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STOCHASTIC PROCESSES & OTIMIZATION IN MACHINE LEARNING

Unsupervised Learning

K-Means Clustering

Principal Component Analysis (PCA)

Autoencoders

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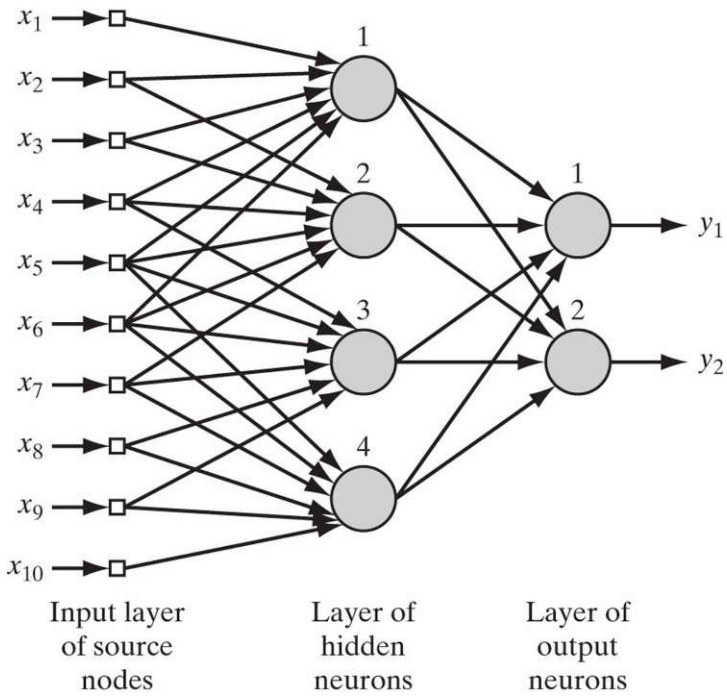
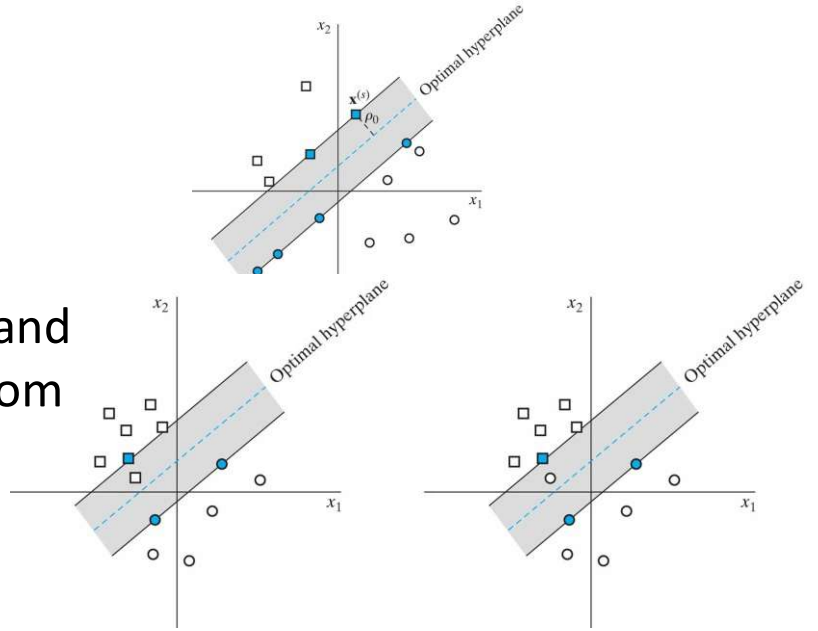
STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Some Special Neural Network Configurations - Supervised Learning

Convolutional Neural Networks (CNN): *Multilayer Perceptron* category preferred for classification of two-dimensional examples (e.g. *pattern recognition* of images) via *supervised learning*. The CNN simplification results by decoupling the net into loosely connected parts with common *receptive fields* among subsets of input element features and exhibiting *convolutional induced local fields*



Support Vector Machines (SVM): Binary classification into regions of maximum linear separation via *supervised learning*. Regions are separated by linear *neutral border zones* as wide as possible, defined by *support vectors* as shown in the two-dimensional adjacent figure. Sample elements belong in two classes, depicted as blue squares and circles. In case of *non-separable patterns*, regions result from the training sample that minimize classification errors



STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Some Special Neural Network Configurations – Unsupervised Learning & LLM

K- Means Clustering: Self-organization of observed sample elements $\mathbf{x}_i$ into K *clusters* via *unsupervised learning*, e.g. clustering based on proximity of Euclidean Distances $\|\mathbf{x}_i - \mathbf{x}_j\|^2$

Principal Components Analysis (PCA): *Unsupervised learning* used to map sample vectors of high dimensionality, e.g. images, $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ into output vectors $\mathbf{y} = [y_1\ y_2\ \dots\ y_l]^{\mathrm{T}}$ of $l \ll m$ *Principal Components* by selecting the most important features (*feature engineering*). Used to overcome the *curse of dimensionality* for image reconstruction, pattern classification…

Self-Organizing Maps (SOM): Neurons are placed on vertices of a two-dimensional *lattice* and converge into maps of location-based significant traits (features) via *competitive unsupervised learning*. Identification of *active neurons* is learned by boosting or attenuating weights of paths between neurons in the lattice, aiming at the final winner selection (*winner takes all*)

Large Language Models (LLM): Used to identify missing words (*masked tokens*) or sentences, generate (via *GenAI*) answers to *chatbot* and/or *search engine* queries, *translate* to alternate natural languages… They employ *Natural Language Processing* (*NLP*) algorithms (e.g. *Attention Mechanism* based *Transformers*), may rely on special hardware (e.g. *GPUs*) and can require extensive *pre-training* in massive datacenters (possibly months of parameter tuning with billions of data elements). Offered (free or for-a-fee) to tens of millions of end-users as a *cloud service* via the Web, usually with a *reasoning* option. Users may upload reduced models in their machines (e.g. laptops). Very recent killer applications: *ChatGPT* (OpenAI), *DeepSeek.* Risks include prediction errors - hallucinations, IPR infringement, plagiarism, excessive reliance to black-box *Artificial Intelligence* methods…

Tutorial by *Mirella Lapata* https://www.youtube.com/watch?v=_6R7Ym6Vy_I&t=1894s

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Unsupervised Learning

- Unsupervised learning is based on estimating *a-priori* probabilities $p(\mathbf{x})$ of *sample elements* (vectors) $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ with m *features* x_i (e.g. *K-Means Clustering* – selection of K *centers of gravity* or *cluster centroids* and assignment of vectors $\mathbf{x}$ into closest centroids)
- It is based on input *feature* statistics estimated from *unlabeled training examples* and assumptions of the environment behavior (e.g. *Hebb's* rule). The system assigns an output $y = h_{\mathbf{w}}(\mathbf{x})$ (e.g. compressed image or class of $\mathbf{x}$) consistent with models inferred from user requirements and conforming to pre-stored experience
- Apart from *training* & *validation examples* used to design the system, *test* data are normally added to assess a trained model $h_{\mathbf{w}}(\cdot)$ *generalization* capability and overfitting risk
- Unsupervised learning is a widely employed method of self organization (e.g. *Self-Organizing Maps* - *SOM*, *Autoencoders*) and of *principal component filtering* for efficient storage - processing – classification of *sample vectors* with massive number of features (typical in *speech - text - image processing* applications and *pattern recognition* models

Note: Definition of Sample, Sample Elements & Sample Space in Statistics
A *sample* is defined as a subset of a superset, referred to as *sample space*, that approximately exhibits its statistical properties. It consists of N *sample elements* (examples), typically vectors $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ with coordinates x_i encoding the m *features* (characteristics) of $\mathbf{x}$

