Redes neuronais artificiais

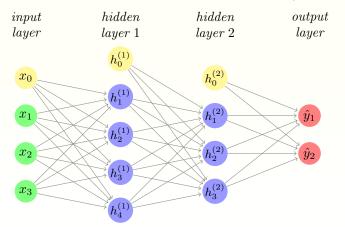
Gaspar J. Machado

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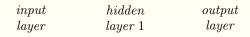
março de $2024\,$

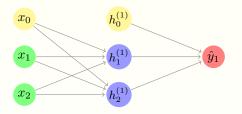
RNA

- Como tratar bases de dados que não são linearmente separáveis?
 - Linearização dos dados aumentando a dimensão do espaço dos atributos.
 - Redes neuronais artificiais RNA (ou Perceptron multicamada multilayer Perceptron, MLP, que é um nome enganador).



RNA | XOR (i)





$$\tilde{U} = \begin{bmatrix} \tilde{u}_{01} & \tilde{u}_{02} \\ \tilde{u}_{11} & \tilde{u}_{12} \\ \tilde{u}_{21} & \tilde{u}_{22} \end{bmatrix} \qquad \tilde{V} = \begin{bmatrix} \tilde{v}_0 \\ \tilde{v}_1 \\ \tilde{v}_2 \end{bmatrix}$$

RNA | XOR (ii)

$$\tilde{U} = \begin{bmatrix} \tilde{u}_{01} & \tilde{u}_{02} \\ \tilde{u}_{11} & \tilde{u}_{12} \\ \tilde{u}_{21} & \tilde{u}_{22} \end{bmatrix} = \begin{bmatrix} -\frac{1}{4} & \frac{5}{4} \\ 1 & -1 \\ 1 & -1 \end{bmatrix} \qquad \tilde{V} = \begin{bmatrix} \tilde{v}_{0} \\ \tilde{v}_{1} \\ \tilde{v}_{2} \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ 1 \\ 1 \end{bmatrix}$$

$$h_{1}(=h_{1}^{(1)}) = \operatorname{sgn}(\tilde{U}(:,1)^{\top}\tilde{x}) = \operatorname{sgn}\left(-\frac{1}{4} + x_{1} + x_{2}\right)$$

$$h_{2}(=h_{2}^{(1)}) = \operatorname{sgn}(\tilde{U}(:,2)^{\top}\tilde{x}) = \operatorname{sgn}\left(\frac{5}{4} - x_{1} - x_{2}\right)$$

$$\hat{y}(=\hat{y}_{1}) = \operatorname{sgn}(\tilde{V}^{\top}\tilde{h}) = \operatorname{sgn}\left(-\frac{1}{2} + h_{1} + h_{2}\right)$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad h_{2} \qquad \hat{y}$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad h_{2} \qquad \hat{y}$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad h_{2} \qquad \hat{y}$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad h_{2} \qquad \hat{y}$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad h_{2} \qquad \hat{y}$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad h_{2} \qquad \hat{y}$$

$$\frac{x_{1}}{4} = \frac{x_{2}}{4} \qquad h_{1} \qquad \operatorname{sgn}(\frac{3}{4}) = +1 \qquad \operatorname{sgn}(\frac{3}{2}) = +1$$

$$\frac{1}{4} \qquad h_{1} \qquad \operatorname{sgn}(\frac{3}{4}) = +1 \qquad \operatorname{sgn}(\frac{3}{4}) = +1 \qquad \operatorname{sgn}(\frac{3}{2}) = +1$$

$$\frac{1}{4} \qquad h_{1} \qquad \operatorname{sgn}(\frac{3}{4}) = +1 \qquad \operatorname{sgn}(\frac{3}{4}) = +1 \qquad \operatorname{sgn}(\frac{3}{2}) = -1$$

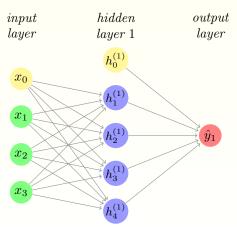
$$\frac{1}{4} \qquad h_{1} \qquad \operatorname{sgn}(\frac{3}{4}) = +1 \qquad \operatorname{sgn}(\frac{3}{4}) = -1 \qquad \operatorname{sgn}(\frac{3}{2}) = -1$$

