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Dimensionality Reduction and Data Visualisation

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Abstract – Dimension reduction has long been associated with retinotopic mapping for understanding cortical maps and neural information processing. Multisensory information is perceived, propagated and mapped onto the 2-D cortex in a near-optimal information preserving manner. Data visualization, inspired by this mechanism, is playing an increasingly important role in many applications involving feature and data reduction, from biology, neuroscience, decision support, social science, to management science. The topic has also attracted a great deal of attention in computer vision and pattern recognition. Classic linear methods include principal component analysis (PCA), factor analysis, projection pursuit and independent component analysis. Recently there have been considerable efforts and advances in developing methodologies and techniques for nonlinear dimensionality reduction. A number of novel projection methods have been proposed from statistics, geometry theory and neural networks. Two fundamental approaches are multidimensional scaling and nonlinear PCA. This tutorial will provide an introduction to this challenging and demanding topic. Various methods along these lines such as, self-organising maps, kernel PCA, principal manifold, metric and non-metric scaling, isomap, local linear embedding, Laplacian eigenmap, as well as spectral clustering will be explained and discussed. It will also attempt to unify these methods under a constrained self-organising framework. Examples and applications will be shown to illustrate the usefulness and strengthen of various methods, as well their weakness and limitation.

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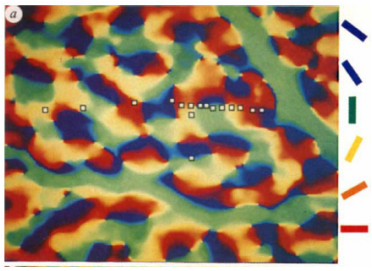
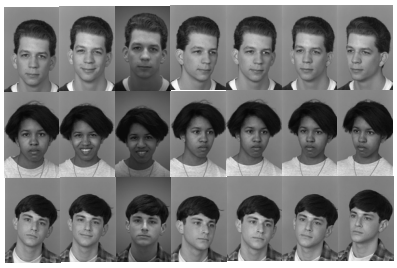
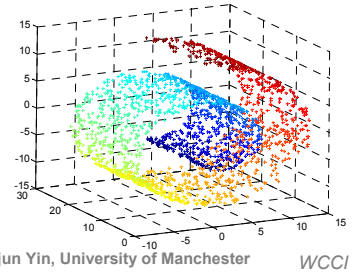
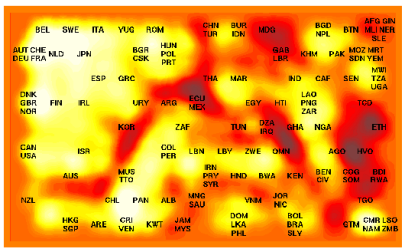
Dimensionality Reduction and Data Visualisation









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Dimensionality Reduction and Data Visualisation

- ❑ PCA, MDS, Principal Curve/Surface
- ❑ LLE, ISOMAP, Kernel PCA, Eigenmap
- ❑ SOM & Data Visualisation
- ❑ ViSOM & MDS, Principal Curve/Surface
- ❑ SOMs & Mixture Model, Kernel Method
- ❑ Conclusions

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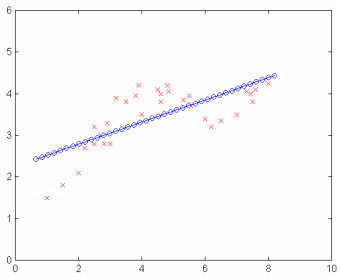
1. PCA, MDS & Principal Curve/Surface

PCA: *A **linear** coordinate transformation*

- To reduce the dimensionality of the data set
- To identify new "meaningful" (hidden) variables

$$\min \sum_{\mathbf{x}} \| X - \sum_{j=1}^{m} (\mathbf{q}_j^T X)\mathbf{q}_j \|^2$$

$$\max \{\mathbf{q}_i^T \mathbf{C} \mathbf{q}_i = \sigma_i^2\},\ \mathbf{q}_i \perp \mathbf{q}_j, i \neq j$$



