CBA 2008 CONGRESSO BRASILEIRO DE AUTOMÁTICA

**Juiz de Fora, 14 a 17 de Setembro de 2008**

**Minicurso:**

# *Componentes Principais Generalizadas Via Redes Neurais*

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**Resumo:**

A Análise por Componentes Principais (PCA) ou Transformada de Kahunen-Löeve é provavelmente o método mais utilizado para compactação de informação. Vantagens adicionais além da redução da dimensionalidade são (a) o fornecimento de componentes ortogonais, descorrelacionadas, o que facilita uma série de processamentos posteriores da informação, e eventualmente (b) a redução do ruído presente na informação. Entretanto este tipo de compactação otimiza apenas a reconstrução da informação. Se uma informação $\underline{x}$ é compactada e preservada é porque, na maioria das vezes, ela vai ser utilizada para gerar algum resultado específico $\underline{y}$ , isto é, utilizada como entrada para um mapeamento $M\text{:}\ \underline{x} \rightarrow \underline{y}$. E nem sempre a compactação que otimiza a reconstrução de $\underline{x}$ é a ótima para gerar $\underline{y}$. Neste mini-curso discutimos a utilização de redes neurais para compactar a informação $\underline{x}$ de modo a otimizar o resultado final desejado $\underline{y}$ mantendo as vantagens adicionais (a) e (b) mencionadas acima.

# Representação por Componentes Principais

PCA - Principal Components Analysis

- Generalização

$$\underline{x} \xrightarrow{\mathcal{M}} \underline{y}$$

$$\underline{x} \xrightarrow{\mathcal{M}_1} \underline{z} \xrightarrow{\mathcal{M}_2} \underline{\tilde{y}}$$

$$\dim \underline{z} < \dim \underline{x} \,,\ \dim \underline{y}$$

$$\dim \underline{z} < \dim \underline{x} \,,\ \dim \underline{y}$$

Compressão da Informação

Redução da Dimensionalidade

Descorrelação

$$r(z_i, z_j) = 0 \qquad \forall\, i, j$$

$$\underline{x} \xrightarrow{\mathcal{M}} \underline{y}$$

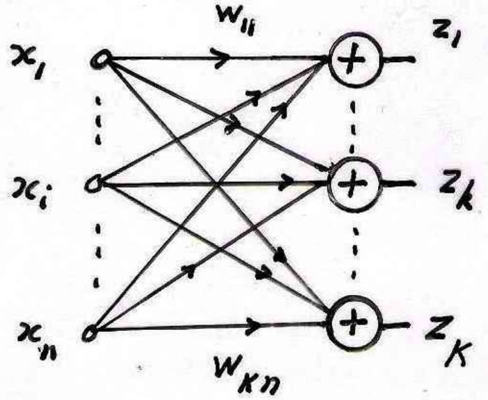
$$\underline{x} \xrightarrow{\mathcal{M}_1} \underline{z} \xrightarrow{\mathcal{M}_2} \underline{\tilde{y}}$$

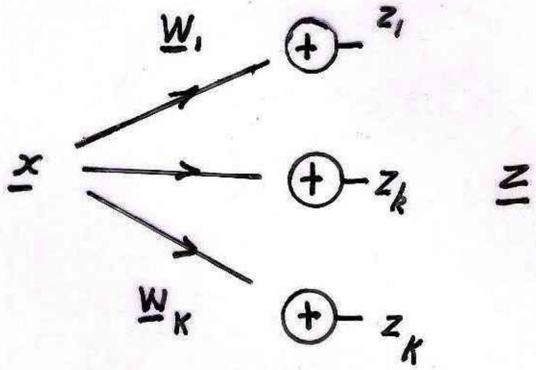
Tipos de mapeamentos:

| $\mathcal{M}$ | $\mathcal{M}_1$ | $\mathcal{M}_2$ | |
|---|---|---|---|
| Linear | L | L | * |
| | NL | NL | |
| Não Linear | L | NL | * |
| | NL | L | |
| | NL | NL | |

# Implementação dos mapeamentos

$\mathcal{M}_1$ linear $\quad \underline{z} = \underline{W}\,\underline{x}$



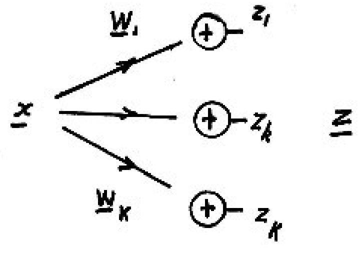




neurônios SEM BIAS

$$z_k = \underline{x}^t\,\underline{w}_k$$

$$\underline{w}_k = \begin{bmatrix} w_{k1} \\ w_{k2} \\ \vdots \\ w_{kn} \end{bmatrix}$$

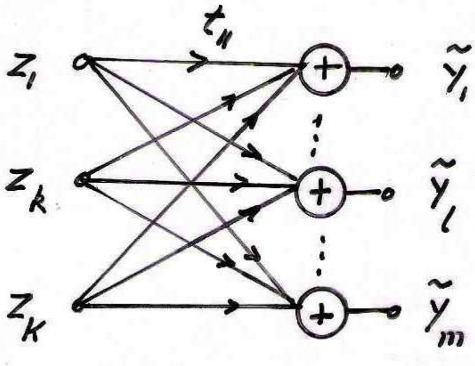
in-star de Grossberg

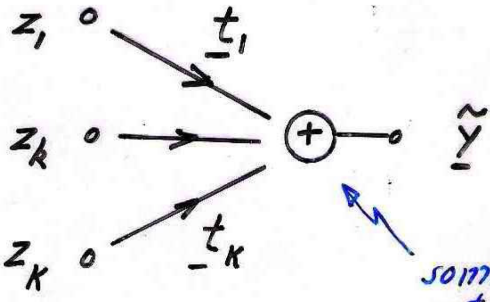



$$\underline{W} = [w_{ij}] = \begin{bmatrix} \underline{w}_1^t \\ \underline{w}_2^t \\ \vdots \\ \underline{w}_K^t \end{bmatrix}$$