RNA1 (i)

- Contexto: classificador binário com a base de dados $D = (x^n, y^n)_{n=1}^N, x^n \in \mathbb{R}^I, y^n \in \{-1, +1\}.$
- Neste curso vamos considerar redes neuronais artificiais do tipo feed-forward com uma camada oculta (shallow neural network), ou seja, com três camadas:
 - \blacksquare a camada de entrada (input layer) com I (+1) nós;
 - uma camada oculta ($hidden\ layer$) com $J\ (+1)$ nós (é um hiperparâmetro da ML);
 - a camada de saída (output layer), com 1 nó, pois o contexto é o da classificação binária.
- Vamos denotar por RNA1 as redes neuronais artificiais do tipo feed-forward com uma camada oculta.

RNA1 (ii)

■ Exemplo com I = 3 e J = 4:



RNA1 (iii)

■ Parâmetros de uma RNA1: matrizes

$$\tilde{U} = \begin{bmatrix}
\tilde{u}_{01} & \tilde{u}_{02} & \cdots & \tilde{u}_{0J} \\
\tilde{u}_{11} & \tilde{u}_{12} & \cdots & \tilde{u}_{1J} \\
\tilde{u}_{21} & \tilde{u}_{22} & \cdots & \tilde{u}_{2J} \\
\vdots & \vdots & \ddots & \vdots \\
\tilde{u}_{I1} & \tilde{u}_{I2} & \cdots & \tilde{u}_{IJ}
\end{bmatrix} \in \mathbb{R}^{(I+1)\times J} \quad e \quad \tilde{V} = \begin{bmatrix}
\tilde{v}_{0} \\
\tilde{v}_{1} \\
\vdots \\
\tilde{v}_{J}
\end{bmatrix} \in \mathbb{R}^{J+1}.$$

Treinar uma RNA1: determinar as matrizes $\tilde{U}^* \in \mathbb{R}^{(I+1)\times J}$ e $\tilde{V}^* \in \mathbb{R}^{J+1}$ que minimizam uma função custo dada.

RNA1 (iv)

- Arquitetura da ML:
 - inputs: $x \in \mathbb{R}^I$, $\tilde{U} \in \mathbb{R}^{(I+1)\times J}$, $\tilde{V} \in \mathbb{R}^{J+1}$, $f : \mathbb{R} \to \mathbb{R}$, $g : \mathbb{R} \to \mathbb{R}$;
 - $output: \hat{y} \in \mathbb{R};$
 - passos

1.
$$s = \tilde{U}^{\top} \tilde{x}$$
,
2. $h = f(s) \equiv (f(s_1), f(s_2), \dots, f(s_J))^{\top}$,
3. $r = \tilde{V}^{\top} \tilde{h}$,
4. $\hat{y} = g(r)$.

■ Função custo genérica:

$$E(\tilde{U}, \tilde{V}; D) = \frac{1}{N} \sum_{n=1}^{N} E_n(\hat{y}^n; y^n),$$

$$\hat{y}^n = \hat{y}(\tilde{U}, \tilde{V}; x^n).$$

Algoritmo RNA1-MGE

```
Input: D = (x^n, y^n)_{n=1}^N, x^n \in \mathbb{R}^I, y^n \in \{0, 1\}, \ \tilde{U}_{(0)} \in \mathbb{R}^{(I+1) \times J},
                     \tilde{V}_{(0)} \in \mathbb{R}^{J+1}, \, \eta \in \mathbb{R}^+
     Output: \tilde{U}^* \in \mathbb{R}^{(I+1)\times J} e \tilde{V}^* \in \mathbb{R}^{J+1}
1 t \leftarrow 0:
2 while V do
              selecionar n \in \{1, ..., N\} aleatório;
4 \quad \middle| \quad d_{(t)}^{\tilde{v}} \leftarrow \nabla_{\tilde{v}} E_n(\hat{y}^n; y^n), \ \tilde{V}_{(t+1)} \leftarrow \tilde{V}_{(t)} - \eta d_{(t)}^{\tilde{v}};
       d_{(t)}^{\tilde{u}} \leftarrow \nabla_{\tilde{u}} E_n(\hat{y}^n; y^n), \ \tilde{U}_{(t+1)} \leftarrow \tilde{U}_{(t)} - \eta d_{(t)}^{\tilde{u}};
          if CP = V then
          \tilde{U}^* \leftarrow \tilde{U}_{(t+1)}, \ \tilde{V}^* \leftarrow \tilde{V}_{(t+1)}; \mathbf{return} \ (\tilde{U}^*, \ \tilde{V}^*);
```