- X: n-dimensional vector, zero-mean
- $\{\mathbf{q}_j\}$: orthogonal eigenvectors of **covariance** $\mathbf{C}=E[XX^T]$
- $m \leq n$

$|\mathbf{C}-\lambda_i\mathbf{I}|=0$

$(\mathbf{C}-\lambda_i\mathbf{I})\mathbf{q}_i=0$

PCA decomposition

$$\mathbf{Q}^T E[XX^T]\mathbf{Q} = \mathbf{\Lambda}$$

- $\mathbf{Q}=[\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_n]$
- $\mathbf{\Lambda}=\text{diag}\,[\lambda_1, \lambda_2, \ldots \lambda_n]$
- $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$ eigenvalues or variances

☺ *simple, direct visualisation*

☺ *stable (fast) solution*

☹ *linear mapping*

☹ *batch operation*

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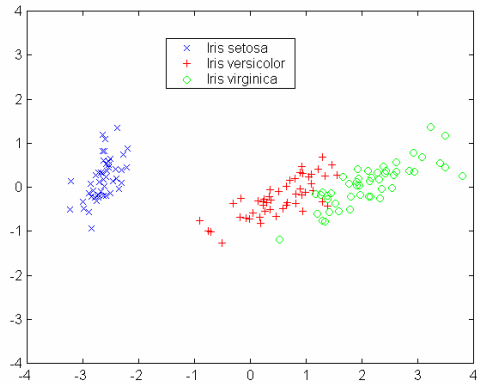
1. PCA, MDS & Principal Curve/Surface

PCA: *Example –Iris data*

- 150 4-D vectors
- 3 categories, 50 points each

4.9	3.0	1.4	0.2
4.7	3.2	1.3	0.2
4.6	3.1	1.5	0.2
5.0	3.6	1.4	0.2
5.4	3.9	1.7	0.4
4.6	3.4	1.4	0.3
……			
7.0	3.2	4.7	1.4
6.4	3.2	4.5	1.5
6.9	3.1	4.9	1.5
5.5	2.3	4.0	1.3
6.5	2.8	4.6	1.5
5.7	2.8	4.5	1.3
……			
6.3	3.3	6.0	2.5
5.8	2.7	5.1	1.9
7.1	3.0	5.9	2.1
6.3	2.9	5.6	1.8
6.5	3.0	5.8	2.2
7.6	3.0	6.6	2.1
……			
……			



Projection onto the 1st×2nd eigenvectors

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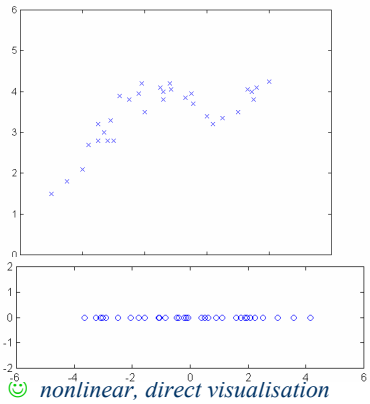
1. PCA, MDS & Principal Curve/Surface

MDS (Multidimensional Scaling)

$$S = \frac{1}{\sum_{i<j} d_{ij}^2} \sum_{i<j} [d_{ij} - D_{ij}]^2$$

$$S_{Sammon} = \frac{1}{\sum_{i<j} d_{ij}} \sum_{i<j} \frac{[d_{ij} - D_{ij}]^2}{d_{ij}}$$



- d_{ij}: *inter-point distance in original space*
  - δ_{ij}: dissimilarity
- D_{ij}: *inter-point distance in projected plot*
- **Classical** MDS: $D_{ij} \approx \delta_{ij}$
- **Metric** MDS: $D_{ij} \approx f(\delta_{ij}) = d_{ij}$
- **Nonmetric** MDS: $\delta_{ij} \le \delta_{kl} \rightarrow D_{ij} \le D_{kl}, \forall i,j,k,l$