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

K- Means Clustering via Unsupervised Learning

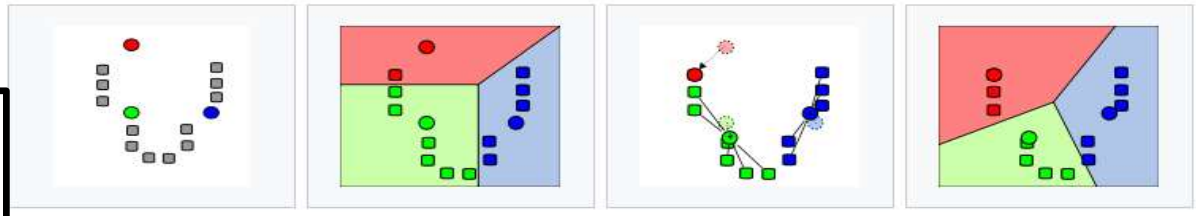
Encoding into K ***clusters*** of N ***unlabeled training*** examples $\mathbf{x}(n) = [x_1(n)\ x_2(n)\ \dots\ x_m(n)]^{\mathrm{T}}$

- **Determination** of ***Encoder*** $C(n) = j$: $\mathbf{x}(n),\ n = 1,2,\dots,N$ belongs to ***cluster*** $j = 1,2,\dots,K$
- **Symmetric Measure of Similarity**: $d(\mathbf{x}(n), \mathbf{x}(n')) = d(\mathbf{x}(n'), \mathbf{x}(n))$
  Example: Euclidean Distance, $d(\mathbf{x}(n), \mathbf{x}(n')) \triangleq \|\mathbf{x}(n) - \mathbf{x}(n')\|^2$
- **Estimation of centroid** $\hat{\boldsymbol{\mu}}_j$ as ***center of gravity*** of ***cluster*** $j = 1,2,\dots,K$: Mean ***Euclidean Distance*** of $\mathbf{x}(i)$ from $\hat{\boldsymbol{\mu}}_j$ for all encoder options $C(n) = j$
- **Cost**: $J(C) = \frac{1}{2}\sum_{j=1}^{K}\sum_{C(n)=j}\sum_{C(n')=j}\|\mathbf{x}(n) - \mathbf{x}(n')\|^2 = \sum_{j=1}^{K}\sum_{C(n)=j}\left\|\mathbf{x}(n) - \hat{\boldsymbol{\mu}}_j\right\|^2$
- **Minimization Criterion**: Variance $\hat{\boldsymbol{\sigma}}_j^2 \triangleq \sum_{C(n)=j}\left\|\mathbf{x}(n) - \hat{\boldsymbol{\mu}}_j\right\|^2,\ \min_C J(C) = \min_C \sum_{j=1}^{K}\hat{\boldsymbol{\sigma}}_j^2$

Self-Organization of N Training Sample Points into K Clusters

- Initialization: Arbitrary selection of hyperparameter K
- Assign the N training sample points $\mathbf{x}(n)$ to the ***closest centroid***
- Update ***centroid selection*** $\hat{\boldsymbol{\mu}}_j, j = 1,2,\dots,K$ & re-evaluate assignment of encoders $C(n) = j$
- Efficient & easy to code algorithm but ***with no formal convergence proof***
- The choice of K may involve several ***trials*** and ***variance*** comparisons by increasing K up to knee of the minimum cost

Example: $K = 3,\ N = 12$
(https://en.wikipedia.org/wiki/K-means_clustering)



Initialize Centroids | Initial Cluster Formation | Determination of New *Centroids* | Next Cluster Formation

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Principal Components Analysis - PCA

The Curse of Dimensionality:

In a *sample space* of vectors $\mathbf{x} = [x_1\ x_2 \dots\ x_m]^{\mathrm{T}}$, encoding of features (categorical or continuous) may lead to a large number of dimensions m (e.g. number of *pixels* in an image)

Rule of Thumb: For statistically meaningful encoding of the m features, it is empirically required a number of N sample vectors that is a multiple of m

(e.g. $N \gg 5m$, https://en.wikipedia.org/wiki/Curse_of_dimensionality)

Reduction of Dimensionality - Principal Components:

A vector space of $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ the m coordinates can be mapped into orthogonal (uncorrelated) *Principal Components*, ordered by their significance. The next step is to truncate insignificant components and obtain an output vector $\mathbf{y} = [y_1\ y_2 \dots\ y_l]^{\mathrm{T}}$ by selecting the $l \ll m$ principal features

Methods for Selecting Principal Components:

- The **Covariance Method**: Statistical analysis of the *training sample space*, linear transformation of its m coordinates using an *orthonormal* basis and selecting the $l \ll m$ principals via *Linear Algebra* methods (similar to the *Karhunen - Loève Expansion* with orthogonal deterministic basis functions in *Time-Series Theory* https://en.wikipedia.org/wiki/Kosambi%E2%80%93Karhunen%E2%80%93Lo%C3%A8ve_theorem)
- The **Hebbian Learning Method**: Via self-organized *Neural Network* models with *Hebbian* local tuning in *unsupervised learning*

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Orthonormal Transformation to Principal Components (1/3)

Covariance Method - Definitions

- **Input**: *Sample elements* (vectors) $\mathbf{x} = [x_1\ x_2 \dots\ x_m]^{\mathrm{T}}$ of m *features* encoded in x_i values
- **Coordinates** x_i: *Sample Values* of *Random Variables* X_i, the coordinates of random vectors $\mathbf{X} = [X_1\ X_2 \dots\ X_m]^{\mathrm{T}}$ of the training sample space. We assume that $\mathrm{E}[\mathbf{X}] = \mathrm{E}[X_i] = 0$
- **Correlation Matrix:** The symmetric matrix $(m \times m)$ $\mathbf{R} = \mathrm{E}[\mathbf{X}\,\mathbf{X}^{\mathrm{T}}]$ with elements $\mathrm{E}[x_i\ x_j]$, *eignevectors* $\mathbf{q}_j$ and *eigenvalues* λ_j: $\mathbf{R}\mathbf{q}_j = \lambda_j \mathbf{q}_j,\ \ j = 1,2, \dots, m$ in decreasing order of λ_j

$$\lambda_j \mathbf{q}_j^{\mathrm{T}} \mathbf{q}_k = \begin{cases} 1, & k = j \\ 0, & k \neq j \end{cases} \quad \text{and} \quad \mathbf{q}_j^{\mathrm{T}} \mathbf{R} \mathbf{q}_k = \begin{cases} \lambda_j, & k = j \\ 0, & k \neq j \end{cases}$$

- **Principal Components:** The eigenvectors $\mathbf{q}_j$ define *Orthonormal Principal* directions that via linear transformation map a random vector $\mathbf{x} = [x_1\ x_2 \dots\ x_m]^{\mathrm{T}}$ of m coordinates x_i into the random vector $\mathbf{a} = [a_1\ \alpha_2 \dots\ \alpha_m]^{\mathrm{T}} = [\mathbf{x}^{\mathrm{T}}\mathbf{q}_1\ \ \mathbf{x}^{\mathrm{T}}\mathbf{q}_2\ \dots\ \mathbf{x}^{\mathrm{T}}\mathbf{q}_m]$ of m coordinates a_i referred to as *Principal Components*
  - ✓ The order of α_j's follows the decreasing order of $\lambda_j = \mathbf{q}_j^{\mathrm{T}} \mathbf{R} \mathbf{q}_j = var(A_j) \triangleq \sigma_j^2$, with A_j a random variable with sample value α_j
  - ✓ The original coordinates x_i are uniquely deduced from the *Principal Components*:

$$\mathbf{x} = \sum_{j=1}^{m} a_j \mathbf{q}_j$$

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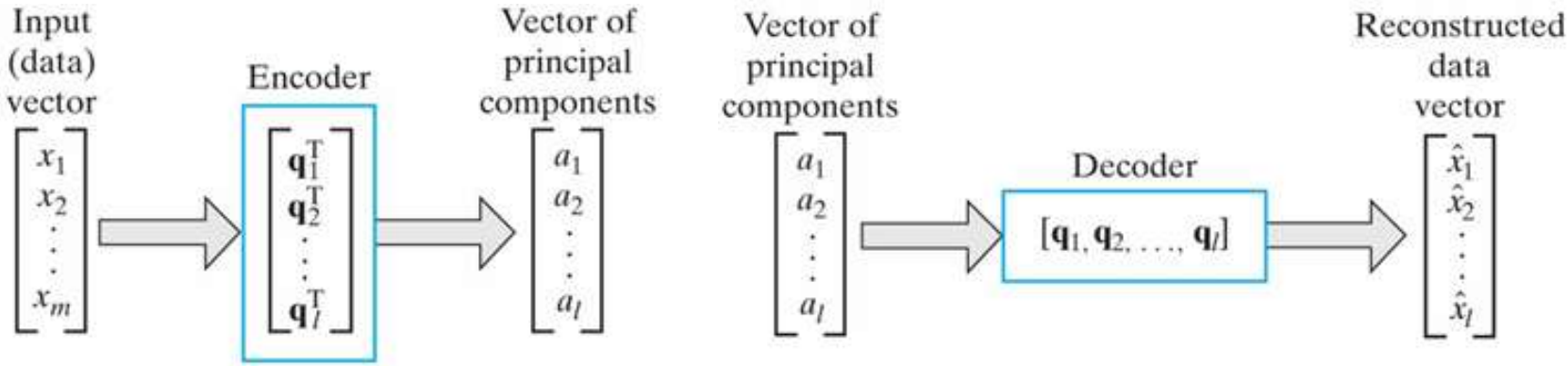
Orthonormal Transformation to Principal Components (2/3)

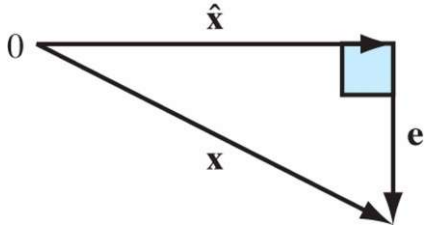
By ignoring *principal components* with smaller variances $\sigma_j^2 = \lambda_j,\ j = l+1, l+2, \ldots, m$ we can approximate (encode) vector $\mathbf{x}$ with $\hat{\mathbf{x}}$ of reduced dimensionality $l < m$

$$\hat{\mathbf{x}} = [\hat{x}_1\ \hat{x}_2\ \ldots\ \hat{x}_l] = [\mathbf{q}_1\ \mathbf{q}_2\ \ldots \mathbf{q}_l][a_1\ a_2\ \ldots\ a_l]^{\mathrm{T}} = \sum_{j=1}^{l} a_j \mathbf{q}_j \text{ for } l < m$$



The error $\mathbf{e} = \mathbf{x} - \hat{\mathbf{x}} = \sum_{i=l+1}^{m} a_i \mathbf{q}_i$ is orthogonal to $\hat{\mathbf{x}}$:

$$\mathbf{e}^{\mathrm{T}}\hat{\mathbf{x}} = \sum_{i=l+1}^{m} a_i\, \mathbf{q}_j^T \sum_{j=1}^{l} a_j \mathbf{q}_j = 0$$



- The total variance of the m *independent* random variables εX_j is $\sum_{j=1}^{m} \sigma_j^2 = \sum_{j=1}^{m} \lambda_j$
- The total variance of the l *Principal Components* A_j is $\sum_{j=1}^{l} \sigma_j^2 = \sum_{j=1}^{l} \lambda_j$

$\Rightarrow$ The total variance of the error $\mathbf{e} = \mathbf{x} - \hat{\mathbf{x}}$ is $\lambda_{l+1} + \lambda_{l+2} + \cdots + \lambda_m$ (the principal components with the smaller variances)

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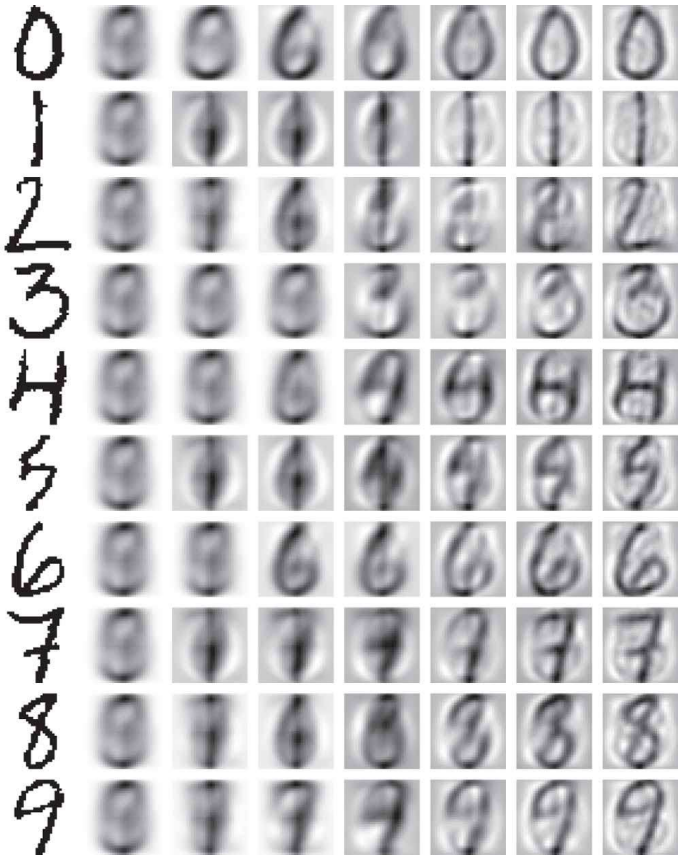
Orthonormal Transformation to Principal Components (3/3)

Application of PCA for Image Compression & Pattern Recognition of Handwritten Numbers



Training Sample:
Scanned images of handwritten numbers $\{0,1,\dots,9\}$
$N = 1700$ elements/number
$m = 32 \times 32 = 1024$ pixels/image (features)

Column 1: Encoding with m binary digits (black or white/pixel)
Column 2: Sample averages for normalization

Evaluation of $l = 64$ principal eigenvectors of the $m \times m = (1024) \times (1024)$ correlation matrix after normalization (subtraction of sample averages)

Reconstruction of Images with $l \leq 64$ Principal Components

$$l \ll m = 32 \times 32 = 1024$$

Column 3: $l = 1$
Column 4: $l = 5$
Column 5: $l = 16$
Column 6: $l = 32$ (acceptable identification of numbers)
Column 7: $l = 64$ (perfect reproducibility under significant compression, $1024 \rightarrow 64$)

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Hebbian Learning of 1st Principal Component (1/2)

Self-Organized Feature Analysis

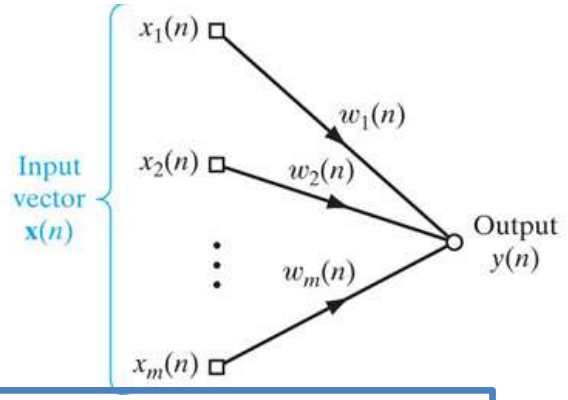
Rule of Hebb: If signals (states) in the borders of a neural synapsis i are *synchronously updated* in step n, the synaptic weight $w_i(n)$ increase. Else it tends to zero (inspired from *neuropsychology learning* context)