RNA1 | Cálculo das derivadas | \tilde{V}

■ Arquitetura da ML:

$$s = \tilde{U}^{\top} \tilde{x}^n, h = f(s), r = \tilde{V}^{\top} \tilde{h}, \hat{y}^n = g(r).$$

■ Seja $j \in \{0, \ldots, J\}$. Então:

$$E_n - \hat{g} - \frac{1}{2} \left(\frac{N_0}{N_0} \right)$$

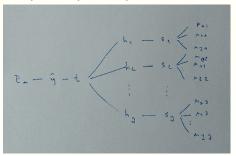
$$\frac{\partial E_n}{\partial \tilde{v}_j}(\hat{y}^n; y^n) = \frac{\mathrm{d}E_n}{\mathrm{d}\hat{y}} \frac{\mathrm{d}\hat{y}}{\mathrm{d}r} \frac{\partial r}{\partial \tilde{v}_j} = \frac{\mathrm{d}E_n}{\mathrm{d}\hat{y}} g'(r) h_j.$$

RNA1 | Cálculo das derivadas | \tilde{U}

■ Arquitetura da ML

$$s = \tilde{U}^{\top} \tilde{x}^n, h = f(s), r = \tilde{V}^{\top} \tilde{h}, \hat{y}^n = g(r).$$

■ Sejam $i \in \{0, ..., J\}$ e $j \in \{1, ..., J\}$. Então:



$$\frac{\partial E_n}{\partial \tilde{u}_{ij}}(\hat{y}^n; y^n) = \frac{\mathrm{d}E_n}{\mathrm{d}\hat{y}} \frac{\mathrm{d}\hat{y}}{\mathrm{d}r} \frac{\partial r}{\partial h_i} \frac{\mathrm{d}h_j}{\mathrm{d}s_j} \frac{\partial s_j}{\partial \tilde{u}_{ij}} = \frac{\mathrm{d}E_n}{\mathrm{d}\hat{y}} g'(r) v_j f'(s_j) x_i.$$

RNA1₁ | função logística + "cross entropy"

■ Sejam:

$$\begin{split} f(z) &= \sigma(z), \\ g(z) &= \sigma(z), \\ E_n(\hat{p}^n; y^n) &= -y^n \ln(\hat{p}^n) - (1 - y^n) \ln(1 - \hat{p}^n). \end{split}$$

- Então:
 - Para $j \in \{0, ..., J\}$:

$$\frac{\partial E_n}{\partial \tilde{v}_j}(\hat{p}^n; y^n) = (\hat{p}^n - y^n) \, \tilde{h}_j.$$

■ Para $i \in \{0, ..., J\}, j \in \{1, ..., J\}$:

$$\frac{\partial E_n}{\partial \tilde{u}_{ij}}(\hat{p}^n; y^n) = (\hat{p}^n - y^n) v_j h_j (1 - h_j) \tilde{x}_i.$$

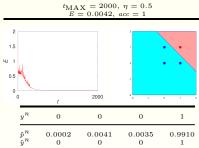
- Backpropagation ...
- Vamos denotar por **RNA1**₁−**MGE** o algoritmo da rede neuronal artificial do tipo *feed-forward* com uma camada oculta cujas funções de ativação são a função logística e cuja função é a "cross entropy"com o MGE.