☺ *nonlinear, direct visualisation*

☺ *stable solution*

☹ *point-point mapping (no function)*

☹ *computational intensive*

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1. PCA, MDS & Principal Curve/Surface

MDS: *Sammon Mapping*

4.9	3.0	1.4	0.2
4.7	3.2	1.3	0.2
4.6	3.1	1.5	0.2
5.0	3.6	1.4	0.2
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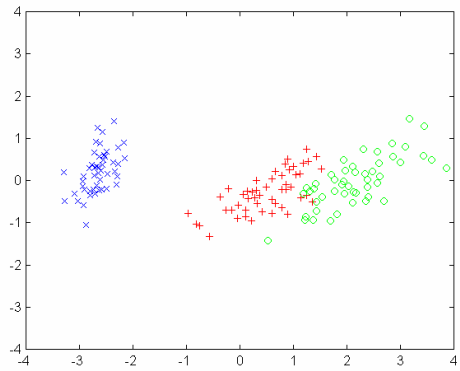
.....			
.....			



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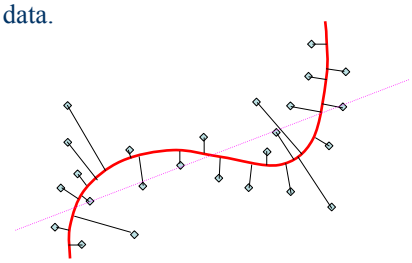
1. PCA, MDS & Principal Curve/Surface

Principal Curve/Surface

-Hastie and Stuetzle (1989)

A smooth and self-consistent curve passing through the "middle" of the data.



Projection:

$$\rho_f(\mathbf{x}) = \sup_{\rho\in\Lambda}\{\rho : \|\mathbf{x} - f(\rho)\| = \inf_{\vartheta}\|\mathbf{x} - f(\vartheta)\|$$

Expectation:

$$f(\rho) = E[\mathbf{X} \mid \rho_f(\mathbf{X}) = \rho]$$

Kernel smoothing:

$$F(\rho) = \frac{\sum_i^S \mathbf{x}_i \kappa(\rho, \rho_i)}{\sum_i^S \kappa(\rho, \rho_i)}$$

☺ *principled nonlinear extension of PCA*

☺ *smooth mapping function*

☹ *lack good algorithm, esp. in 2D*

☹ *boundary problems*

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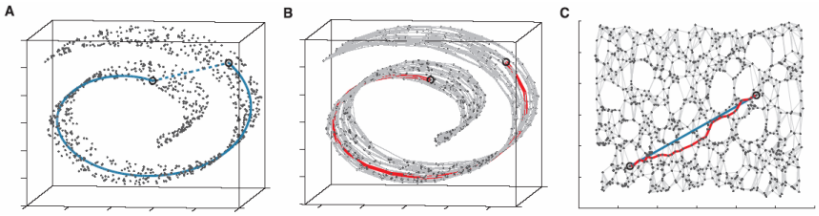
2. Isomap, LLE, Eigenmap & Kernel PCA

- **Isomap**: *Tenenbaum, Silva and Langford (2000)*
  for nonlinear dimensional scaling (dimensionality reduction).
  - **Construct neighbourhood graph:** by $d_X(i,j)<\varepsilon$ or k nearest neighbours.
  - **Compute the shortest (geodesic) paths:** $\min\{d_G(i,j), d_G(i,k)+ d_G(k,j)\}$.
  - **Construct low dimension embedding:** by applying **MDS**,



☺ *nonlinear, direct visualisation*
☺ *global geometric structure*

☹ *point-point mapping (no function)*
☹ *difficult choice of k or ε*

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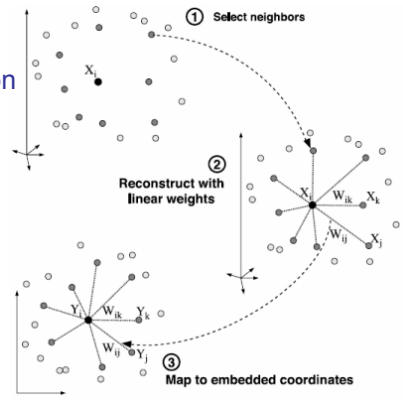
2. Isomap, LLE, Eigenmap & Kernel PCA