$\mathcal{M}_2$ linear

$$\underline{\tilde{y}} = \underline{T}\ \underline{z}$$




somador vetorial

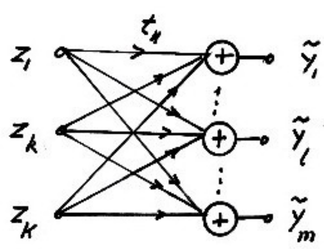
neurônios SEM BIAS

$$\underline{\tilde{y}} = \sum_{k=1}^{K} z_k\ \underline{t}_k$$

$$\underline{\tilde{y}} = \sum_{k=1}^{K} z_k\ \underline{t}_k$$

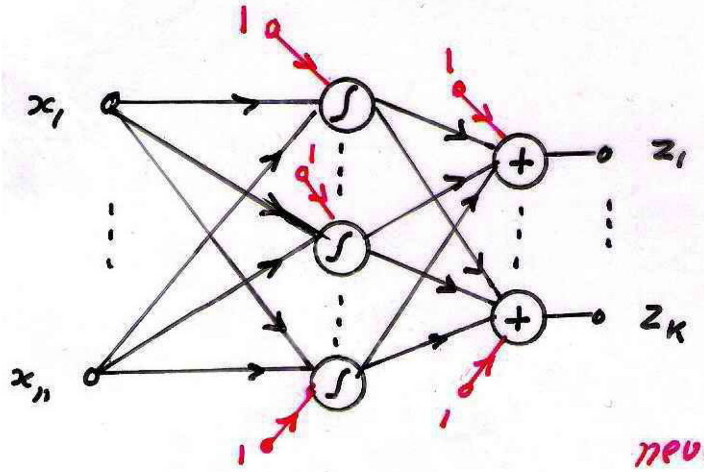
$$\underline{t}_k = \begin{bmatrix} t_{k1} \\ t_{k2} \\ \vdots \\ t_{kK} \end{bmatrix}$$

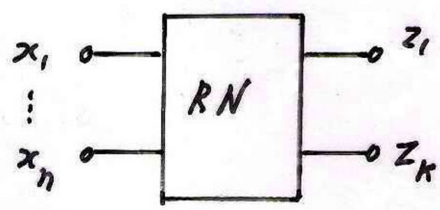
out-star de Grossberg




$$\underline{T} = [\ \underline{t}_1\ \ \underline{t}_2\ \dots\ \underline{t}_K\ ]$$

$\mathcal{M}_1$ não linear $\quad \underline{z} = \varphi(\underline{x})$

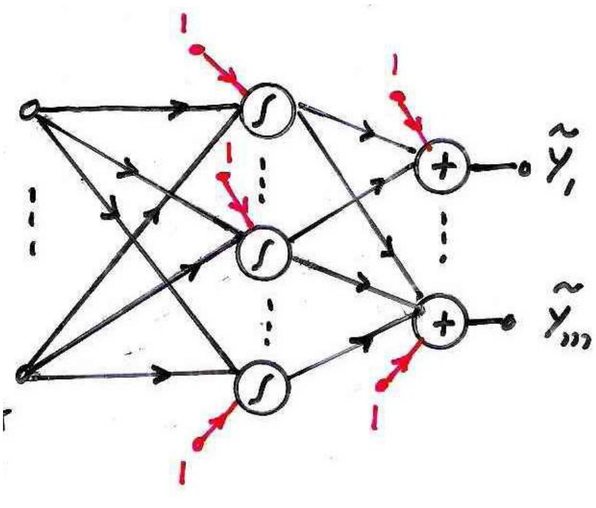


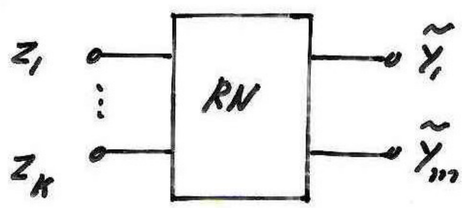




neurônios COM BIAS

$\mathcal{M}_2$ não linear $\quad \tilde{y} = \phi(\underline{z})$

similar

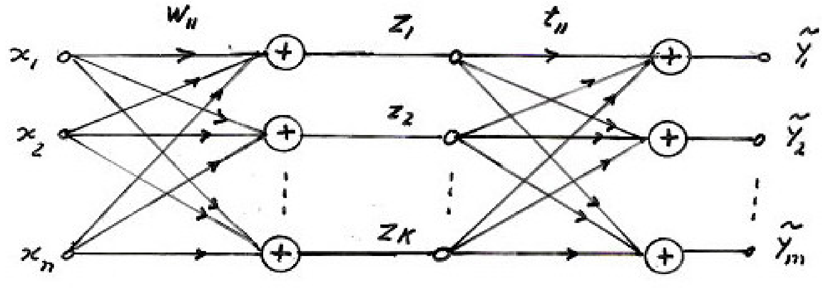


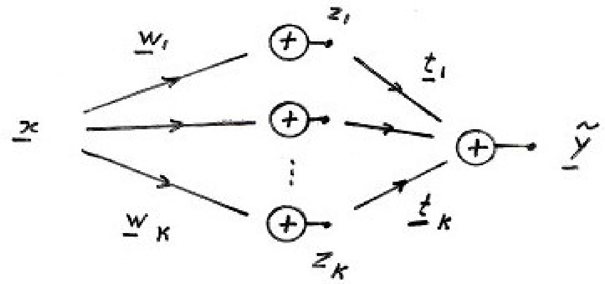



# Mapeamento Linear

$\mathcal{M}_1$ linear $\qquad \underline{z} = \underline{W}\,\underline{x}$

$\mathcal{M}_2$ linear $\qquad \underline{\tilde{y}} = \underline{T}\,\underline{z}$




## Primeira componente


$$z_1 = \underline{x}^t \underline{w}_1 = \sum_{i=1}^{n} x_i\, w_{1i}$$

$$\underline{\tilde{y}} = z_1\, \underline{t}_1 \qquad \tilde{y}_j = z_1\, t_{j1}$$

Critério

$\underline{w}_1\,,\ \underline{t}_1 \quad /$

$$F = E\,|\underline{y} - \underline{\tilde{y}}|^2 \quad \text{mínimo}$$

$$\Rightarrow \quad \nabla_{\underline{w}_1} F = \underline{0}$$

$$\nabla_{\underline{t}_1} F = \underline{0}$$

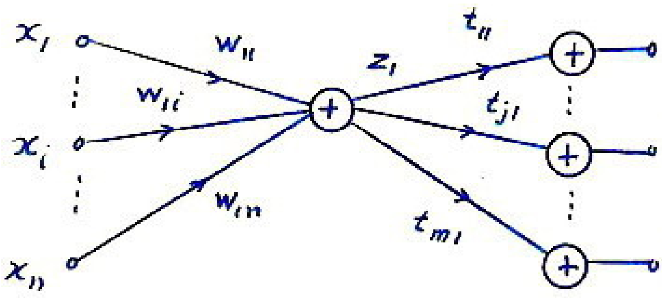
$$\Rightarrow \quad \frac{\partial F}{\partial w_{1i}} = 0 \quad \forall i$$

$$\frac{\partial F}{\partial t_{j1}} = 0 \quad \forall j$$

# Treinamento da Rede - Primeira Componente

$(\underline{x}, \underline{y}) \longrightarrow \underline{\tilde{y}} \simeq \underline{y}$ $\qquad$ P pares

$$F = \sum_{\forall (\underline{x}, \underline{y})} |\underline{y} - \underline{\tilde{y}}|^2$$