Competition Principle: The most active synapses tend to eliminate weak ones

Hebbian-based Maximum Eigenfilter

Linear Neural Network:

$$y(n) = v(n) = \sum_{i=1}^{m} w_i(n)x_i(n) \text{ at step } n$$



Hebbian Learning:

Weights increase at step $n \to n+1 \leq N$ if $y(n)x_i(n) > 0$

$$w_i(n+1) = w_i(n) + \eta y(n)x_i(n),\ i = 1,2,\dots,m,\ \eta \textit{ learning-rate hyperparameter}$$

To enforce stabilization (avoid unlimited growth) in every step (based on the **Competition Principle**) we normalize by summing over all synapses associated with the neuron:

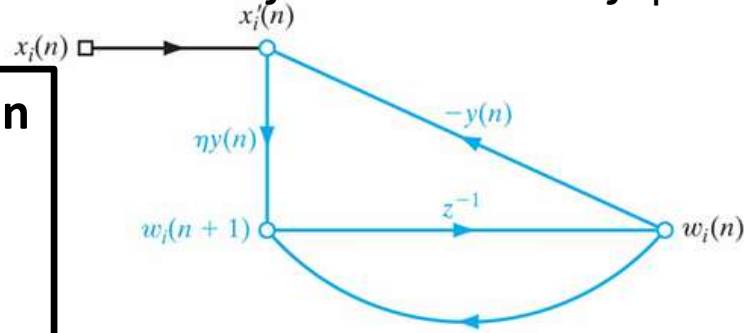
$$w_i(n+1) = \frac{w_i(n) + \eta y(n)x_i(n)}{\left(\sum_{k=1}^{m}[w_k(n) + \eta y(n)x_k(n)]^2\right)^{1/2}} \cong w_i(n) + \eta y(n)[x_i(n) - y(n)w_i(n)]$$

the approximation is valid for small values of η

Signal-flow Graph of Maximum Eigenfilter with Normalization

Positive feedback $y(n)x_i(n)$ is countered by $y(n)w_i(n)$

$$w_i(n+1) = w_i(n) + \eta y(n)x_i'(n),$$
$$x_i'(n) = x_i(n) - y(n)w_i(n)$$



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Hebbian Learning of 1st Principal Component (2/2)

Convergence Issues of Self-Organized Algorithm

Definitions of Vectors

$\mathbf{x}(n) = [x_1(n)\ x_2(n)\ \ldots\ x_m(n)]^{\mathrm{T}}$

$\mathbf{w}(n) = [w_1(n)\ w_2(n)\ \ldots\ w_m(n)]^{\mathrm{T}}$

Unsupervised Learning via Self-Organization Algorithm:

$$y(n) = \mathbf{w}^{\mathrm{T}}(n)\mathbf{x}(n),\ \mathbf{w}(n+1) = \mathbf{w}(n) + \eta y(n)[\mathbf{x}(n) - y(n)\mathbf{w}(n)] \Rightarrow$$

$$\mathbf{w}(n+1) = \mathbf{w}(n) + \eta[\mathbf{x}(n)\mathbf{x}^{\mathrm{T}}(n)\mathbf{w}(n) - \mathbf{w}^{\mathrm{T}}(n)(\mathbf{x}(n)\mathbf{x}^{\mathrm{T}}(n))\mathbf{w}(n)\mathbf{w}(n)]$$

- Factors $\mathbf{x}(n)\mathbf{x}^{\mathrm{T}}(n)$ represent the *Correlation Matrix* $\mathbf{R} = \mathrm{E}[\mathbf{X}\,\mathbf{X}^{\mathrm{T}}]$ at training iteration step $n \to n+1 \leq N$ without mean values. It leads to convergence properties of the algorithm using non-linear stochastic difference equations (*beyond the scope of the lectures*)

- There is no external influence to the self-organized unsupervised learning algorithm, except the a-priori setting of the training *hyperparameter* η

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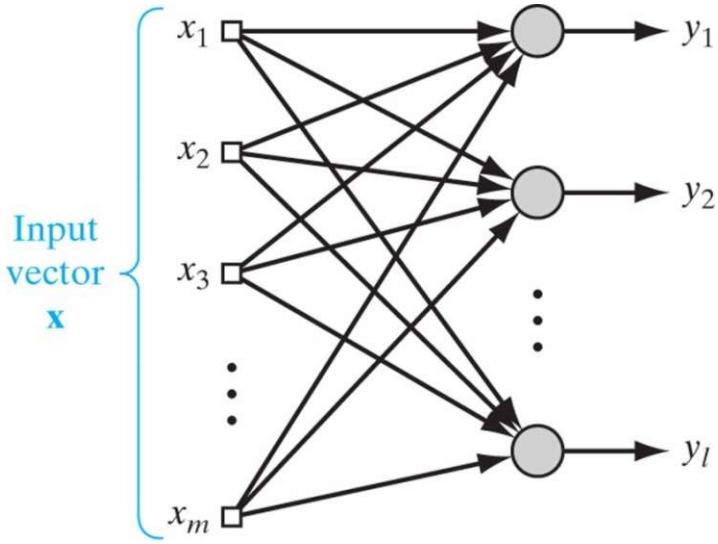
Generalized Hebbian-based Principal-Component Analysis (1/3)

Generalization of Hebbian-based Maximum Eigenfilter:

Linear Feedforward Single Layer Neural Network of l output neurons associated with the most important Principal Components of input sample vectors of dimensionality m, $l < m$

$$y_j(n) = v_j(n) = \sum_{i=1}^{m} w_{ji}(n)x_i(n), \qquad j = 1,2,\dots,l$$



Hebbian Learning: Weights $w_{ji}(n)$ from input $x_i(n)$, $i = 1,2,\dots,m$ to the *Principal Component* $y_j(n)$, $j = 1,2,\dots,l$ change by $\Delta w_{ji}(n)$ in iteration $n \to n+1$

$$\Delta w_{ji}(n) = \eta\left[y_j(n)x_i(n) - y_j(n)\sum_{k=1}^{j} w_{ki}(n)y_k(n)\right], j = 1,2,\dots,l \;\&\; i = 1,2,\dots,m$$

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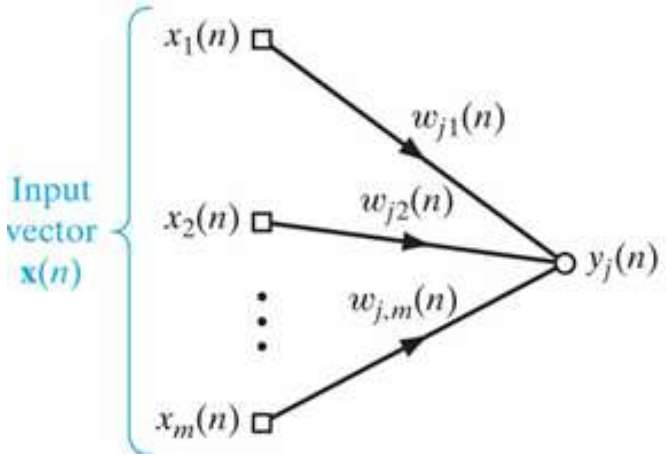
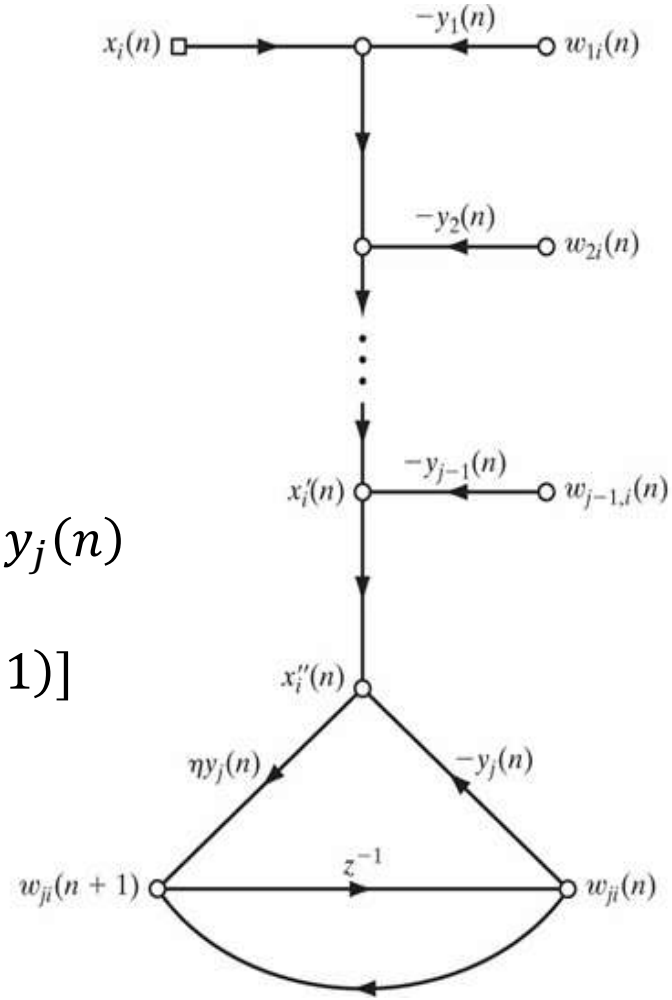
Generalized Hebbian-based Principal-Component Analysis (2/3)