- **LLE (Local Linear Embedding):**
  - Roweis and Saul (2000)
  for nonlinear dimensionality reduction



- **Select neighbourhood graph:**
  k nearest neighbours.
- **Reconstruct linear weights:**
  $$\varepsilon(W) = \min \sum_i \| X_i - \sum_j W_{ij} X_j \|^2$$
- **Compute embedding coordinates Y:**
  $$\Phi(Y) = \min \sum_i \| Y_i - \sum_j W_{ij} Y_j \|^2$$

☺ *nonlinear, direct visualisation*
☺ *stable, single pass solution*

☹ *point-point mapping (no function)*
☹ *computational intensive*

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2. Isomap, LLE, Eigenmap & Kernel PCA

- **Laplacian Eigenmap:** *Belkin and Niyogi (2003)* for dimensionality reduction.
  - **Select neighbourhood graph:**

    k nearest neighbours or ε rule.
  - **Construct the weightings (heat kernel):**

$$W_{ij} = e^{-\frac{\|X_i - X_j\|^2}{t}}$$

Affinity matrix

Spectral Clustering – *Weiss 1999; Ng, Jordan and Weiss 2002*

  - **Eigenmap: compute the embedding**

$$L\mathbf{f} = \lambda D\mathbf{f} \qquad D_{ii} = \sum_j W_{ji}, \ and \ \ L = D - W$$

$$X_i \to (\mathbf{f}_1(i), \mathbf{f}_2(i), \ldots, \mathbf{f}_m(i))$$

Objective function: $\min \sum_{ij} (Y_i - Y_j)^2 W_{ij}$

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2. Isomap, LLE, Eigenmap & Kernel PCA

- **Kernel PCA:** *Shölkopf, Smola and Müller (1998)* for nonlinear PCA.
  - **Kernel method has become popular.**

$$\phi : X \to F, \qquad \mathbf{x} \mapsto \phi(\mathbf{x})$$

$$\kappa : X \times X \in \Re, \qquad \kappa(\mathbf{x};\mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle$$

  - **PCA**

$$\mathbf{Cq} = \lambda \mathbf{q}, \qquad \mathbf{C} = \frac{1}{n}\sum_i \mathbf{x}_i \mathbf{x}_i^T, \qquad \mathbf{q} = \sum_i \alpha_i \mathbf{x}_i,$$

  - **Kernel PCA**

$$\mathbf{K}\boldsymbol{\alpha} = \lambda \boldsymbol{\alpha}, \qquad K_{ij} := \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle, \qquad \boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots\ldots \alpha_n]^T,$$

$$\mathbf{q} = \sum_i \alpha_i \phi(\mathbf{x}_i), \qquad \langle \phi(\mathbf{x}_k), \mathbf{q} \rangle = \sum_i \alpha_i \kappa(\mathbf{x}_k, \mathbf{x}_i),$$

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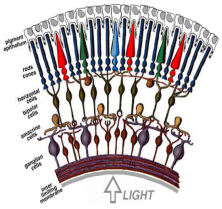
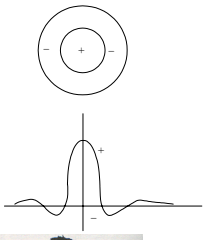
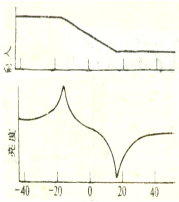
3. Self-Organising Maps

