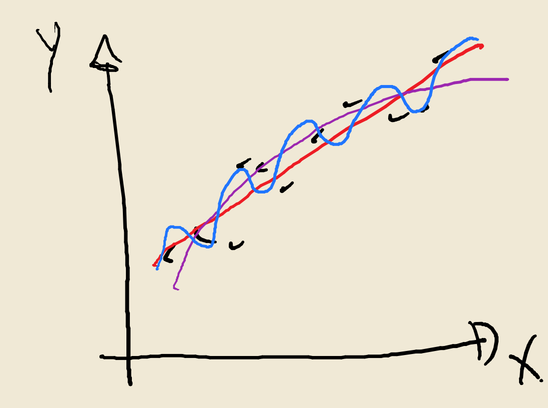
05/06 - Quadrados Mínimos



modelo: $y = \beta_0 + \beta_1 x$

$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x$

$y = \beta_0 + \beta_1 \sin(Lx) + \beta_2 \cos(Lx)$

Modelo: $h(x;\beta) = \sum_{j=1}^{p} \beta_j \varphi_j(x)$ base do modelo

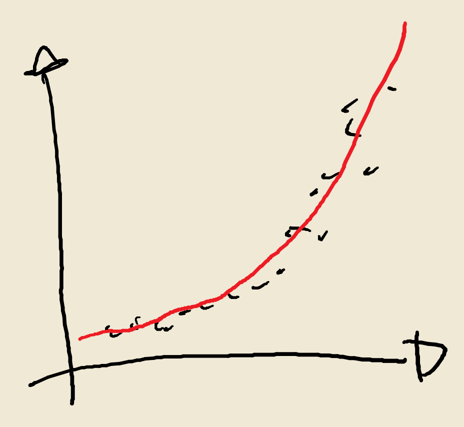
$$X = \begin{bmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \cdots & \varphi_p(x_1) \\ \vdots & \vdots & & \vdots \\ \varphi_1(x_n) & \varphi_2(x_n) & \cdots & \varphi_p(x_n) \end{bmatrix} \in \mathbb{R}^{n\times p}$$

→ Jacobiana de $F(\beta) = y - X\beta$

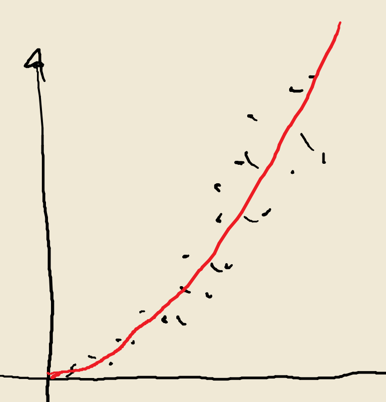
Problema: $\min_\beta \frac{1}{2}\|\underbrace{y - X\beta}_{\text{resíduo}}\|^2$

equiv. $X^T X \beta = X^T y$ equações normais

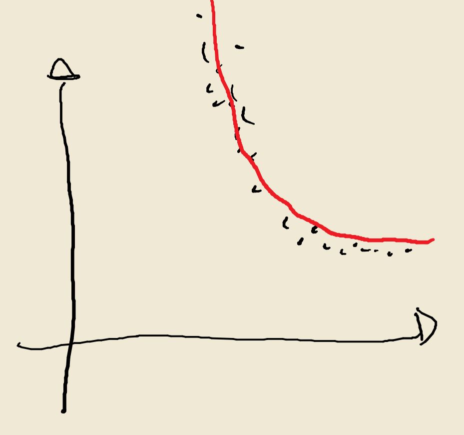
Não-linear linearizável



$y_i = \exp(\beta_0 + \beta_1 x_i)$



$y_i = \beta_0 x_i^{\beta_1}$



$y_i = \dfrac{1}{\beta_0 + \beta_1 x_i}$

Ex.: $h(x;\beta) = e^{\beta_0 + \beta_1 x}$

$\underbrace{\ln h(x;\beta) = \beta_0 + \beta_1 x}_{\psi(x;\beta)}$

$y_i \approx h(x_i;\beta) \Rightarrow \underbrace{\ln y_i}_{z_i} \approx \ln h(x_i;\beta) = \psi(x_i;\beta) = \beta_0 + \beta_1 x_i$

Ajuste $\{(x_i, z_i),\ i=1,\dots,n\}$

Ex.:

x	1	2	3	4
y	2.1	4.4	7.3	15.9

Ajuste d modelo $y = e^{\beta_0 + \beta_1 x}$ ← ñ sei

Veja que $\ln y = \beta_0 + \beta_1 x$, daí ← sei

x	1	2	3	4
ln y	0.7419	1.4816	1.9879	2.7663

Resolvendo criando X e y'

$$X = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix} \qquad y' = \begin{bmatrix} 0.7419 \\ 1.4816 \\ 1.9879 \\ 2.7663 \end{bmatrix}$$

$\beta_0 \cdot 1 + \beta_1 \cdot x$ ln y

$$X^T X = \begin{bmatrix} 4 & 10 \\ 10 & 30 \end{bmatrix} \qquad X^T y = \begin{bmatrix} 6.9777 \\ 20.734 \end{bmatrix}$$

$(X^T X)\beta = X^T y \Rightarrow \beta = (X^T X)^{-1} X^T y$

$$\hat{\beta} = \frac{1}{20}\begin{bmatrix} 30 & -10 \\ -10 & 4 \end{bmatrix}\begin{bmatrix} 6.9777 \\ 20.734 \end{bmatrix} = \begin{bmatrix} 0.0996 \\ 0.6580 \end{bmatrix}$$

$\hat{y} = \exp(X\hat{\beta})$ (y predito/estimado)

$$\hat{y} = \exp\left(\begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \\ 1 & 4 \end{bmatrix}\begin{bmatrix} 0.0996 \\ 0.6580 \end{bmatrix}\right) = \begin{bmatrix} 2.1332 \\ 4.1190 \\ 7.9534 \\ 15.3573 \end{bmatrix} \quad \begin{matrix} 2.1 \\ 4.4 \\ 7.3 \\ 15.9 \end{matrix}$$

resíduo: $y - \hat{y} = y - X\hat{\beta}$ (erro)

real → medido, aprox. p/ ajustar

O modelo: $y \approx \exp(0{,}0996 + 0.6580x)$

Avaliando o modelo

SQR = Soma dos Quadrados dos Resíduos

$= \sum_{i=1}^{n} (y_i - \underbrace{h(x_i;\beta)}_{\hat{y}_i})^2$

Métrica R^2

$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$

$SQT = \sum_{i=1}^{n} (y_i - \bar{y})^2$ Soma Total

$R^2 = 1 - \dfrac{SQR}{SQT} = 1 - \dfrac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$

$R^2 \in [0,1]$

Ex.: $y_i \approx \beta_0 x_i^{\beta_1}$

$\ln y_i \approx \underbrace{\ln \beta_0}_{\gamma_0} + \underbrace{\beta_1}_{\gamma_1} \ln x_i$ → linear em γ

Ex.: $y_i \approx \dfrac{1}{\beta_0 + \beta_1 x_i}$

$\dfrac{1}{y_i} \approx \beta_0 + \beta_1 x_i$