

Ajuste de Curvas (Parte II)

Prof. Americo Cunha

Universidade do Estado do Rio de Janeiro – UERJ

americo.cunha@uerj.br

www.americocunha.org



 @AmericoCunhaJr



@AmericoCunhaJr



@AmericoCunhaJr



Resolvendo o problema de mínimos quadrados (computacionalmente)



Mínimos quadrados via fatoração Cholesky

$$\begin{cases} A^T A \mathbf{x} = A^T \mathbf{b} \\ A^T A = G G^T \end{cases} \iff \begin{cases} G \mathbf{y} = A^T \mathbf{b} \\ G^T \mathbf{x} = \mathbf{y} \end{cases}$$

Receita computacional

1. Construir $A^T A$ e $A^T \mathbf{b}$
2. Calcular $A^T A = G G^T$
3. Resolver $G \mathbf{y} = A^T \mathbf{b}$
4. Resolver $G^T \mathbf{x} = \mathbf{y}$

$$\begin{matrix} G & \mathbf{y} & A^T \mathbf{b} \\ n \times n & n \times 1 & n \times 1 \end{matrix}$$
$$\begin{matrix} G^T & \mathbf{x} & \mathbf{y} \\ n \times n & n \times 1 & n \times 1 \end{matrix}$$

$$\text{flops (MQ Cholesky)} \sim m n^2 + \frac{1}{3} n^3$$

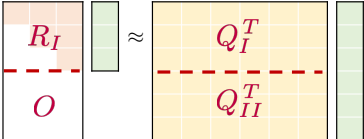


Mínimos quadrados via fatoração QR

$$\begin{cases} A^T A \mathbf{x} = A^T \mathbf{b} \\ A = QR \end{cases} \iff \begin{cases} R_I \mathbf{x} = Q_I^T \mathbf{b} \end{cases}$$

Receita computacional

1. Calcular $A = QR$
2. Calcular $Q_I^T \mathbf{b}$
3. Resolver $R_I \mathbf{x} = Q_I^T \mathbf{b}$

$$\begin{array}{cc} R & \mathbf{x} \\ m \times n & n \times 1 \end{array} \approx \begin{array}{cc} Q^T & \mathbf{b} \\ m \times m & m \times 1 \end{array}$$




$$\mathbf{x} = A \setminus \mathbf{b}$$

“backslash” usa fatoração QR para sistemas retangulares

$$\text{flops}(\mathbf{MQ QR}) \sim 2mn^2 - \frac{2}{3}n^3 + nm + n^2$$

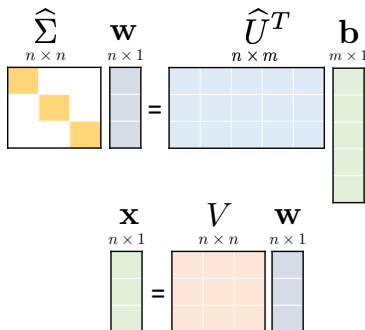


Mínimos quadrados via fatoração SVD

$$\begin{cases} A^T A \mathbf{x} = A^T \mathbf{b} \\ A = \hat{U} \hat{\Sigma} V^T \end{cases} \iff \begin{cases} \hat{\Sigma} \mathbf{w} = \hat{U}^T \mathbf{b} \\ \mathbf{x} = V \mathbf{w} \end{cases}$$

Receita computacional

1. Calcular $A = \hat{U} \hat{\Sigma} V^T$
2. Calcular $\hat{U}^T \mathbf{b}$
3. Resolver $\hat{\Sigma} \mathbf{w} = \hat{U}^T \mathbf{b}$
4. Calcular $\mathbf{x} = V \mathbf{w}$



$$\text{flops}(\mathbf{MQ\ SVD}) \sim 2 m n^2 + 11 n^3 + m^2 + n + n^2$$



Custo do problema de mínimos quadrados ($m \gg n$)

fatoração	flops	estabilidade	custo
Cholesky	$\sim m n^2 + \frac{1}{3} n^3$	***	1 × \$
QR	$\sim 2 m n^2 - \frac{2}{3} n^3$	****	2 × \$
SVD	$\sim 2 m n^2 + 11 n^3$	*****	2 × \$



Podemos usar outra noção de erro?