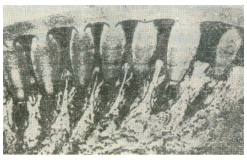
SOM: *Background–lateral inhibition*

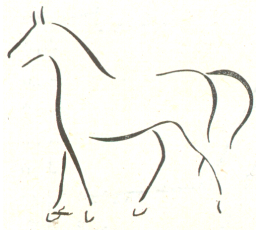


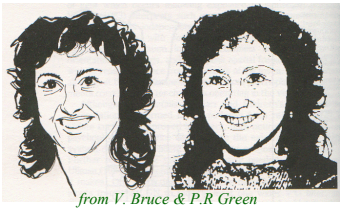




Hartline, et al. 1960s







from V. Bruce & P.R Green

It explains Mach-band effect and abstraction purpose

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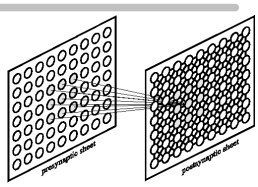
3. Self-Organising Maps

SOM: *Model*



Hebbian learning (Hebb 1949) $\Delta w = \alpha x y$

von der Malsburg and Willshaw's model (1973, 1976)

$$\frac{\partial y_i(t)}{\partial t} + c y_i(t) = \sum_j w_{ij}(t) x_i(t) + \sum_k e_{ik} y_k^*(t) - \sum_{k'} b_{ik'} y_{k'}^*(t)$$

$$\frac{\partial w_{ij}(t)}{\partial t} = \alpha x_i(t) y_j{}^*(t), \quad \text{subject to } \sum w_{ij} = \text{constant}$$

$$y_j{}^*(t) = \begin{cases} y_j(t) - \theta, & \text{if } y_j(t) > \theta \\ 0 & \text{otherwise} \end{cases}$$

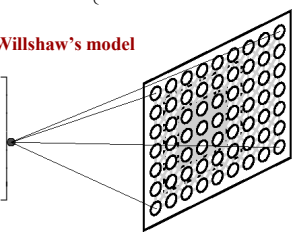
Kohonen's model (1982) is an abstraction of von der Malsburg and Willshaw's model

$$y_j(t+1) = \varphi\left(\mathbf{w}_j^T \mathbf{x}(t) + \sum_i h_{ij} y_i(t)\right)$$

$$\frac{\partial w_{ij}(t)}{\partial t} = \alpha y_j(t) x_i(t) - \beta y_j(t) w_{ij}(t)$$

$$= \alpha[x_i(t) - w_{ij}(t)] y_j(t) = \begin{cases} \alpha[x_i(t) - w_{ij}(t)], & \text{if } j \in \eta(t) \\ 0 & \text{if } j \notin \eta(t) \end{cases}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_n \end{bmatrix}$$



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3. Self-Organising Maps

SOM: *Algorithm*

- *At each time t, present an input,* $\mathbf{x}(t)$*, select the winner.*

$$v = \arg\min_{c \in \Omega} \left\| \mathbf{x}(t) - \mathbf{w}_c \right\|$$

- *Updating the weights of winner and its neighbours.*

$$\Delta \mathbf{w}_k(t) = \alpha(t)\eta(v,k,t)[\mathbf{x}(t) - \mathbf{w}_v(t)]$$

- *Repeat until the map converges.*

Typical neighbourhood function: $\eta(v,k,t) \propto \exp[-\frac{\|v-k\|^2}{2\sigma(t)^2}]$

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3. Self-Organising Maps

SOM: *Quantisation, topology & cost function*

Topologically "ordered" map

$$E(\mathbf{w}_1,\ldots\mathbf{w}_N) = \sum_i \int_{V_i} \sum_k h_{i,k} \left\| \mathbf{x} - \mathbf{w}_k \right\|^2 p(\mathbf{x}) d\mathbf{x}$$

(Heskes, 1999)

"*Error tolerant*" coding -HVQ (Luttrell, NC 1994)

"*Minimum wiring*" (Mitchison, NC 1995), (Durbin&Mitchson, Nature1990)