Generalized Hebbian Algorithm (GHA)

$$\Delta w_{ji}(n) = \eta y_j(n)\left[x_i'(n) - w_{ji}(n)y_j(n)\right], \qquad j = 1,2,\dots,l \text{ και } i = 1,2,\dots,m$$

$$x_i'(n) = x_i(n) - \sum_{k=1}^{j-1} w_{ki}(n)y_k(n)$$





$\Delta w_{ji}(n) = \eta y_j(n)x_i''(n)$ όπου $x_i''(n) = x_i'(n) - w_{ji}(n)y_j(n)$

$w_{ji}(n+1) = w_{ji}(n) + \Delta w_{ji}(n)$, $w_{ji}(n) = z^{-1}[w_{ji}(n+1)]$

Vector Form of GHA:

$\Delta \mathbf{w}_j(n) = \eta y_j(n)\mathbf{x}_i'(n) - \eta y_j^2(n)\mathbf{w}_j(n), j = 1,2,\dots,l$

where $\mathbf{x}'(n) = \mathbf{x}(n) - \sum_{k=1}^{j-1} \mathbf{w}_k(n)y_k(n)$

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Generalized Hebbian-based Principal-Component Analysis (3/3)

$$\mathbf{x}'(n) = \mathbf{x}(n) - \sum_{k=1}^{j-1} \mathbf{w}_k(n) y_k(n), \qquad j = 1,2,\ldots,l$$

For $j = 1$: $\mathbf{x}'(n) = \mathbf{x}(n)$

Evaluation of 1st *Principal Component* $y_1(n)$

For $j = 2$: $\mathbf{x}'(n) = \mathbf{x}(n) - \mathbf{w}_1(n) y_1(n)$

Evaluation of 2nd *Principal Component* $y_2(n)$ as 1st component after subtracting $y_1(n)$

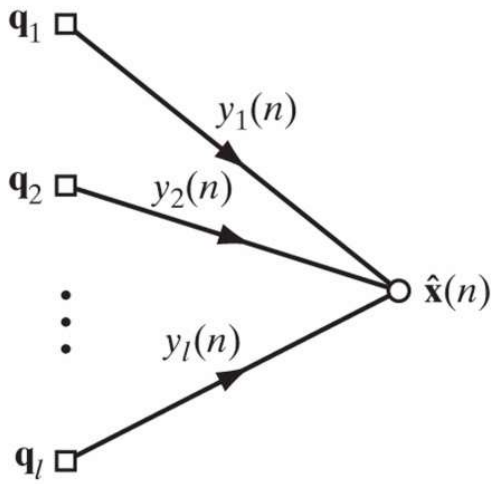
For $j = 3$: $\mathbf{x}'(n) = \mathbf{x}(n) - \mathbf{w}_1(n) y_1(n) - \mathbf{w}_2(n) y_2(n)$

Evaluation of 3rd *Principal Component* $y_3(n)$ as 1st component after subtracting $y_1(n)$ and $y_2(n)$

.....

The l most significant *Principal Components* correspond to the eigenvectors $\mathbf{q}_k$ of the *Correlation Matrix* $\mathbf{R} = \mathrm{E}[\mathbf{X}\mathbf{X}^{\mathrm{T}}]$, $k = 1,2,\ldots,l$ oredered by decreasing order of eigenvalues $\lambda_1 > \lambda_2 > \cdots > \lambda_l$ and provide the estimate $\hat{\mathbf{x}}(n)$ of input sample element $\mathbf{x}(n)$ of $m > l$ characteristics

$$\hat{\mathbf{x}}(n) = \sum_{k=1}^{l} y_k(n) \mathbf{q}_k \quad \text{για} \quad l < m$$



STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Generalized Hebbian Algorithm (GHA): Image Coding Example (1/2)

- **Training Sample**: 2000 scanned pictures of **Lena** 256×256 pixels, 256 gray levels as in the **1st *Original Image***
- **Training Sample Elements**: Images segmented to 1024 non-overlapping ***Blocks*** of size 8×8 pixels: $m = 64$ features/block
- Every block corresponds to sample input vector of m features (pixels) encoded into 256 gray levels (8 bits/pixel):

$$\mathbf{x}(n) = [x_1(n)\ x_2(n)\ \dots\ x_m(n)]^{\mathrm{T}} \qquad n = 1,2,\dots,N$$

- The sample vectors are fed into a ***Linear Feedforward Network*** with $l = 8$ outputs
- The $m \times l = 64 \times 8$ synaptic weights $w_{ji}(n)$ converge to 8 ***Significant Principal Components*** at its output nodes:

$$y_j(n) = \sum_{i=1}^{m} w_{ji}(n)x_i(n), \qquad j = 1,2,\dots,l$$

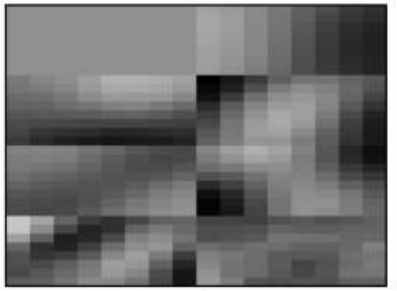
- The ***Learning Rate***) is set to $\eta = 10^{-4}$
- The ***weights*** after convergence are depicted in the **2nd *Image*** with $4 \times 2 = 8$ regions (***masks***), 64 segments/mask, total $64 \times 8 = 1024$ segments representing the contribution of 64 features of the sample input to the 8 outputs. White color signifies positive contribution, black negative and gray no contribution
- The **3rd *Image*** is a reconstruction of the ***Original*** using only $l = 8$ most significant ***Principal Components***

$$\hat{\mathbf{x}}(n) = \sum_{k=1}^{l} y_k(n)\mathbf{q}_k\,, \quad \mathbf{q}_k = \lim_{n} \mathbf{w}_k(n)\,, \qquad \mathbf{w}_k(n) = [w_{k1}(n)\ w_{k2}(n)\ \dots\ w_{km}(n)]^{\mathrm{T}}$$

- The **4th *Image*** is a compressed version of the **3rd *Image*** with quantized values according to the logarithm of the 8 output variances (***final compression*** $11:1$)

