061, \gamma \rightarrow 0.751851 \} \}
min rss: {38.8924}
 \mbox{min model fun: } -0.589475 + 0.393061 \\ \mbox{Cos} \left[ 0.177491 \\ \mbox{t} \right] - 0.751851 \\ \mbox{Sin} \left[ 0.177491 \\ \mbox{t} \right] 
   2
   0
                                                                                                                                                                                                                                   100
                                                  20
                                                                                                                                                                                       80
-2
-3<sup>L</sup>
Â: {0.848397}
\hat{\phi}: {2.05251}
```

TODO: exibir (e resolver) a NE (equações normais) em forma matricial. Valores M, τ, β, γ estão vazando para o global e contaminando as funções.

Testes de **tS**.

Aparentemente, mudar a razão de tS só vai escalonar o eixo X.

O problema é usar o valor de **tS** para acessar os índices dos dados.

Os dados têm de ser acessados pelos índices de ts, não por seus valores.

Mas neste caso, ts não vai servir para mais absolutamente nada.

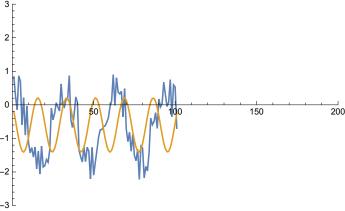
Ou, criar os pontos (indexar) dos dados por **tS**.

In[*]:= fmodelparam1

```
\textit{Out[*]=} \; \; \text{Function} \left[ \left. \left\{ \textbf{t, M, } \tau \textbf{, } \beta \textbf{, } \gamma \right\} \textbf{, M} + \beta \, \text{Cos} \left[ \frac{2 \, \pi \, \textbf{t}}{\tau} \right] - \gamma \, \text{Sin} \left[ \frac{2 \, \pi \, \textbf{t}}{\tau} \right] \right] \right]
//n[*]:= Module[{dta, ts, dtapoints},
            dta = points1;
            ts = Range[0, (Length[dta] - 1) * 2, 2];
            Print[Length[ts]];
            Print[ts];
            dtapoints = Table[{i - 1, dta[[i]]}, {i, Range[1, Length[ts]]}];
            Print[dtapoints];
            mdl = Table[fmodelparam1[t, vpar1["M"], vpar1["\tau"], vpar1["\beta"], vpar1["\beta"]], {t, ts}];
           Print[mdl];
           Print[ListLinePlot[{dta, mdl}, ImageSize → Medium, PlotRange → {{0, 200}, {-3, 3}}]];
```