Algoritmo RNA1₁-MGE

10

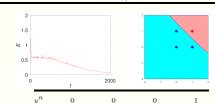
```
Input: D = (x^n, y^n)_{n=1}^N, x^n \in \mathbb{R}^I, y^n \in \{0, 1\}, \ \tilde{U}_{(0)} \in \mathbb{R}^{(I+1) \times J},
                      V_{(0)} \in \mathbb{R}^{J+1}, \, \eta \in \mathbb{R}^+
     Output: \tilde{U}^* \in \mathbb{R}^{(I+1)\times J} e \tilde{V}^* \in \mathbb{R}^{J+1}
1 t \leftarrow 0:
   while V do
               selecionar n \in \{1, ..., N\} aleatório;
4 s \leftarrow \tilde{U}_{(t)}^{\top} \tilde{x}^n, h \leftarrow \sigma(s), r \leftarrow \tilde{V}_{(t)}^{\top} \tilde{h}, \hat{p}^n \leftarrow \sigma(r);
       d_{i,(t)}^{\tilde{v}} \leftarrow (\hat{p}^n - y^n) \tilde{h}_j, \ \tilde{v}_{i,(t+1)} \leftarrow \tilde{v}_{i,(t)} - \eta d_{i,(t)}^{\tilde{v}}, \ j = 0, \dots, J;
              d_{ij}^{\tilde{u}}(t) \leftarrow (\hat{p}^n - y^n) v_{j,(t)} h_j (1 - h_j) \tilde{x}_i,
                   \tilde{u}_{ij,(t+1)} \leftarrow \tilde{u}_{ij,(t)} - \eta d_{ii,(t)}^{\tilde{u}}, \ i = 0, \dots, I, \ j = 1, \dots, J;
                if CP = V then
                 \tilde{U}^* \leftarrow \tilde{U}_{(t+1)}, \ \tilde{V}^* \leftarrow \tilde{V}_{(t+1)}; \mathbf{return} \ (\tilde{U}^*, \ \tilde{V}^*);
                else
                   t \leftarrow t + 1;
```

ex1 (AND) | RNA1₁-MGE | J=2



$$t_{\text{MAX}} = 10000, \ \eta = 0.5$$

 $E = 0.0006, \ acc = 1$

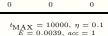


0.0043

0

 $t_{\text{MAX}} = 2000, \ \eta = 0.1$

E = 0.0750, acc = 1

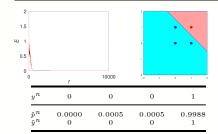


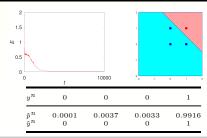
0.0800

0.0595

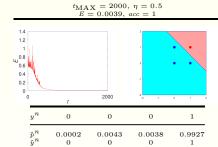
0

0.8600



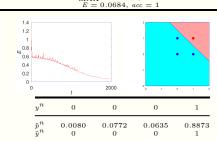


ex1 (AND) | RNA1₁-MGE | J = 3

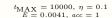


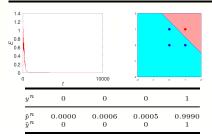
$$t_{\text{MAX}} = 10000, \ \eta = 0.5$$

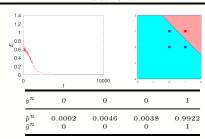
 $E = 0.0005, \ acc = 1$



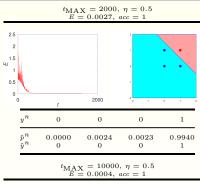
 $t_{\text{MAX}} = 2000, \ \eta = 0.1$



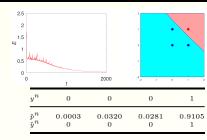




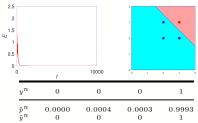
ex1 (AND) | RNA1₁-MGE | J = 10

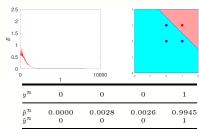


 $\begin{array}{c} t_{\hbox{MAX}} = 2000, \: \eta = 0.1 \\ E = 0.0388, \: acc = 1 \end{array}$