Original Image

Weights



Using First 8 Components

11 to 1 compression

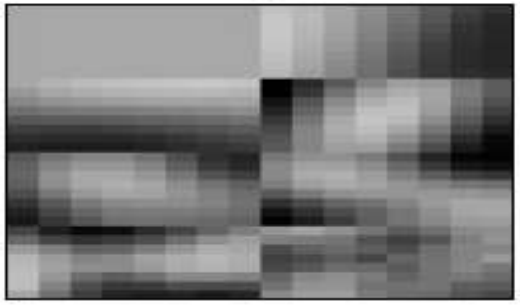
STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Generalized Hebbian Algorithm (GHA): Image Coding Example (2/2)

Original Image (Peppers): 256×256 pixels (features), 256 gray levels

Original Image

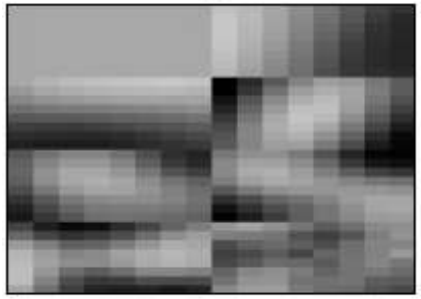
Weights



Using First 8 Components

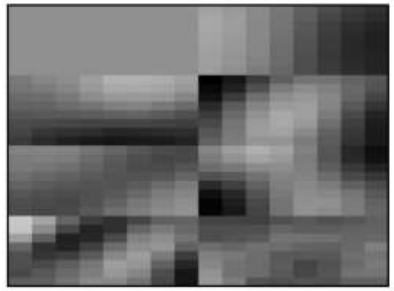
12 to 1 compression via quantization of weights into 8 **Significant Principal Components** determined for **Peppers**

Weights



12 to 1 compression via quantization of weights into 8 **Significant Principal Components** determined for **Lena** but applied for **Peppers** (***GENERALIZATION*** **?**)

Weights



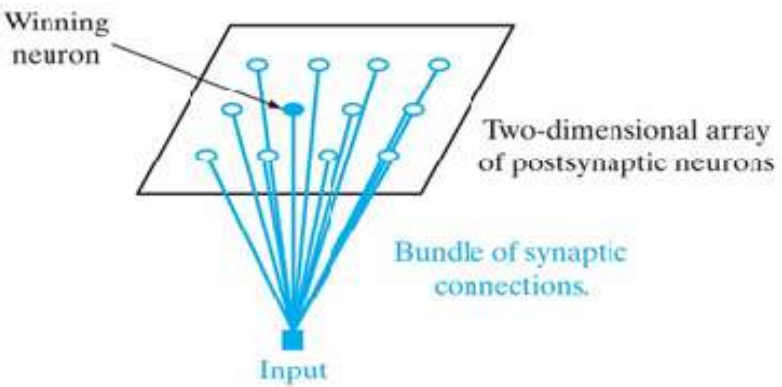
STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Overview of Self-Organizing Maps (SOM)

- Self-Organized Maps (**SOM**) refer to *nonlinear* Neural Networks with m–dimensional inputs $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ (*Sample Vectors, Examples*)
- By analogy to mammal brain functions, ***Kohonen*** suggested in 1982 a *Feedforward Neural Network* of a Single Layer of neurons $j = 1,2, \dots, l$ placed in a *Feature Map Lattice*
- Input nodes interact with *postsynaptic* lattice neurons with weights $\mathbf{w}_j = [w_{j1}\ w_{j2}\ \dots\ w_{jm}]^{\mathrm{T}}$
- The activated states of *postsynaptic* neurons reflect the system estimate for $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ regarding the closest resemblance to *patterns* stored in SOM regions
- Regions are neighborhoods of active neurons, determined via *Competitive Unsupervised Learning* around the closest neuron (*winner*) to input vector $\mathbf{x}$

SOM Applications

- Selection of dominant features in multi-dimensional sample spaces
- Image compression by identification of similar regions
- Pattern recognition, classification of images
- Reconstruction of images, filtering of interference and noise
- Completion of partially damaged examples



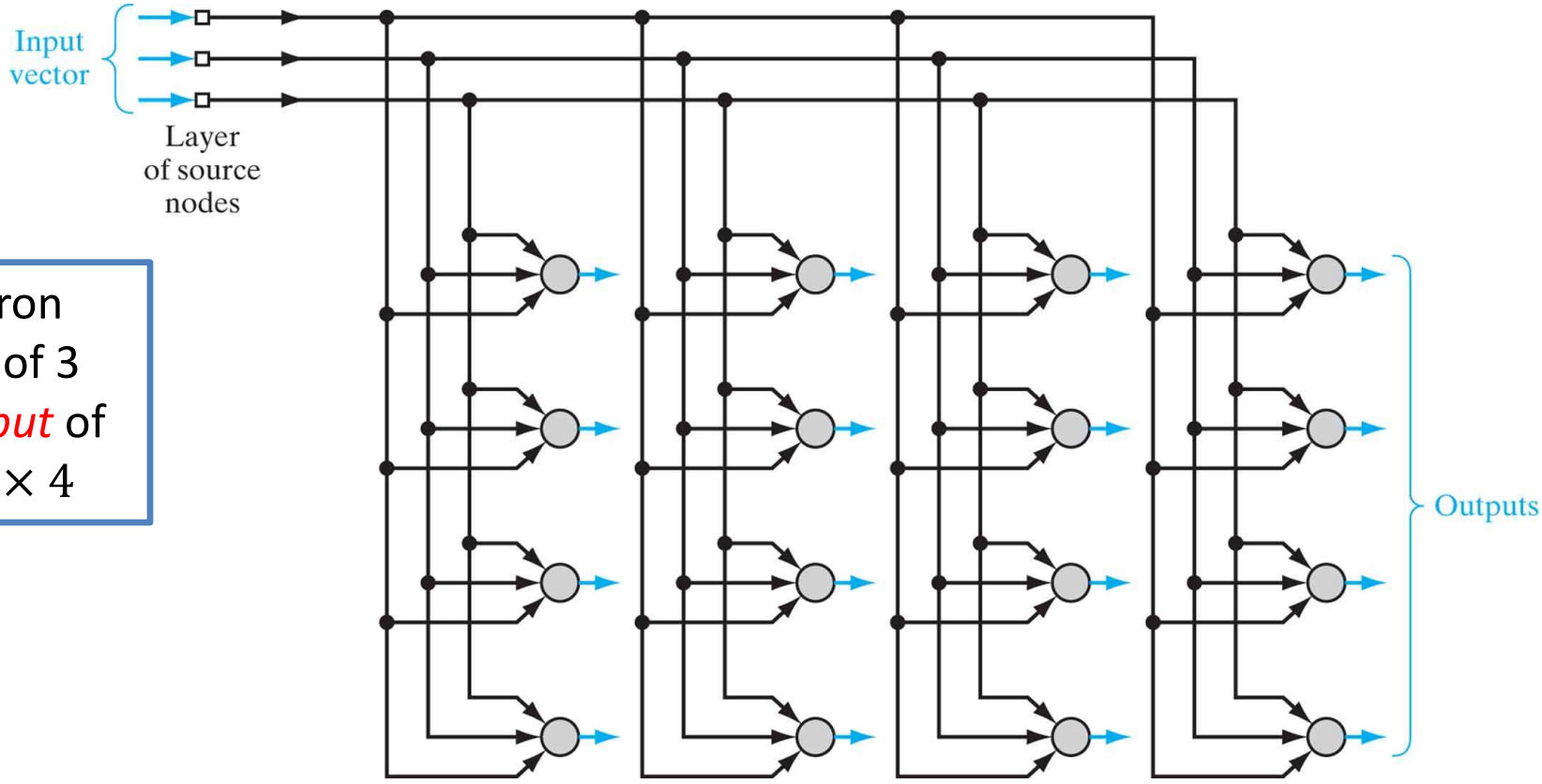
SOM Model, *Kohonen* 1982

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

SOM Configuration (1/5)

- Algorithm of *feature map* configuration is based on ***Hebb*** principles for topological self-organization of neural nets into *postsynaptic neuron grids* (arrays, lattices)
- It saves via unsupervised learning *patterns* in the training data by selscting $l \ll m$ features (*data compression*, *dimensionality reduction*)
- After configuration **SOM** attempts to reconstruct incomplete or distorted due to noise new examples, based on statistical similarity to pre-stored patterns
- Comparison with K-Means Clustering: With an adequate number of neurons *SOM* also identifies K as the number of *winning neurons*, without the need for repeated trials!