Ajuste de curva robusto

Outras medidas de erro são possíveis (e pertinentes):

- Erro médio quadrático

$$E_2 = \left(\frac{1}{m} \sum_{k=1}^m (y_k - f(x_k))^2 \right)^{1/2}$$

- Erro médio

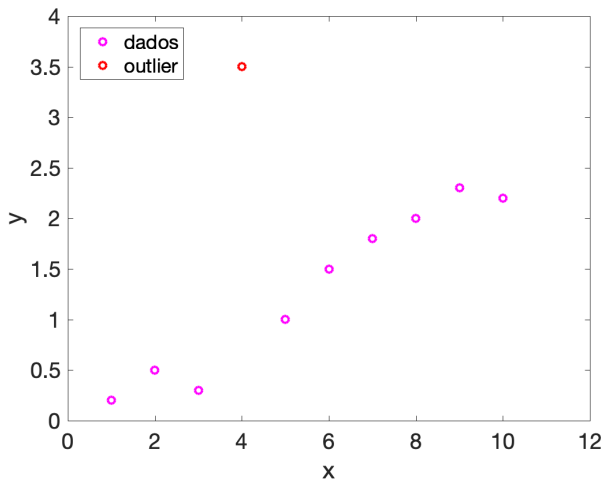
$$E_1 = \frac{1}{m} \sum_{k=1}^m |y_k - f(x_k)|$$

- Erro máximo

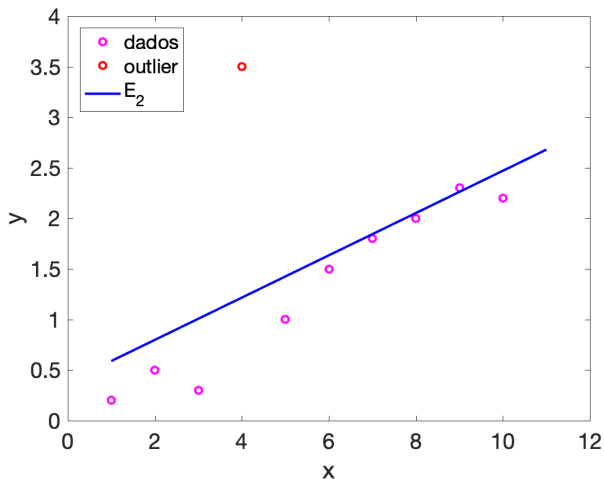
$$E_\infty = \max_{1 \leq k \leq m} |y_k - f(x_k)|$$