Gradiente descendente

$$\Delta w_{1i} = -\alpha \frac{\partial F}{\partial w_{1i}}$$

$$\Delta t_{j1} = -\alpha \frac{\partial F}{\partial t_{j1}}$$

$$\varepsilon^2 = |\underline{y} - \underline{\tilde{y}}|^2 = \sum_{l=1}^{m} (y_l - \tilde{y}_l)^2$$

$$= \sum_l \varepsilon_l^2$$

$$\frac{\partial \varepsilon^2}{\partial t_{j1}} = 2 \sum_l \varepsilon_l \frac{\partial \varepsilon_l}{\partial t_{j1}} = -2 \sum_l \varepsilon_l \frac{\partial \tilde{y}_l}{\partial t_{j1}}$$

$$\tilde{y}_l = z_1 t_{l1} \qquad \frac{\partial \varepsilon^2}{\partial t_{j1}} = -2 \varepsilon_j z_1$$

$$\frac{\partial \varepsilon^2}{\partial w_{1i}} = -2 \sum_{l} \varepsilon_l \frac{\partial \tilde{y}_l}{\partial w_{1i}}$$

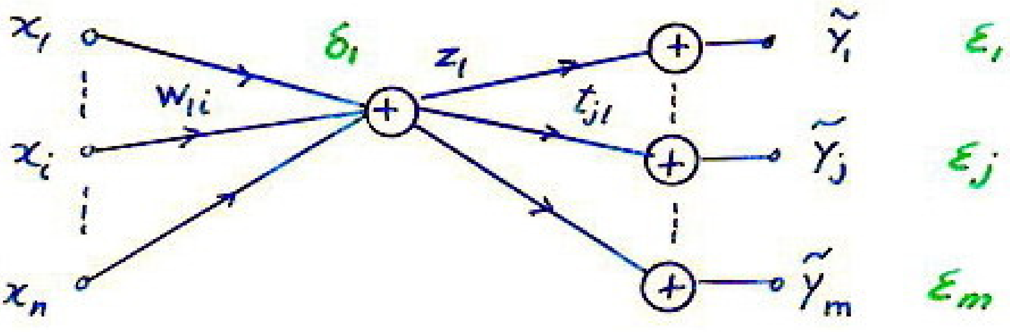
$$\tilde{y}_l = t_{l1}\, z_1 = t_{l1} \sum_{j=1}^{n} w_{1j}\, x_j$$

$$\frac{\partial \varepsilon^2}{\partial w_{1i}} = -2 \sum_{l} \varepsilon_l\, t_{l1}\, x_i = -2\, x_i \underbrace{\sum_{l} \varepsilon_l\, t_{l1}}_{\delta_1}$$

$$\delta_1 = \sum_{l} \varepsilon_l\, t_{l1}$$

$$\frac{\partial \varepsilon^2}{\partial w_{1i}} = -2\, x_i\, \delta_1$$

$$\delta_1 = \sum_{l=1}^{m} \varepsilon_l\, t_{l1}$$




$$\Delta w_{1i} = 2 \alpha\, x_i\, \delta_1$$

$$\Delta t_{j1} = 2 \alpha\, z_1\, \varepsilon_j$$

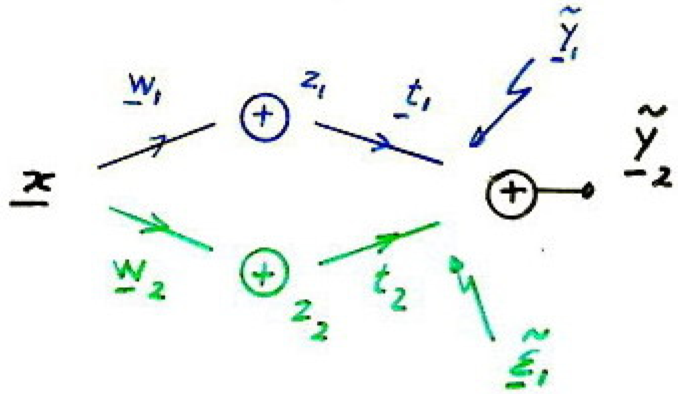
## Normalização

$$\tilde{\underline{y}}_1 = z_1 \, \underline{t}_1 = \underline{x}^t \, \underline{w}_1 \, \underline{t}_1$$

$$\underline{w}_1 \longrightarrow \frac{1}{|\underline{w}_1|} \, \underline{w}_1$$

$$\underline{t}_1 \longrightarrow |\underline{w}_1| \, \underline{t}_1$$

## Segunda componente




$$\underline{\varepsilon}_2 = \underline{y} - \tilde{\underline{y}}_2$$

$$\varepsilon_2^2 = |\underline{\varepsilon}_2|^2$$

$$\varepsilon_2^2 < \varepsilon_1^2$$

## Treinamento

- "Congelar" $\underline{w}_1$ e $\underline{t}_1$

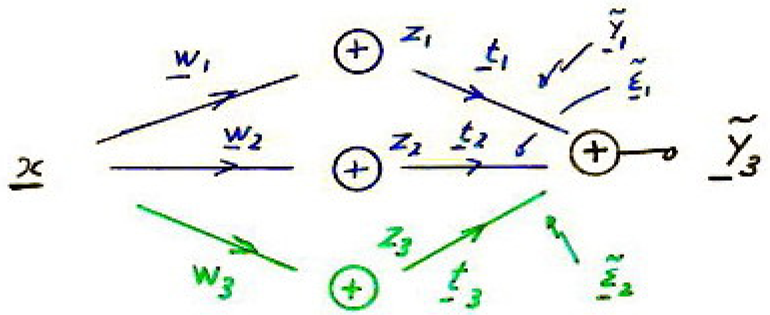
- Treinar $\underline{w}_2$ e $\underline{t}_2$

Terceira componente

Introduzir $\underline{w}_3$ e $\underline{t}_3$

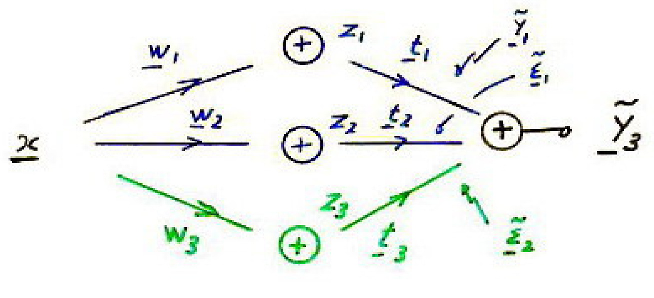
Congelar $\underline{w}_1$ , $\underline{t}_1$ , $\underline{w}_2$ e $\underline{t}_2$

Treinar $\underline{w}_3$ e $\underline{t}_3$




$$\underline{\tilde{Y}}_1 \simeq \underline{Y} \qquad \underline{\varepsilon}_1 = \underline{Y} - \underline{\tilde{Y}}_1$$

$$\underline{\tilde{\varepsilon}}_1 \simeq \underline{\varepsilon}_1 \qquad \underline{\tilde{Y}}_2 = \underline{\tilde{Y}}_1 + \underline{\tilde{\varepsilon}}_1$$




$$_2 = \underline{Y} - \underline{\tilde{Y}}_2 =$$

$$\underline{Y} - (\underline{\tilde{Y}}_1 + \underline{\tilde{\varepsilon}}_1) =$$