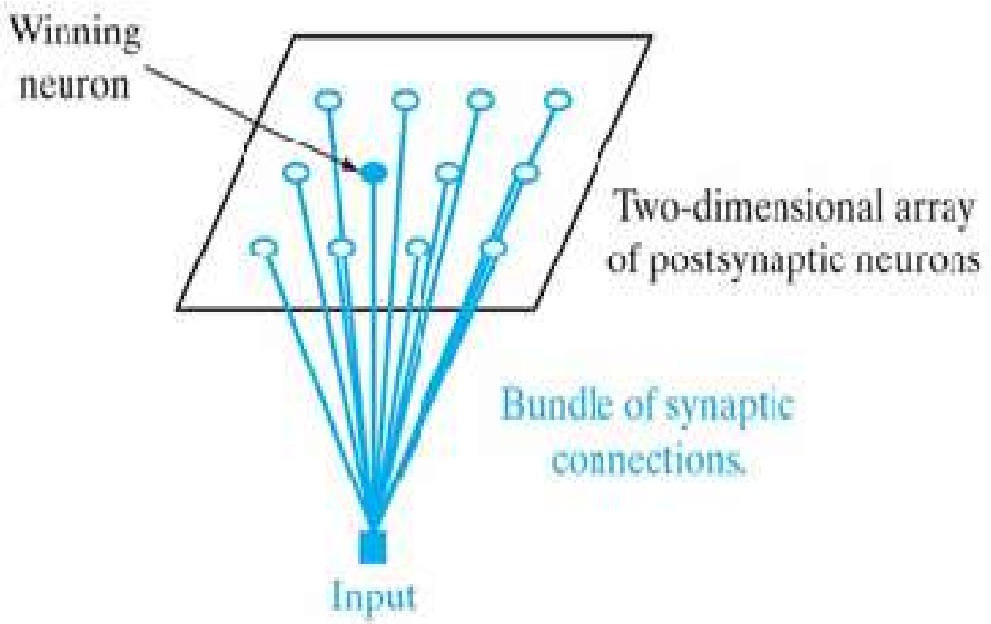
Formation of Neuron *Lattice* with *Input* of 3 Features and *Output* of Dimensionality 4×4



STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

SOM Configuration (2/5)

- An *unsupervised learning* algorithm identifies the closest neuron (*winning neuron*) for every input training vector $\mathbf{x}$ via a **Competition Process** that maximizes a *discriminant function*
- The *winner* determines a region of active neurons via a **Cooperation Process** with postsynaptic neighbors in the two-dimensional array, resulting in topological *feature map* of active neurons via *self-organization*
- In the *Hebbian* self-organization the weight vector $\mathbf{w}_j$ is updated with each training input vector $\mathbf{x}$. For *stability* of the iterative learning an **Adaptive Process** may guarantee that weights do not increase in uncontrollable fashion



SOM Model, *Kohonen* 1982

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

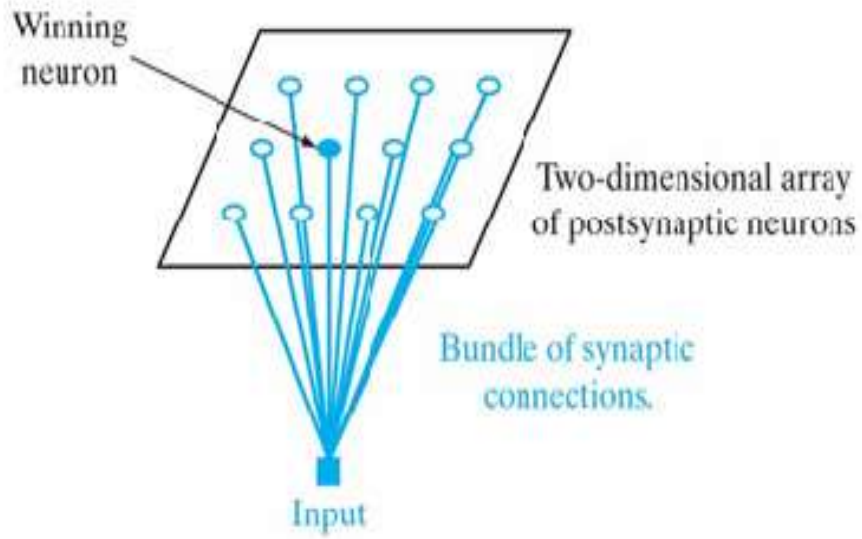
SOM Configuration (3/5)

Competition Process

During *training* it identifies the closest postsynaptic neuron j (*winner*) for every input $\mathbf{x}$ via competition that maximizes a *discriminant function* of the inner product $\mathbf{w}_j^{\mathrm{T}}\mathbf{x}$

- $\forall\ \mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$ select $\mathbf{w}_j = [w_{j1}\ w_{j2}\ \dots\ w_{jm}]^{\mathrm{T}}$ for *postsynaptic neurons* $j = 1,2,\dots,l$
- Select *winning neuron* $i(\mathbf{x})$ as the one with the maximum $\mathbf{w}_j^{\mathrm{T}}\mathbf{x}$ (the activation center within the array). Its selection is equivalent to identifying the minimum Euclidean distance between vectors $\mathbf{x}$ and $\mathbf{w}_j$. If $\|\mathbf{w}_j\| = 1$:

$$i(\mathbf{x}) = \arg\min_j \|\mathbf{x} - \mathbf{w}_j\|$$



Μοντέλο SOM, *Kohonen* 1982

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

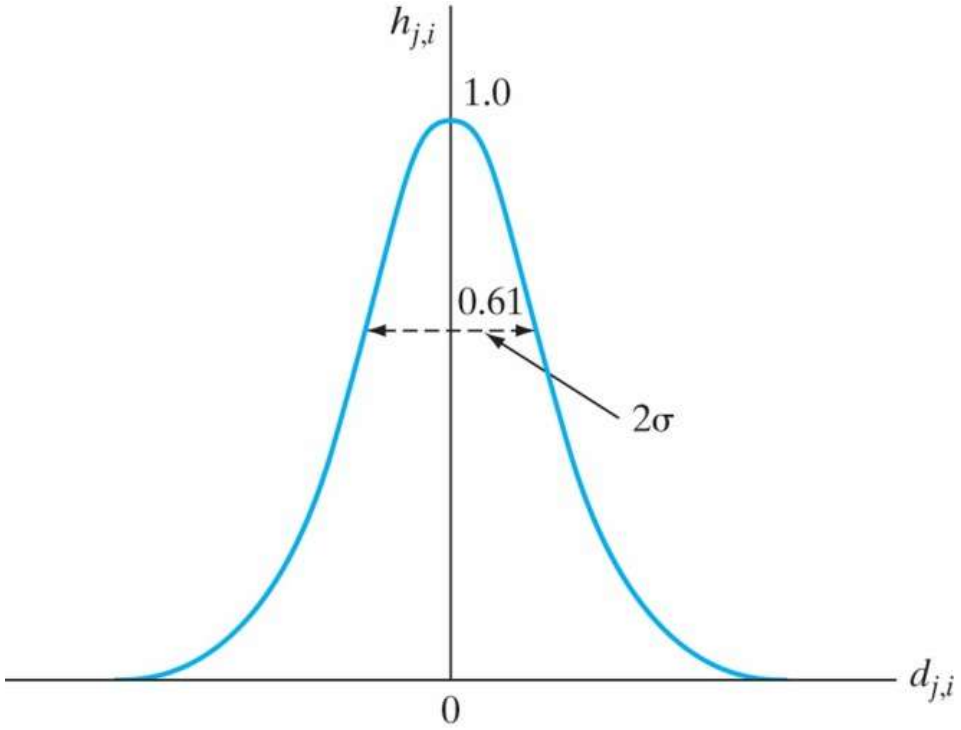
SOM Configuration (4/5)