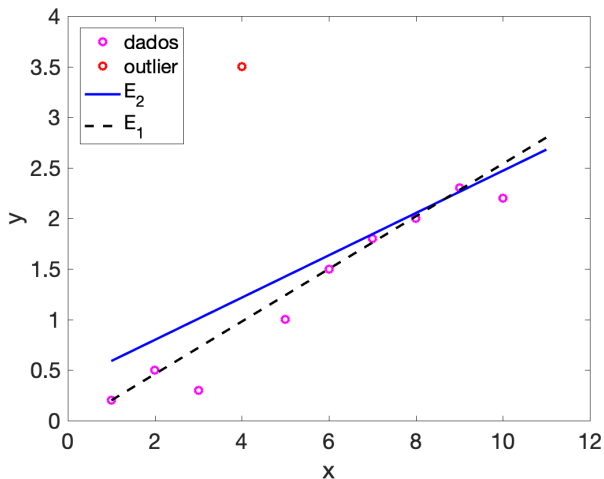
Ajuste de curva robusto



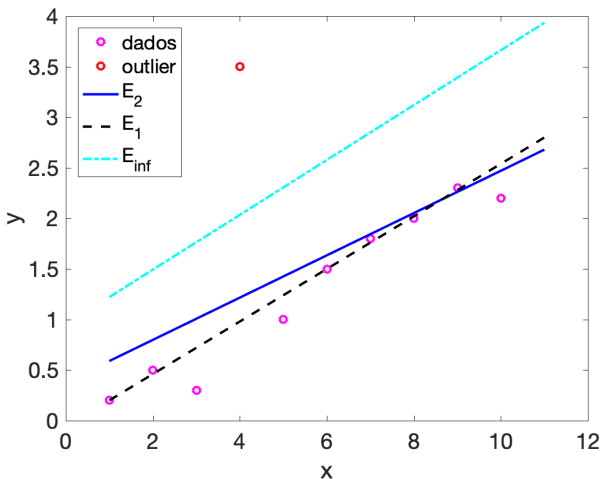
Ajuste de curva robusto



Ajuste de curva robusto



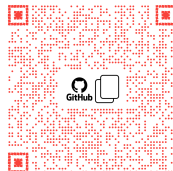
Ajuste de curva robusto



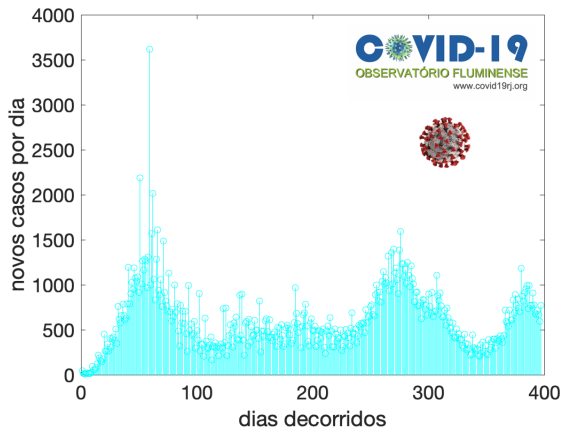
Ajuste de curva robusto

MainRegressionExample3.m

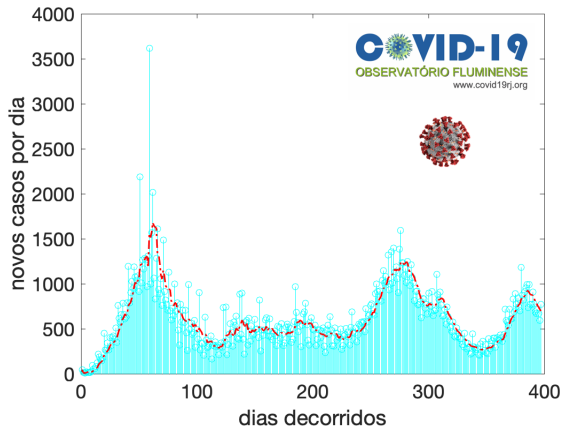
```
1  clc; clear; close all;
2
3  m = 10;
4  xd = [1 2 3 4 5 6 7 8 9 10];
5  yd = [0.2 0.5 0.3 3.5 1.0 1.5 1.8 2.0 2.3 2.2];
6
7  E_2 = @(p) sqrt(sum(abs(p(1)*xd+p(2)-yd).^2)/m);
8  E_1 = @(p)      sum(abs(p(1)*xd+p(2)-yd))/m;
9  E_inf = @(p) max(abs(p(1)*xd+p(2)-yd));
10 p_2 = fminsearch(E_2,[1 1]);
11 p_1 = fminsearch(E_1,[1 1]);
12 p_inf = fminsearch(E_inf,[1 1]);
13
14 xfit = 1:0.01:11;
15 y_2 = polyval(p_2,xfit);
16 y_1 = polyval(p_1,xfit);
17 y_inf = polyval(p_inf,xfit);
18
19 plot(xd,yd,'om',xd(4),yd(4),'or','LineWidth',2);
20 hold on
21 plot(xfit,y_2,'-b','LineWidth',2);
22 plot(xfit,y_1,'--k','LineWidth',2);
23 plot(xfit,y_inf,'-.c','LineWidth',2);
24 hold off
25 xlabel('x'); ylabel('y');
26 set(gca,'FontSize',18);
27 legend('dados','outlier','E_2','E_1','E_{inf}')
```