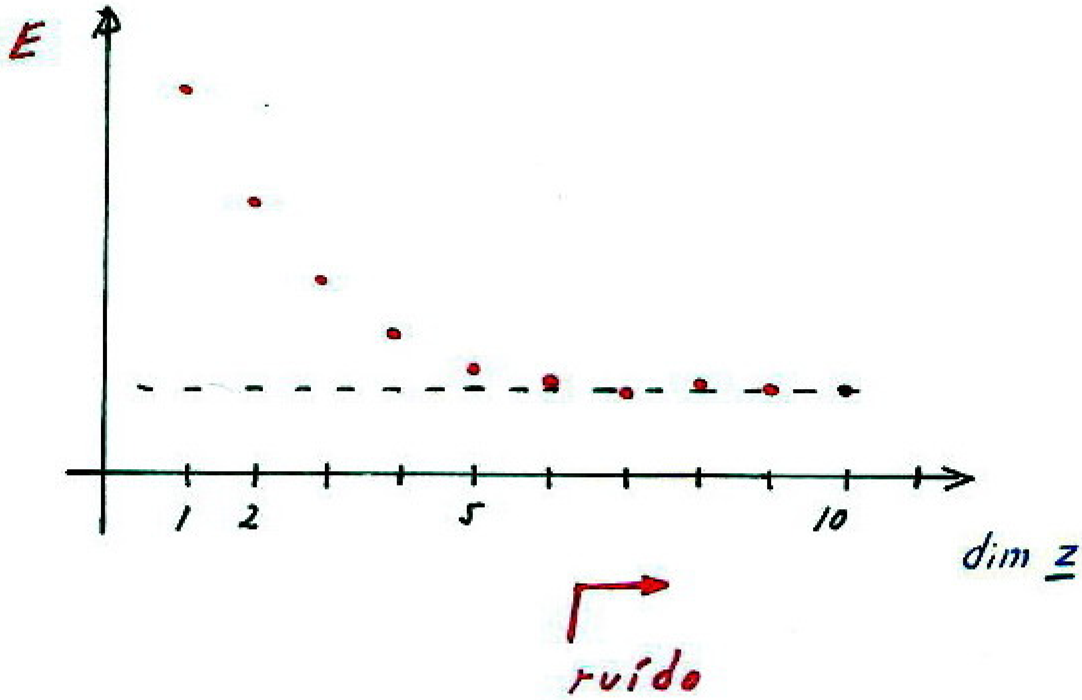
$$\underline{Y} - [\underline{Y} - \underline{\varepsilon}_1 + \underline{\tilde{\varepsilon}}_1] =$$

$$\underline{\varepsilon}_1 - \underline{\tilde{\varepsilon}}_1$$

$$\underline{\tilde{\varepsilon}}_2 \simeq \underline{\varepsilon}_2 \qquad \underline{\tilde{Y}}_3 = \underline{\tilde{Y}}_2 + \underline{\tilde{\varepsilon}}_2$$

Erro $E\,|\underline{y} - \underline{\tilde{y}}|^2$ versus

nº de componentes dim $\underline{z}$




Normalização

$$\underline{\tilde{y}}_1 = \underline{x}^t\, \underline{w}_1\, \underline{t}_1$$

$$\underline{w}_1 \longrightarrow \frac{1}{|\underline{w}_1|}\, \underline{w}_1$$

$$\underline{t}_1 \longrightarrow |\underline{w}_1|\, \underline{t}_1$$

e

$$\underline{w}_2 \longrightarrow \frac{1}{|\underline{w}_2|}\, \underline{w}_2$$

$$\underline{t}_2 \longrightarrow |\underline{w}_2|\, t_2$$

etc...

Ortogonalidade

$\underline{w}_1\ ,\ \underline{t}_1 \quad / \quad |\underline{\varepsilon}_1|$ mínimo

$$\tilde{\underline{y}}_1 = \underline{x}^t\,\underline{w}_1\,\underline{t}_1 = \underline{y}_1 - \underline{\varepsilon}_1$$

$$\tilde{\underline{y}}_2 = \underbrace{\underline{x}^t\,\underline{w}_1\,\underline{t}_1}_{\tilde{\underline{y}}_1} + \underbrace{\underline{x}^t\,\underline{w}_2\,\underline{t}_2}_{\tilde{\underline{\varepsilon}}_1}$$

Se $\quad \underline{w}_2 = \alpha\,\underline{w}_1 + \underline{w}_\perp$

$$\tilde{\underline{y}}_2 = \underline{x}^t\,\underline{w}_1\,\underline{t}_1 + \underline{x}^t\alpha\,\underline{w}_1\,t_2 + \underline{x}^t\,\underline{w}_\perp\,\underline{t}_2$$

$$= \underline{x}^t\,\underline{w}_1\underbrace{(\underline{t}_1 + \alpha\,\underline{t}_2)}_{=\,\underline{t}_1} + \underline{x}^t\,\underline{w}_\perp\,\underline{t}_2$$

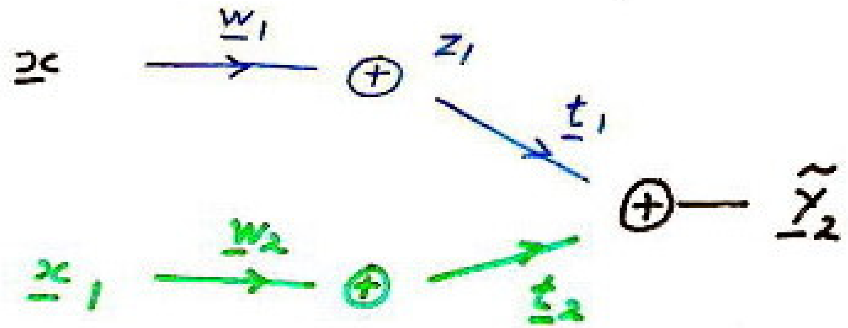
$\therefore \quad \alpha = 0 \qquad \underline{w}_2 = \underline{w}_\perp$

## Garantindo a ortogonalidade

$$\underline{w}_{2\,inicial} = \underline{r} - \underline{r}^t \underline{w}_1 \underline{w}_1$$

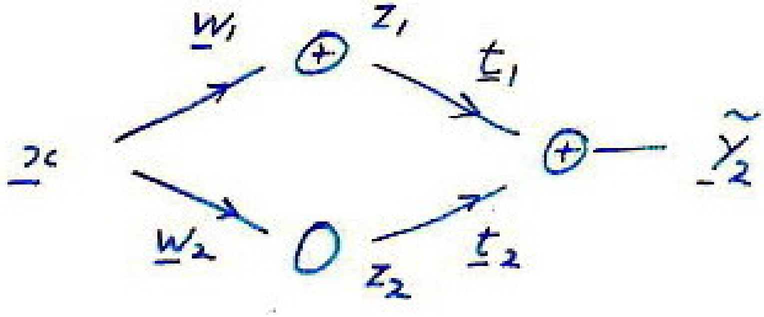
$$\underline{r} = \text{randomico}$$

## Treinamento de $\underline{w}_2$




$$\underline{x}_1 = \underline{x} - \underline{x}^t \underline{w}_1 \underline{w}_1$$