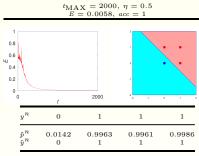








ex2 (OR) | RNA1₁-MGE | J = 2



0

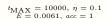
0.1219

0

 $t_{\text{MAX}} = 2000, \ \eta = 0.1$

E = 0.0562, acc = 1

 $t_{\text{MAX}} = 10000, \ \eta = 0.5$ $E = 0.0010, \ acc = 1$



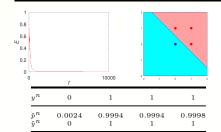
0.9614

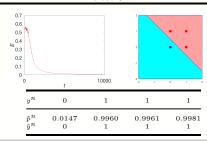
1

0.9613

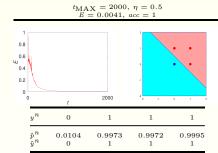
1

0.9843

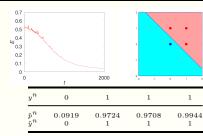




ex2 (OR) | RNA1₁-MGE | J = 3



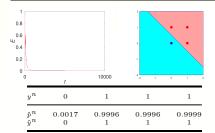
 $\begin{array}{c} t_{\hbox{\scriptsize MAX}} = 2000, \; \eta = 0.1 \\ E = 0.0399, \; acc = 1 \end{array}$

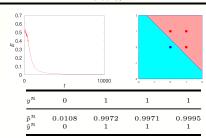


$$t_{\text{MAX}} = 10000, \ \eta = 0.5$$

 $E = 0.0007, \ acc = 1$



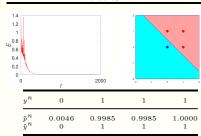


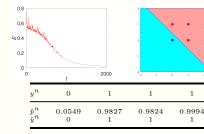


ex2 (OR) | RNA1₁-MGE | J = 10



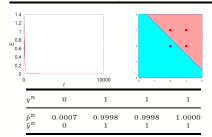
 $\begin{array}{c} t_{\hbox{\scriptsize MAX}} = 2000, \; \eta = 0.1 \\ E = 0.0231, \; acc = 1 \end{array}$

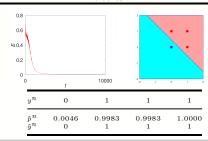




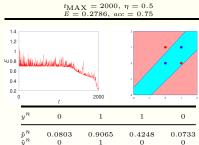
$$t_{\mbox{MAX}} = 10000, \; \eta = 0.5 \\ E = 0.0003, \; acc = 1$$

 $\begin{array}{l} t_{\hbox{\scriptsize MAX}} = 10000, \; \eta = 0.1 \\ E = 0.0020, \; acc = 1 \end{array}$

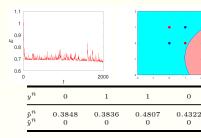




ex3 (XOR) | RNA1₁-MGE | J = 2



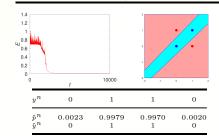
 $t_{\text{MAX}} = 10000, \ \eta = 0.5$ $E = 0.0023, \ acc = 1$

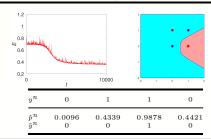


 $t_{\text{MAX}} = 2000, \eta = 0.1$

E = 0.6857, acc = 0.50

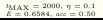
 $t_{\mbox{MAX}} = 10000, \; \eta = 0.1 \\ E = 0.3601, \; acc = 0.75$

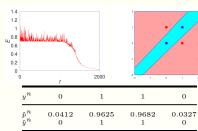


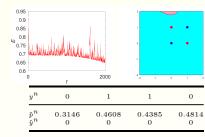


ex3 (XOR) | RNA1₁-MGE | J = 3





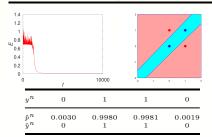


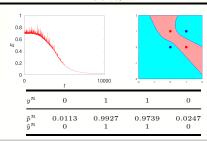


$$t_{\text{MAX}} = 10000, \ \eta = 0.5$$

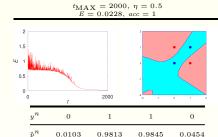
 $E = 0.0022, \ acc = 1$

 $t_{\mbox{MAX}} = 10000, \; \eta = 0.1 \\ E = 0.0175, \; acc = 1$





ex3 (XOR) | RNA1₁-MGE | J = 10

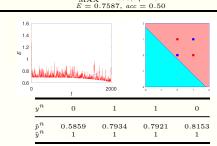


 \hat{y}^n

0

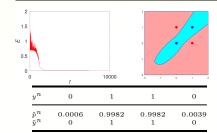
$$t_{\mbox{MAX}} = 10000, \; \eta = 0.5$$