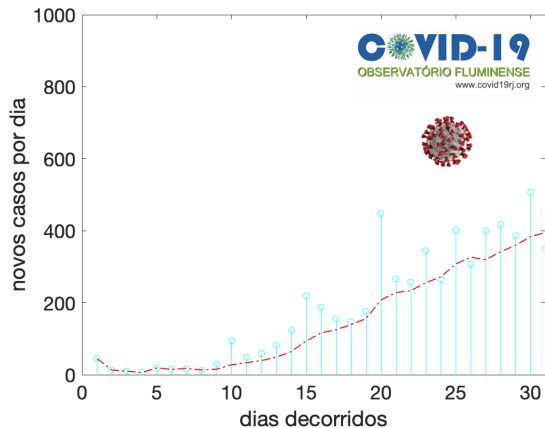
COVID-19 na cidade do Rio de Janeiro



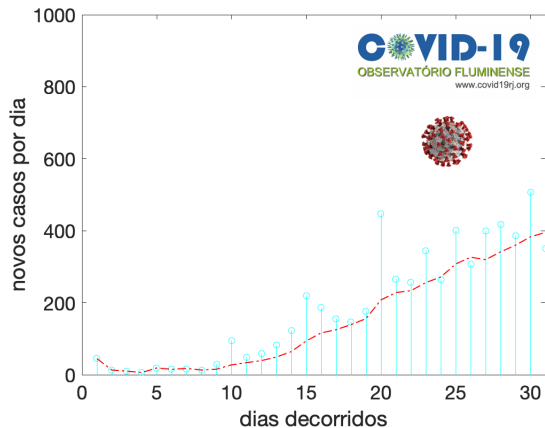
COVID-19 na cidade do Rio de Janeiro



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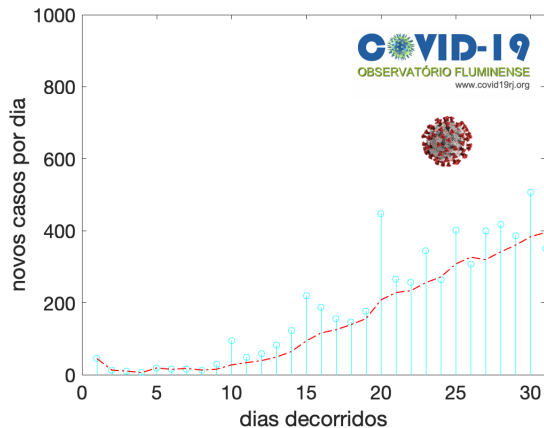


(fase de expansão)

$$\text{novos casos} \sim N \exp(\beta t)$$



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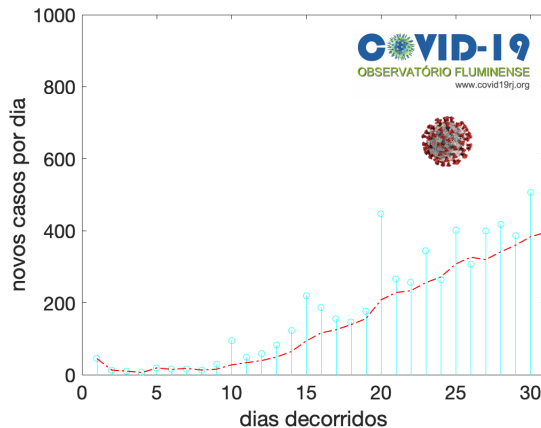
(fase de expansão)

$$\text{novos casos} \sim N \exp(\beta t)$$

$$y = N \exp(\beta t)$$



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(fase de expansão)

$$\text{novos casos} \sim N \exp(\beta t)$$

$$y = N \exp(\beta t) \implies \ln y = \beta t + \ln N$$



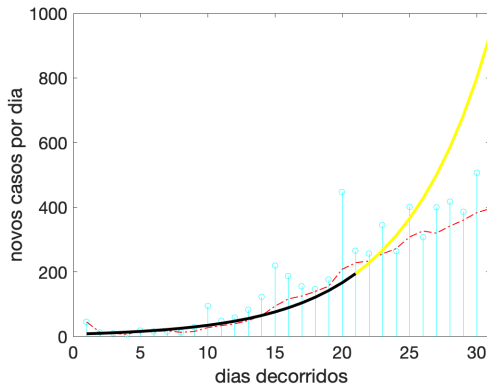
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MainRegressionExample4.m

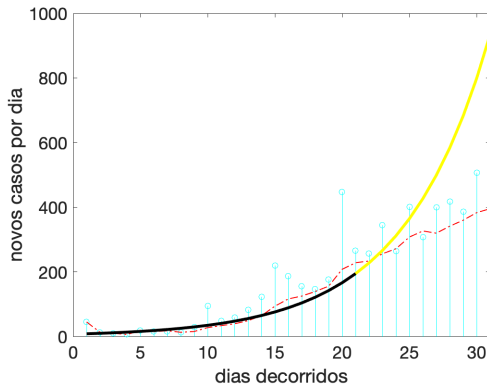
```
1  clc; clear; close all;
2
3  dados = load('covid19_casos_rio_2020_2021.csv');
4
5  mm7 = dados;
6  for j=7:length(dados)
7      mm7(j) = sum(dados(j-6:j))/7;
8  end
9
10 xdata = 1:21; ydata = mm7(xdata)';
11 A      = [xdata; ones(size(xdata))];
12 b      = log(ydata)';
13 x      = A\b;
14 yfit   = @(z) exp(x(2))*exp(x(1)*z);
15
16 stem(dados(1:31), 'oc', 'LineWidth', 0.5);
17 hold on
18 plot(1:31, mm7(1:31), '-.r', 'LineWidth', 1);
19 plot(yfit(1:31), '-y', 'LineWidth', 3);
20 plot(yfit(1:21), '-k', 'LineWidth', 3);
21 hold off
22 xlabel('dias decorridos'); ylabel('novos casos por dia');
23 set(gca, 'FontSize', 18);
```



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Outra possibilidade, curva logística (via regressão não linear):

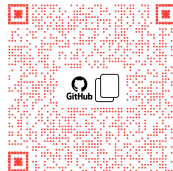
$$I(x) = \frac{\alpha L e^{-\alpha(t-t_m)}}{(1 + e^{-\alpha(t-t_m)})^2}$$