## Operação

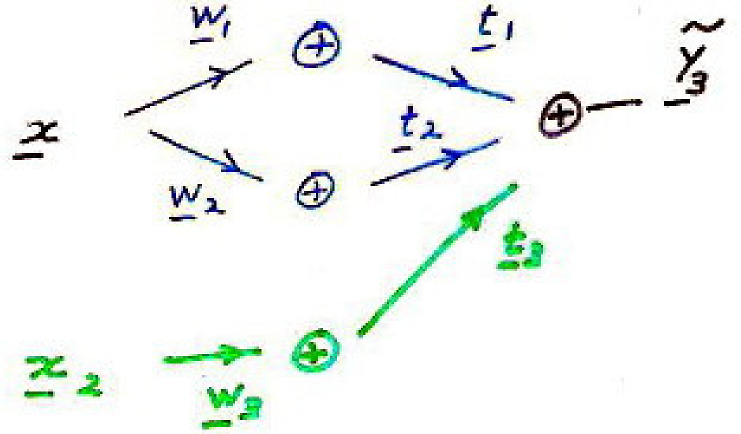


Treinamento de $\underline{w}_3$

$\underline{w}_{3\ inicial} =$

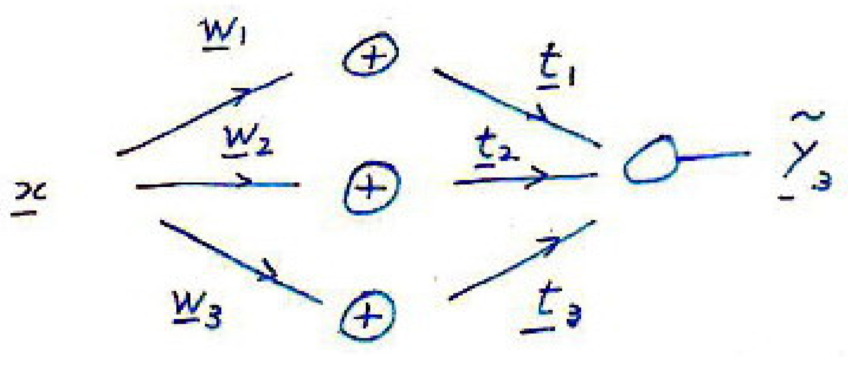
$\underline{r} - \underline{r}^t \underline{w}_1 \underline{w}_1 - \underline{r}^t \underline{w}_2 \underline{w}_2$

Treinamento

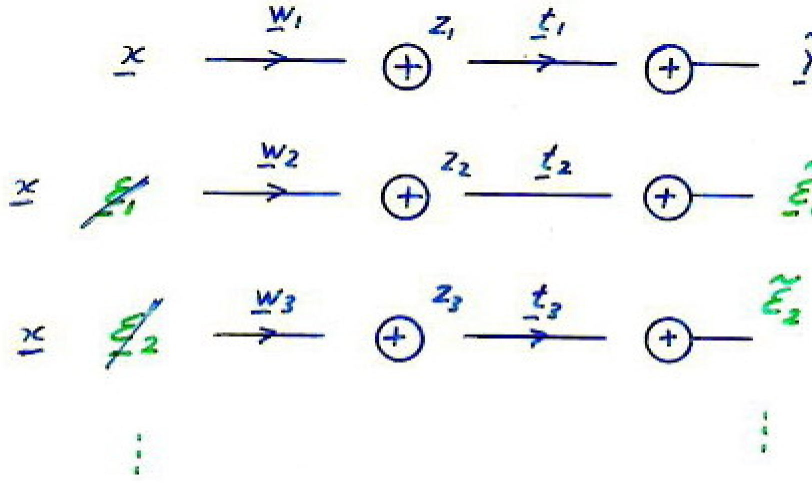



$\underline{x}_2 = \underline{x}_1 - \underline{x}_1^t \underline{w}_2 \underline{w}_2$

Operação



## Treinamento alternativo




$\underline{\varepsilon}_1 = \underline{y} - \tilde{\underline{y}}_1$

$\underline{\varepsilon}_2 = \underline{\varepsilon}_1 - \tilde{\underline{\varepsilon}}_1$

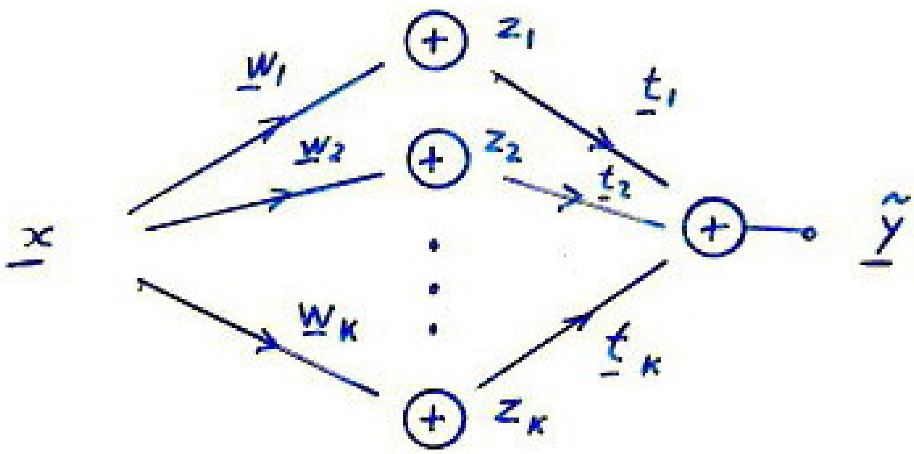
$\underline{\varepsilon}_3 = \underline{\varepsilon}_2 - \tilde{\underline{\varepsilon}}_2$

convergência mais rápida

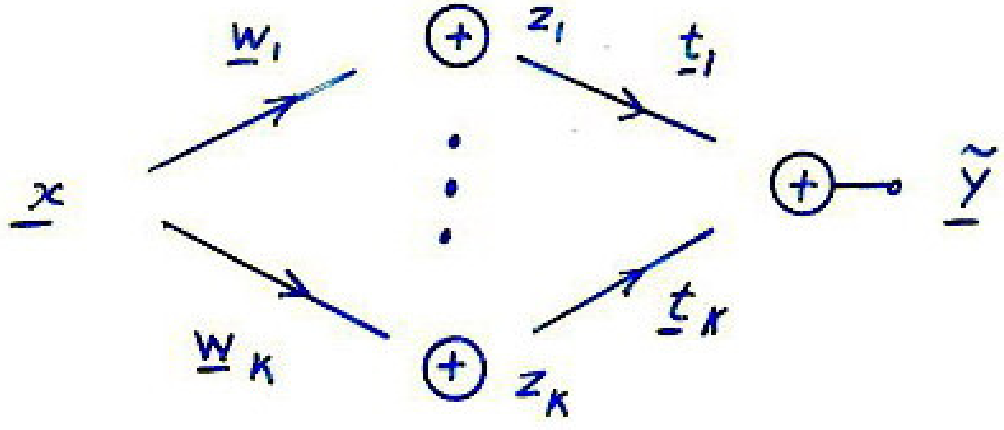
processamento paralelo

## Operação

$$\tilde{\underline{y}} = \tilde{\underline{y}}_K = \tilde{\underline{y}}_1 + \tilde{\underline{\varepsilon}}_1 + \tilde{\underline{\varepsilon}}_2 + \dots + \tilde{\underline{\varepsilon}}_{K-1}$$



# Outro treinamento alternativo




Treinamento simultaneo de todas as sinapses

↳ mais rápido

[$\underline{W}$] é apenas uma base para o espaço das componentes principais.