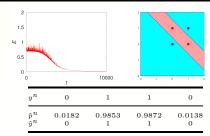
 $E = 0.0020, \; acc = 1$



 $t_{\text{MAX}} = 2000, \ \eta = 0.1$

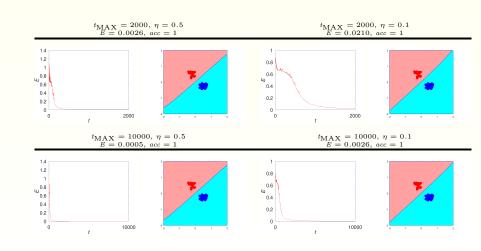




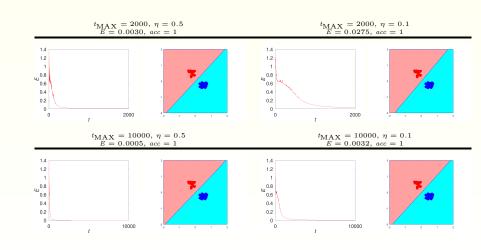


0

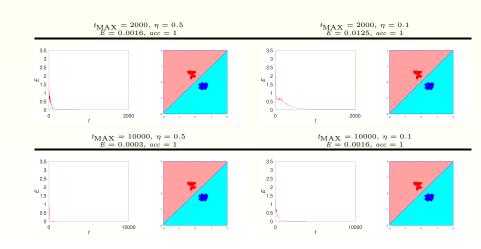
$ex4 \mid RNA1_1 - MGE \mid J = 2$



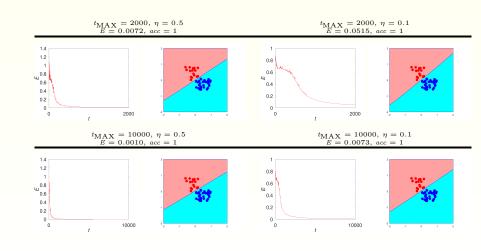
$ex4 \mid RNA1_1 - MGE \mid J = 3$



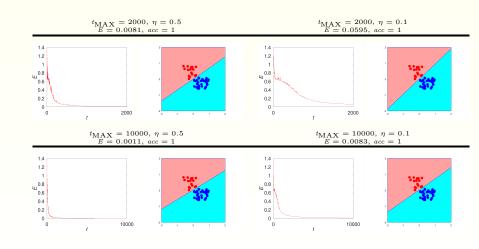
$ex4 \mid RNA1_1 - MGE \mid J = 10$



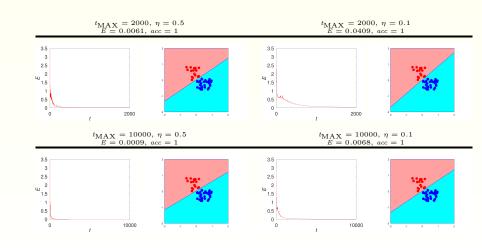
$ex5 \mid RNA1_1 - MGE \mid J = 2$

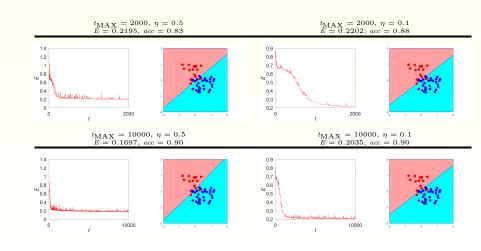


$ex5 \mid RNA1_1 - MGE \mid J = 3$

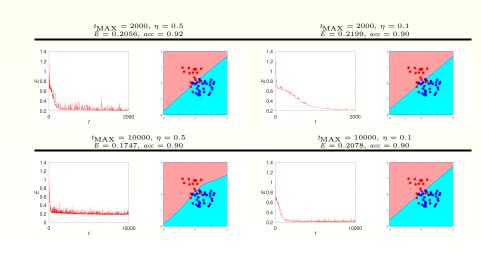


$ex5 \mid RNA1_1 - MGE \mid J = 10$

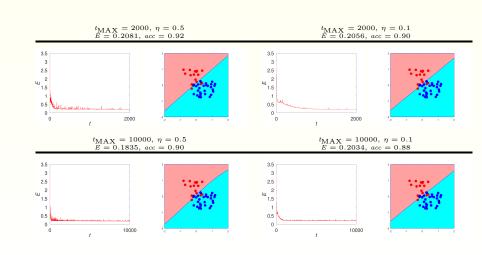


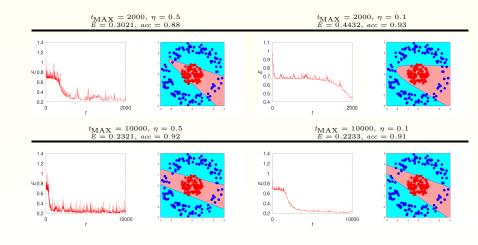


$ex6 \mid RNA1_1 - MGE \mid J = 3$

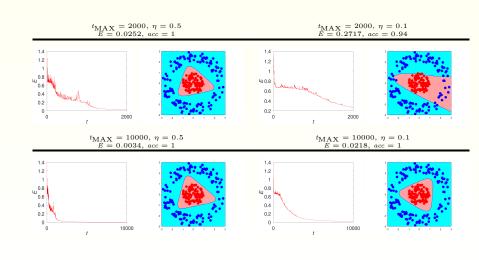


$ex6 \mid RNA1_1 - MGE \mid J = 10$

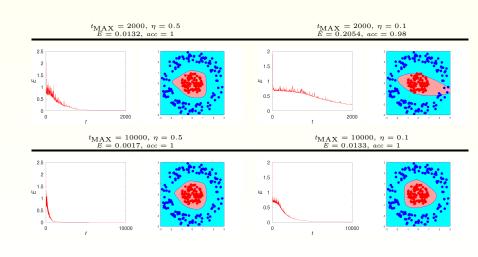




ex8 | RNA1₁-MGE | J = 3



ex8 | RNA1₁-MGE | J = 10



Exercícios

Exercício 1. Sejam:

$$\begin{split} f(z) &= \sigma(z), \\ g(z) &= \sigma(z), \\ E_n(\hat{p}^n; y^n) &= -y^n \ln(\hat{p}^n) - (1 - y^n) \ln(1 - \hat{p}^n). \end{split}$$

(a) Seja $j \in \{0, \dots, J\}$. Mostre que:

$$\frac{\partial E_n}{\partial \tilde{v}_j}(\hat{p}^n; y^n) = (\hat{p}^n - y^n) \, \tilde{h}_j.$$

(b) Sejam $i \in \{0, ..., J\}$ e $j \in \{1, ..., J\}$. Mostre que:

$$\frac{\partial E_n}{\partial \tilde{u}_{ij}}(\hat{p}^n; y^n) = (\hat{p}^n - y^n) v_j h_j (1 - h_j) \tilde{x}_i.$$

Exercícios

Exercício 2. Considere a base de dados binária $D = (x^n, y^n)_{n=1}^6$ (I=2) com

$$\begin{split} x^1 &= (-1,1)^\top & y^1 &= 0, \\ x^2 &= (-1,-1)^\top & y^2 &= 1, \\ x^3 &= (0,0)^\top & y^3 &= 1, \\ x^4 &= (1,1)^\top & y^4 &= 1, \\ x^5 &= (-1,0)^\top & y^5 &= 0, \\ x^6 &= (1,-1)^\top & y^6 &= 0. \end{split}$$

Aplique o Algoritmo RNA1₁–MGE e $J=2,\ t_{\rm max}=3,\ \eta=0.1$ e n dado pela sequência 3, 2, 5 à base de dados D, indicando a accuracy que se obteve. Inicialize as matrizes pesos com matrizes nulas.

Exercício 3. Implemente o algoritmo RNA 1_1 -MGE.