Cooperation Process

- During training, the *winning neuron* $i(\mathbf{x})$ defines a region $h_{j,i(\mathbf{x})}$ of activated neighbors within a *lateral distance* $d_{j,i(x)}$

- A usual choice: *Gaussian Function* $h_{j,i(\mathbf{x})} = \exp\left(-\frac{d_{j,i(x)}^2}{2\sigma^2}\right)$

- The standard deviation σ may decrease as training proceeds, attenuating spatial *correlations* of nodes in the array and accelerating convergence of *synaptic weights*



STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

SOM Configuration (5/5)

Adaptive Process

The *Hebbian* based self-organized learning algorithm requires corrections while iterating towards a finite weight vector $\mathbf{w}_j$ for each example $\mathbf{x}$. A remedy is to adjust its coordinates via a *forgetting term* proportional to the output in each iteration

- Definition of **Forgetting Term**: $g(y_i)\mathbf{w}_j$ with $g(y_i)$ a non-negative function of output y_i with $g(y_i) = 0$ for $y_i = 0$
- Updates are guided by differences $\Delta\mathbf{w}_j = \eta y_i \mathbf{x} - g(y_i)\mathbf{w}_j$ where:

  η: *learning hyperparameter*,
  $y_i\mathbf{x}$: *Hebbian term*
  $g(y_i)\mathbf{w}_j$: *forgetting term*
- With linear *forgetting term* $g(y_i) = \eta y_i$ and $y_i = h_{j,i(\mathbf{x})}$ we obtain:

  $\Delta\mathbf{w}_j = \eta h_{j,i(\mathbf{x})}(\mathbf{x} - \mathbf{w}_j)$ with $i(\mathbf{x})$ the *winning neuron* for input $\mathbf{x}$
- In iteration $n \to n+1$ and with decreasing hyperparameter $\eta(n)$:

$$\mathbf{w}_j(n+1) = \mathbf{w}_j(n) + \eta(n) h_{j,i(\mathbf{x})}(n)(\mathbf{x}(n) - \mathbf{w}_j(n))$$

The synaptic weights to the *winning neuron* converge to input sample vector $\mathbf{x}$ and those of the neighboring neurons reflect the distribution of the training sample

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Autoencoders (1/2)

Encoder:

Input $\mathbf{x} = [x_1\ x_2\ \dots\ x_m]^{\mathrm{T}}$

Output $\mathbf{h} = \mathbf{F_e}(\mathbf{x}) = [h_1\ h_2\ \dots\ h_l]^{\mathrm{T}},\ l \ll m$ (*code*, *latent variables*)

Decoder:

Input $\mathbf{h} = [h_1\ h_2\ \dots\ h_l]^{\mathrm{T}}$

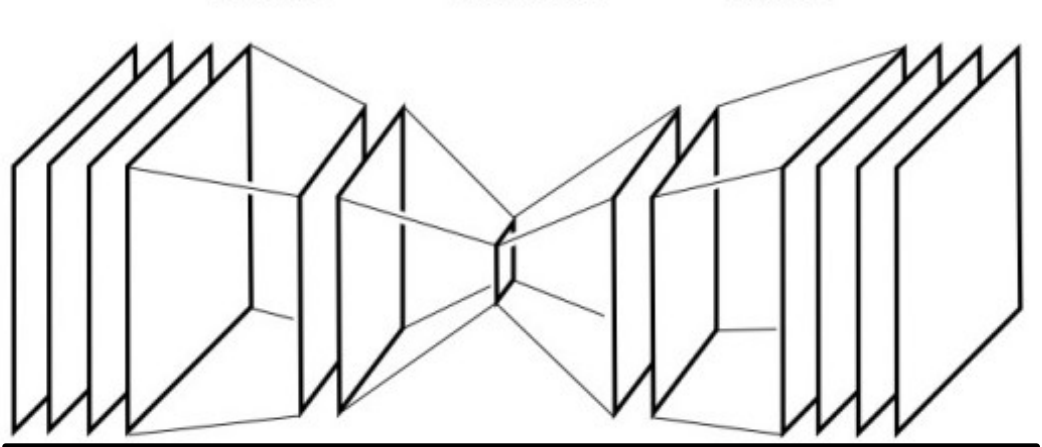
Output $\mathbf{x}' = \mathbf{F_d}(\mathbf{h}) = [x_1'\ x_2'\ \dots\ x_m']^{\mathrm{T}}$ (*reconstruction* of $\mathbf{x}$)

Bottleneck:

Middle layer of hidden nodes reflecting l *latent variables*

Unsupervised Learning Algorithm:

MSE minimization $\|\mathbf{x} - \mathbf{x}'\|^2$ via *backpropagation* for *unlabeled* training sample elements



The *decoder* layers are not used **after** the *encoder* parameter tuning (training) stage for applications relying on determination of *latent variables*, e.g. for dimensionality reduction and compression

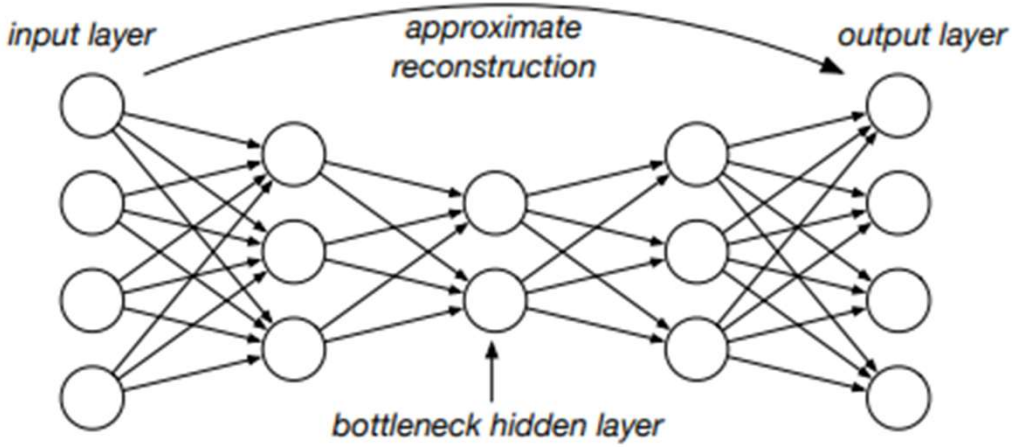
- The *latent variables* reveal *reduced feature maps*. With linear neural nets and zero *bias* they estimate the l *Principal Components* of *unlabeled* sample sets
- Applications include *image compression*, *pattern recognition*, correction and completion of distorted (noisy) images, anomaly detection from *unlabeled training datasets*

STOCHASTIC PROCESSES & OPTIMIZATION IN MACHINE LEARNING

Autoencoders (2/2)

Autoencoder Use for Anomaly Detection

- Used to identify **outliers,** rare invalid *anomalies* hidden among many *normal unlabeled* sample elements
- The autoencoder parameters in all stages are tuned by *back-propagation* with **normal** examples as input training elements
- Close *reconstruction* of input elements at the output layer is considered as the test for a test (or new) element to be classified as normal or dismissed as a statistical outlier
- Critical hyperparameters: *Reconstruction deviation* (e.g. MSE) and *threshold* classifying an element as *statistically normal* or as an *outlier*



https://saketsathe.net/downloads/autoencode.pdf

Note: All layers of the Autoencoder are employed in the post-training phase of its operation as Anomaly Detector