Compressão da informação

para (auto) reprodução

$$\begin{tikzcd}
\underline{x} \arrow[rr, "L"] \arrow[dr, "L_1"'] & & \underline{x} \\
& \underline{z} \arrow[r, "L_2"'] & \tilde{\underline{x}}
\end{tikzcd}$$

$L$ $\qquad \underline{x} = [I]\, \underline{x}$

$L_1$ $\qquad \underline{z} = [\underline{W}]\, \underline{x}$

$L_2$ $\qquad \tilde{\underline{x}} = [T]\, \underline{z} = [W^{-1}]\, \underline{z}$

Transformada de Karhunen-Loève

Componentes Principais propriamente ditas

Rede: BP auto supervisionada

Outros processos neurais

Oja , Sanger-Oja

Se normalizarmos

$$|\underline{w}_i| = \underline{w}_i^t\,\underline{w}_i = 1 \quad \forall i$$

E como $\underline{w}_i$'s são ortogonais

$$\underline{w}_i^t\,\underline{w}_j = 0 \quad \forall i \neq j$$

[W] é "ortogonal"

$$[W]\,[\underline{W}^t] = [I] \quad \text{ou}$$

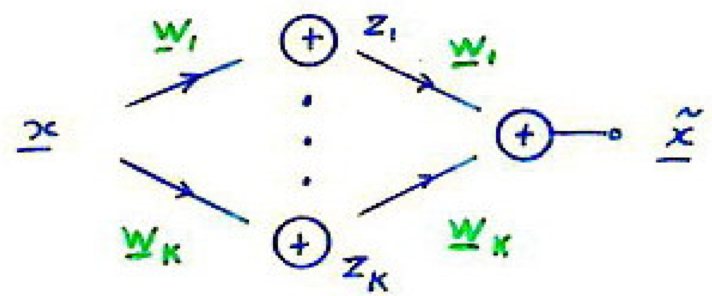
$$[W^{-1}] = [W^t]$$

logo

$$[T] = [W^{-1}] = [W^t]$$

ou

$$\underline{t}_i = \underline{w}_i \quad \forall i$$



Treinamento BP - Regra delta

$$\underline{x} \xrightarrow{\underline{w}} \oplus \, z \xrightarrow{\underline{w}} \oplus \; \tilde{\underline{y}}$$

$$z = \sum_j w_j x_j \qquad \tilde{y}_i = z\, w_i$$

$$\frac{d\tilde{y}_i}{dw_k} = \begin{cases} w_i \dfrac{dz}{dw_k} = w_i\, x_k & i \neq k \\[2ex] z + w_k \dfrac{dz}{dw_k} = z + w_k\, x_k & i = k \end{cases}$$

$$\varepsilon^2 = \sum_i \varepsilon_i^2 = \sum_i (y_i - \tilde{y}_i)^2$$

$$\frac{d\varepsilon^2}{dw_k} = \sum_i 2\,\varepsilon_i \frac{d\varepsilon_i}{dw_k} = -2 \sum_i \varepsilon_i \frac{d\tilde{y}_i}{dw_k} =$$

$$= -2 \left[ \sum_{i \neq k} \varepsilon_i \frac{d\varepsilon_i}{dw_k} + \varepsilon_k \frac{d\varepsilon_k}{dw_k} \right] =$$

$$= -2 \left[ \sum_{i \neq k} \varepsilon_i\, w_i\, x_k + \varepsilon_k \left( z + w_k x_k \right) \right]$$

$$= -2 \left[ \varepsilon_k\, z + x_k \sum_i \varepsilon_i\, w_i \right]$$

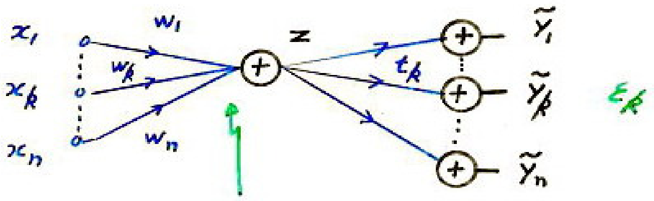
$$\Delta w_k = E \left\{ -\alpha \frac{d\varepsilon^2}{dw_k} \right\} =$$

$$= 2\alpha\, E \left\{ z\, \varepsilon_k + x_k \sum_i \varepsilon_i\, w_i \right\}$$

Obs: $|\underline{W}_{inicial}| = 1$

Obs:

Sinapses independentes




$$\delta = \sum_i \varepsilon_i t_i$$

$$\Delta t_k = 2\alpha \, E\{z \, \varepsilon_k\} \qquad (1)$$

$$\Delta w_k = 2\alpha \, E\{x_k \, \delta\} \qquad (2)$$

Sinapses iguais $\quad t_k = w_k$

$$\Delta w_k = \Delta t_k = 2\alpha \, E\{z \, \varepsilon_k + x_k \, \delta\}$$

(1) + (2)

Obs:

Mapeamento linear

$\Downarrow$

F quadratica

$\hookrightarrow$ treinamento

$\downarrow$

rapido

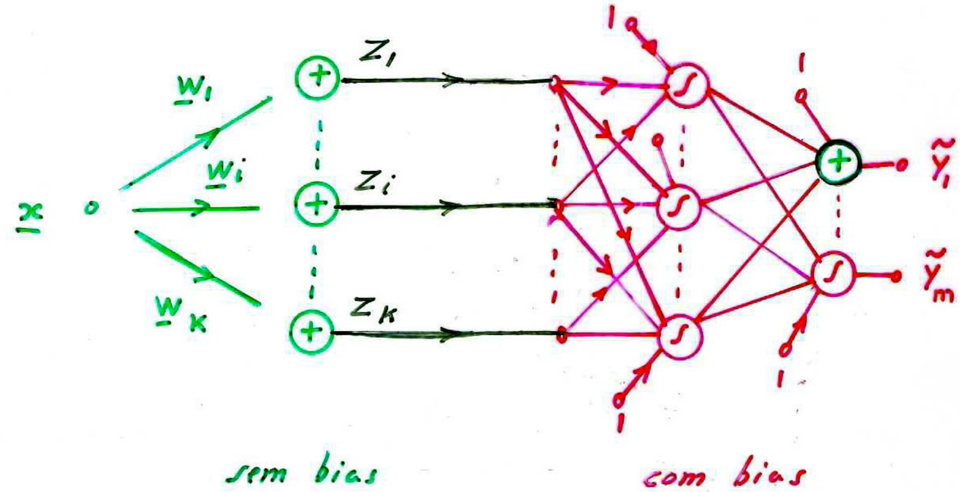
sem minimos locais

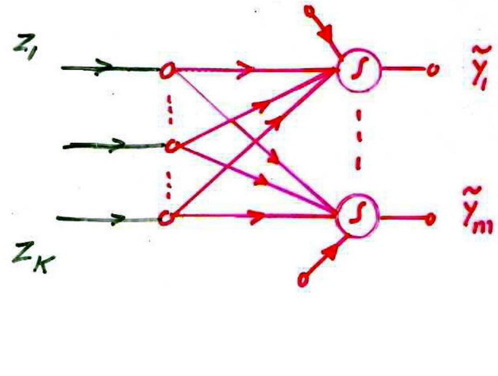
sem overtraining

$\exists$ solução analitica

# Mapeamento não Linear I

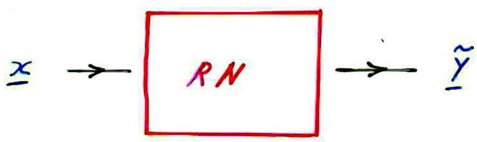
$$\begin{tikzcd} \underline{x} \arrow[rr, "\eta L"] \arrow[dr, "L"'] & & \underline{y} \\ & \underline{z} \arrow[r, "\eta L"'] & \underline{\tilde{y}} \end{tikzcd}$$



Dimensionando a RN

Mapear SEM comprimir




1 - 2 camadas

$Q$ # neurônios camada intermediária

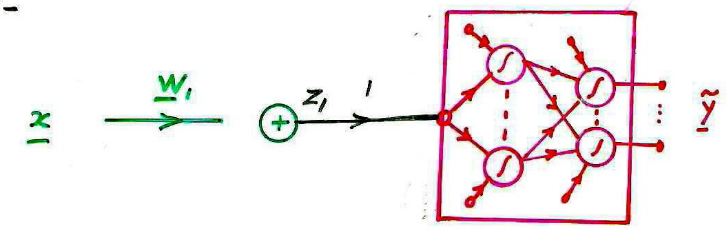
$$\Rightarrow \quad \dim \underline{z} \leq Q$$

1 camada $\Rightarrow \dim \underline{z} \leq \dim \underline{y}$

Componentes para

ATUAÇÃO independente

1-




RN com uma entrada

Treinar todas as sinapses,

$\underline{W}_1$ e RN

normalizar $\underline{W}_1 \longrightarrow \dfrac{\underline{W}_1}{|\underline{W}_1|}$

2 - Segunda Componente

$$\underline{x}_1 = \underline{x} - \underline{x}^t \underline{w}_1 \, \underline{w}_1$$

$$\underline{w}_{2\ inicial} = \underline{r} - \underline{r}^t \underline{w}_1 \, \underline{w}_1$$

retornar ao passo 1 fazendo

$$\underline{x}_1 \longrightarrow \underline{x}$$

$$\underline{w}_2 \longrightarrow \underline{w}_1$$

$$z_2 \longrightarrow z_1$$

3 - Terceira Componente

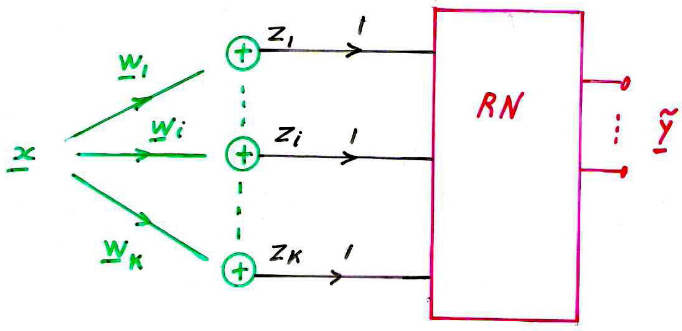
. . .

Rede para ATUAÇÃO conjunta

1- Determinar $\underline{w}_1 , \underline{w}_2 , \ldots , \underline{w}_k$

2 - Treinar RN ,

mantendo $\underline{w}_i$ congelados



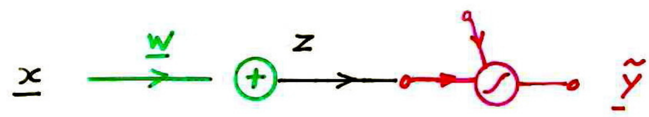

Componentes calculadas para

ATUAÇÃO independente

Usadas em ATUAÇÃO conjunt

Um caso particular:

o classificador linear




CDA - Canonical discrimination analisys

Discriminador linear ótimo

Discriminador de Fischer

Componentes para ATUAÇÃO conjunta ou cooperativa

1 - Passo igual ao treinamento para componentes com atuação independente.

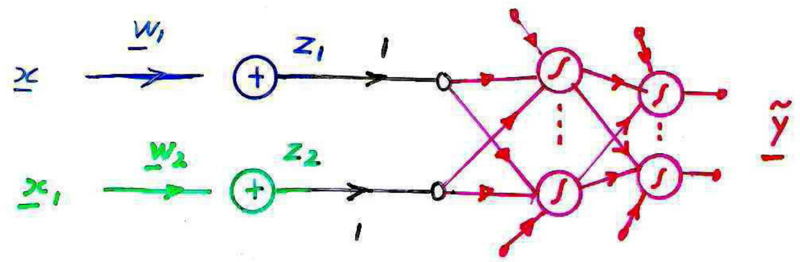
2 - Congelar $\underline{w}_1$ $\quad |\underline{w}_1| = 1$

Acrescentar $\underline{w}_2$ para gerar $z_2$

Acrescentar uma entrada à RN

Treinar $\underline{w}_2$ e TODA a RN

(inclusive as sinapses conectadas a $z_1$)




$$\underline{x}_1 = \underline{x} - \underbrace{\underline{x}^t\,\underline{w}_1}_{z_1}\,\underline{w}_1$$

$$\underline{w}_{2\,inicial} = \underline{r} - \underline{r}^t\,\underline{w}_1\,\underline{w}_1$$

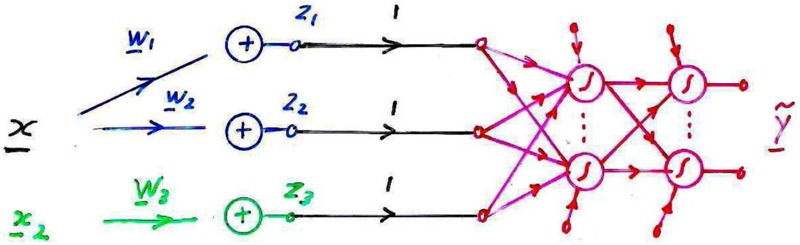
3 - Congelar $\underline{w}_1$ e $\underline{w}_2$ $\quad |\underline{w}_2| = 1$