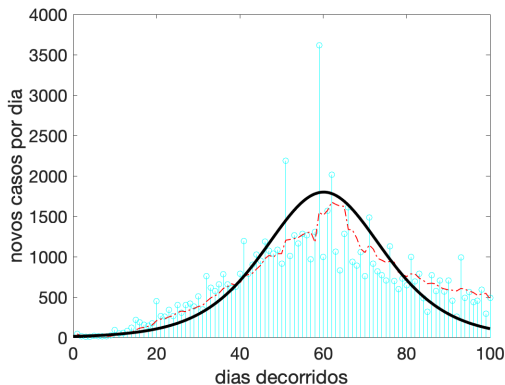
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MainRegressionExample5.m

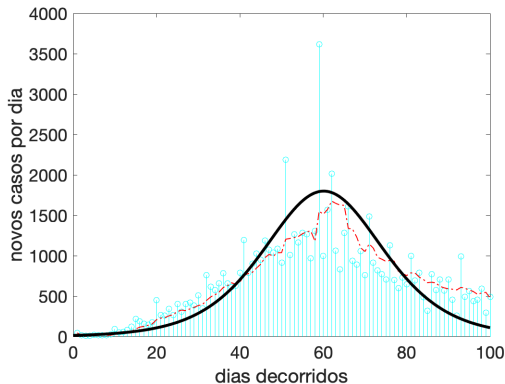
```
1  clc; clear; close all;
2
3  dados = load('covid19_casos_rio_2020_2021.csv');
4
5  mm7 = dados;
6  for j=7:length(dados)
7      mm7(j) = sum(dados(j-6:j))/7;
8  end
9
10 xdata = 1:100; ydata = mm7(xdata)';
11 N      = @(x,p) p(1)*p(2)*exp(-p(1)*(x-p(3)));
12 D      = @(x,p) (1+exp(-p(1)*(x-p(3)))).^2;
13 I      = @(x,p) N(x,p)./D(x,p);
14 E_2    = @(p) sqrt(sum(I(xdata,p) - ydata).^2/length(ydata));
15 p_2    = fminsearch(E_2,[0.1 8e4 55]);
16 yfit   = I(0:0.1:100,p_2);
17
18 stem(dados(1:100),'oc','LineWidth',0.5);
19 hold on
20 plot(1:100,mm7(1:100),'-r','LineWidth',1);
21 plot(0:0.1:100,yfit,'-k','LineWidth',3);
22 hold off
23 xlabel('dias decorridos'); ylabel('novos casos por dia');
24 set(gca,'FontSize',18);
```



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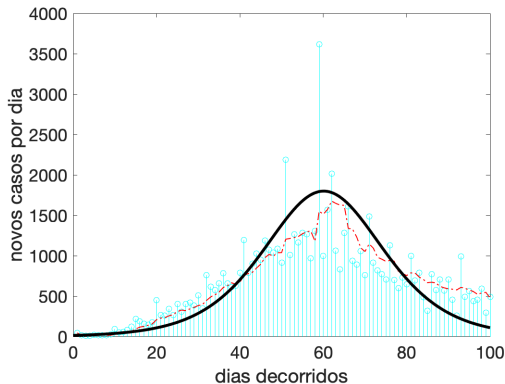
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E para ajustar várias ondas?



COVID-19 na cidade do Rio de Janeiro

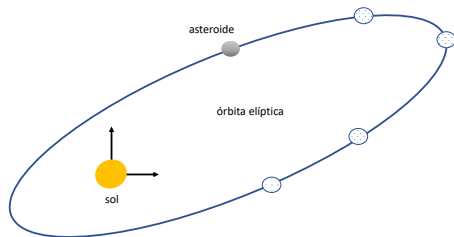


E para ajustar várias ondas?

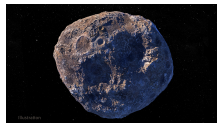
Tente somar várias curvas logísticas!



Órbita de um asteroide



5 observações estão disponíveis



x (ua)	y (ua)
8,025	8,310
10,170	6,355
11,202	3,212
10,736	0,375
9,092	-2,267
ua = unidade astronômica	

$$Ax^2 + Bxy + Cy^2 + Dx + Ey + 1 = 0$$

Determine a equação da órbita!



Algumas bases de dados




Pegue alguns dados nessas bases e construa regressores!

Como citar esse material?

A. Cunha Jr, *Ajuste de Curvas*,
Universidade do Estado do Rio de Janeiro – UERJ, 2024.



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