```
101
```

```
{0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 36, 38, 40, 42, 44,
   46, 48, 50, 52, 54, 56, 58, 60, 62, 64, 66, 68, 70, 72, 74, 76, 78, 80, 82, 84, 86, 88, 90,
   92, 94, 96, 98, 100, 102, 104, 106, 108, 110, 112, 114, 116, 118, 120, 122, 124, 126, 128,
    130, 132, 134, 136, 138, 140, 142, 144, 146, 148, 150, 152, 154, 156, 158, 160, 162, 164,
    166, 168, 170, 172, 174, 176, 178, 180, 182, 184, 186, 188, 190, 192, 194, 196, 198, 200}
{{0,0.828449},{1,0.267377},{2,-0.145871},{3,0.86597},{4,0.699105},{5,-0.593286},
    \{6, 0.21297\}, \{7, -0.901046\}, \{8, -0.0308795\}, \{9, -1.13305\}, \{10, -1.43241\}, \{11, -1.27098\}, \{10, -1.43241\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}, \{11, -1.27098\}
    \{12, -1.55522\}, \{13, -1.25866\}, \{14, -1.90932\}, \{15, -1.3759\}, \{16, -2.06161\}, \{17, -1.23359\},
    \{18, -1.85334\}, \{19, -1.81647\}, \{20, -1.62901\}, \{21, -1.71166\}, \{22, -1.35207\}, \{23, -0.10037\}, \{23, -1.85334\}, \{19, -1.81647\}, \{20, -1.62901\}, \{21, -1.71166\}, \{20, -1.85207\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.81647\}, \{21, -1.8164
    \{24, -0.444725\}, \{25, -0.259657\}, \{26, 0.0628543\}, \{27, -0.0634696\}, \{28, -0.184484\},
    \{35, -0.454881\}, \{36, -0.673642\}, \{37, -0.291191\}, \{38, 0.237324\}, \{39, 0.0717739\}, \{40, -1.35391\},
    \{41, -1.54713\}, \{42, -1.70356\}, \{43, -1.25588\}, \{44, -1.69065\}, \{45, -1.26194\}, \{46, -1.38428\}, \{46, -1.8428\}, \{47, -1.8413\}, \{48, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}, \{49, -1.8413\}
    \{47, -2.20528\}, \{48, -1.26573\}, \{49, -2.0948\}, \{50, -1.70808\}, \{51, -1.35185\}, \{52, -0.961597\},
    \{53, -0.749494\}, \{54, -0.733854\}, \{55, -0.653462\}, \{56, -0.625239\}, \{57, -0.520483\}, \{58, -0.387476\},
    \{59, -0.0575814\}, \{60, 0.118542\}, \{61, 0.898165\}, \{62, -0.0139777\}, \{63, 0.805251\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.37662\}, \{64, 0.376
    \{65, 0.325103\}, \{66, 0.406461\}, \{67, -0.358079\}, \{68, 0.487177\}, \{69, -0.718652\}, \{70, -1.09497\},
    \{71, -0.818308\}, \{72, -1.38016\}, \{73, -0.879561\}, \{74, -1.51713\}, \{75, -1.66477\}, \{76, -1.32329\},
    \{77, -2.21958\}, \{78, -1.2324\}, \{79, -1.2868\}, \{80, -2.17856\}, \{81, -1.83439\}, \{82, -1.96933\},
    \{83, -1.4279\}, \{84, -0.392676\}, \{85, -0.596141\}, \{86, -0.503018\}, \{87, -0.235215\}, \{88, -0.698701\},
    \{89, 0.176379\}, \{90, -0.0599401\}, \{91, 0.0354239\}, \{92, 0.674987\}, \{93, 0.310189\}, \{94, -0.047734\},
    \{95, 0.0676676\}, \{96, 0.754158\}, \{97, -0.354738\}, \{98, 0.594251\}, \{99, 0.529957\}, \{100, -0.695208\}\}
\{-0.2, -0.468241, -0.752911, -1.01851, -1.23193, -1.36655, -1.40558, -1.34416, -1.18995, -0.962178, -1.23193, -1.34055, -1.34416, -1.3895, -0.962178, -1.34056, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.34416, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, -1.3895, 
    -0.689241, -0.405176, -0.145404, 0.0576812, 0.178758, 0.202727, 0.126601, -0.040129, -0.276672,
    -0.553531, -0.836186, -1.08939, -1.28157, -1.38876, -1.3976, -1.30698, -1.1282, -0.883563, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603565, -0.603
    -0.323123, -0.0772054, 0.103522, 0.196524, 0.190204, 0.0853496, -0.104964, -0.357006, -0.639349,
    -0.916784, -1.15472, -1.32348, -1.40203, -1.38057, -1.26178, -1.06047, -0.801735, -0.517849,
    -0.244207, -0.0149298, 0.141392, 0.205266, 0.168728, 0.0363334, -0.175408, -0.440095, -0.72472,
    -0.993794, -1.21376, -1.3572, -1.40622, -1.3547, -1.20908, -0.987513, -0.717622, -0.433064,
    -0.169322, 0.0407168, 0.170862, 0.204884, 0.138542, -0.0198927, -0.250663, -0.524995, -0.808679,
    -1.06634, -1.26585, -1.38234, -1.40127, -1.32029, -1.14949, -0.91017, -0.632176, -0.35017,
    -0.0993171, 0.0891037, 0.191597, 0.195382, 0.0999877, -0.0826916, -0.329877, -0.610744, -0.890273,
    -1.13361, -1.3104, -1.39861, -1.38724, -1.27771, -1.08366, -0.829312, -0.546366, -0.270107}
```



O problema é que o plot como pontos (ListLinePlot) não escala o eixo X.

Só que se resolver por Plot[], como no ActStudio é plotado?

Parte do problema é que a largura do plot por pontos é definida pela lista de dados, e não por um scaling. Se estipularmos uma largura diferente para a discretização do modelo via scaling do ${ t t S}$, ele fica com largura diferente dos dados. Interpolar a lista de dados seria "feio", mas talvez a única solução.