Acrescentar $\underline{w}_3$ para gerar $z_3$

Acrescentar uma entrada a RN

Treinar $\underline{w}_3$ e TODA a RN

(inclusive as sinapses conectadas a $z_1$ e $z_2$)



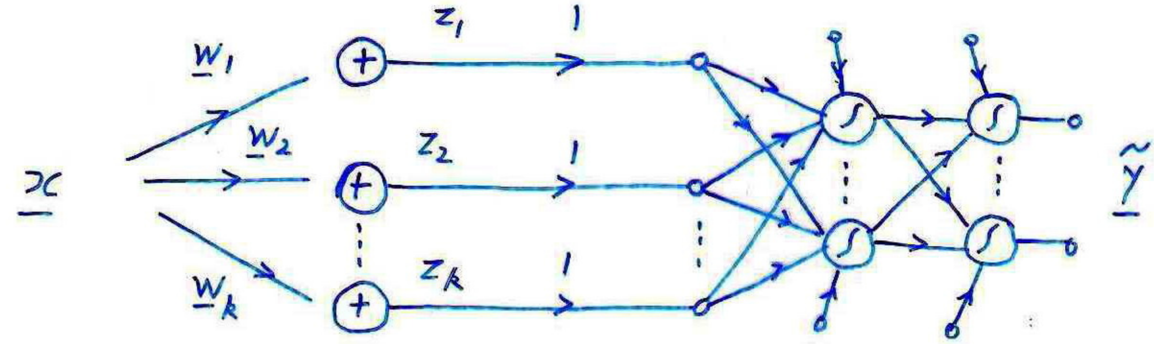

$$\underline{x}_2 = \underline{x}_1 - \underline{x}_1^t\,\underline{w}_1\,\underline{w}_1$$

$$\underline{w}_{3\,inicial} = \underline{r} - \underline{r}^t\,\underline{w}_1\,\underline{w}_1 - \underline{r}^t\,\underline{w}_2\,\underline{w}_2$$

Obs: dim $z$ $\leq$

\# neuronios camada intermediaria

Operação: Última rede treinada




# Mapeamento não Linear II

$$
\begin{tikzcd}
\underline{x} \arrow[rr, "nL"] \arrow[dr, "nL"'] & & \underline{y} \\
& \underline{z} \arrow[r, "L"'] & \tilde{\underline{y}}
\end{tikzcd}
$$

1 - Comprimir $\underline{Y}$

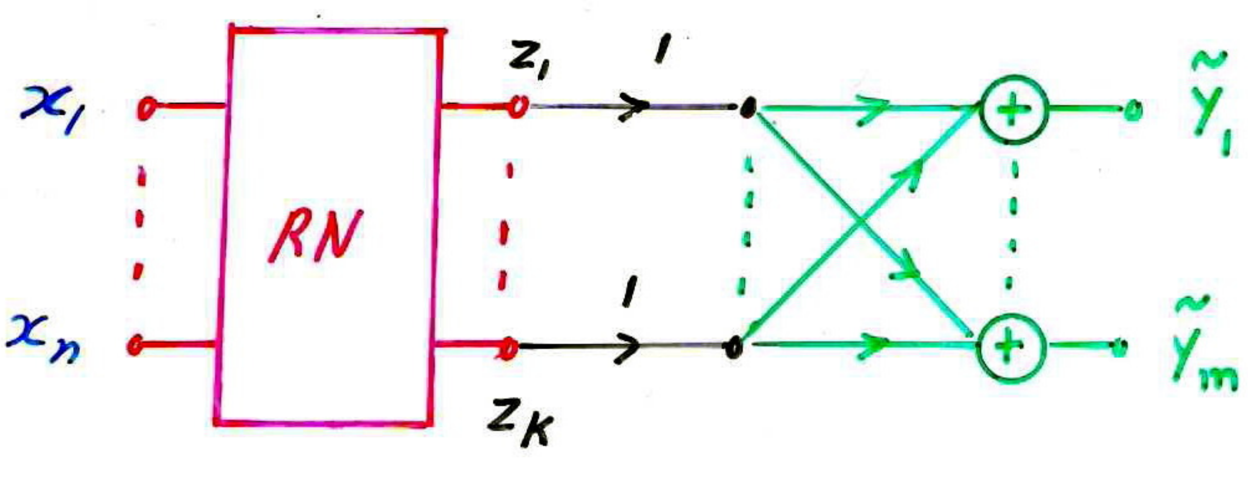
$$\underline{Y} \xrightarrow[\underline{W}]{} \underline{Z} \xrightarrow[\underline{W}^t]{} \underline{\tilde{Y}}$$

$$\underline{Z} = \underline{W}\,\underline{Y} \qquad \underline{\tilde{Y}} = \underline{W}^t\,\underline{Z}$$

2 - Realizar o mapeamento

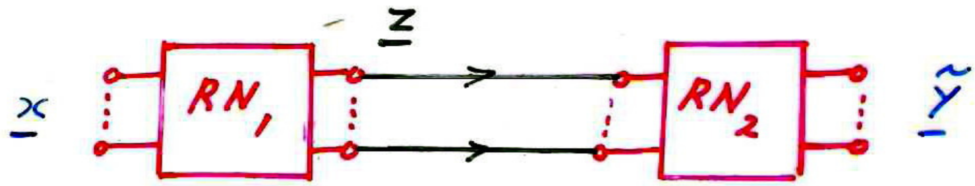
$\underline{Z} = \varphi(\underline{x})$ via RN

3 - Rede final



# Mapeamento não Linear III

$$
\begin{tikzcd}
\underline{x} \arrow[rr, "L \text{ ou } \eta L"] \arrow[dr, "\eta L"'] & & \underline{y} \\
& \underline{z} \arrow[r, "\eta L"'] & \underline{\tilde{y}}
\end{tikzcd}
$$




Como RN são mapeadores universais

$\Downarrow$

teóricamente $\dim \underline{z} = 1$

satisfaz !

# Resumo:

Neste mini-curso discutimos

- A generalização do conceito de componentes principais (PCA) para compressão da informação da entrada $\underline{x}$ ou da saída $\underline{y}$ de um mapeamento qualquer $\underline{x}: \rightarrow \underline{y}$ , linear ou não linear, objetivando minimizar o erro na saída.

- Os métodos de compressão utilizados no processo empregam redes neurais feedforward com aprendizado supervisionado tipo retropropagação do erro.

- Nos casos de mapeamentos não lineares, a não linearidade pode ser introduzida no mapeamento de compressão ou de reconstrução da informação.

- A base (linear) gerada para compressão e/ou reconstrução da informação pode ser ortonormal