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3. Self-Organising Maps

SOM: *Variants & extensions*

- **HSOM** (Miikkulainen 1990), **DISLEX** (1990, 1997)
- **PSOM** (Ritter 1993), **Hyperbolic SOM** (1999), **H²SOM**
- **Temporal Kohonen Map** (Chappell &Taylor 1993)
- **Neural Gas** (Martinetz et al.1991), **Growing Grid** (Fritzke1995)
- **ASSOM** (Kohonen 1997)
- **Recurrent SOM** (Koskela, 1997), RecursiveSOM (Voegtlin2001)
- **SOAR** (Lampinen&Oja 1989), **SOMAR** (Ni&Yin, 2007)
- **Bayesian SOM** & **SOMN** (Yin&Allinson 1995,1997; Utsugi 1997)
- **GTM** (Bishop et al. 1998)
- **GHSOM** (Merkl et al. 2000), **TOC**(TreeSOM) (Freeman&Yin2004)
- **PicSOM** (Laaksonen, Oja, et al., 2000)
- **ViSOM** (Yin 2001, 2002), **gViSOM** (Yin 2007)

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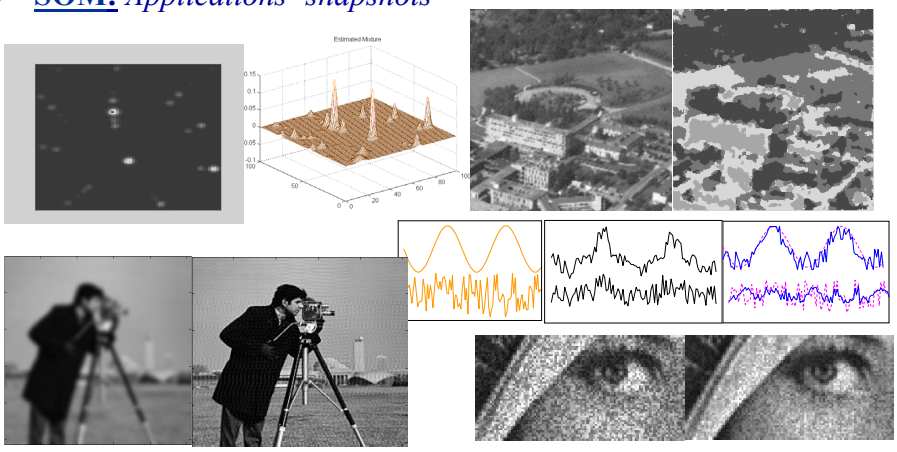
3. Self-Organising Maps

SOM: *Applications -snapshots*



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3. Self-Organising Maps

SOM: *Applications -snapshots*

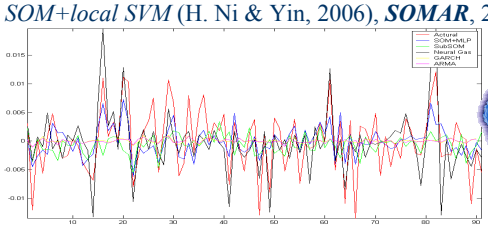
A Temporal Shape Metric :

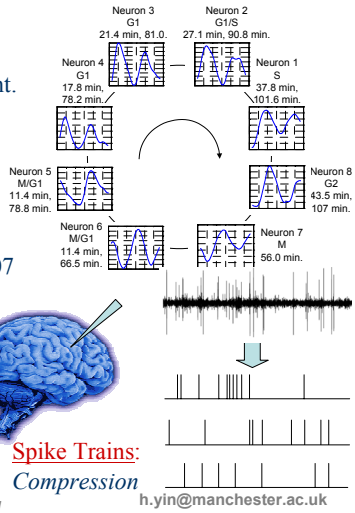
Co-Expression Coefficient (Möller-Levet & Yin, Int. J. Neural Systems, 15: 311-322, 2005)

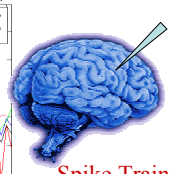
$$ce(x,y) = \frac{\int x' y' dt}{\sqrt{\int x'^2 dt \int y'^2 dt}}$$

Foreign exchange modelling :

SOM+local SVM (H. Ni & Yin, 2006), ***SOMAR***, 2007







Spike Trains:

Compression

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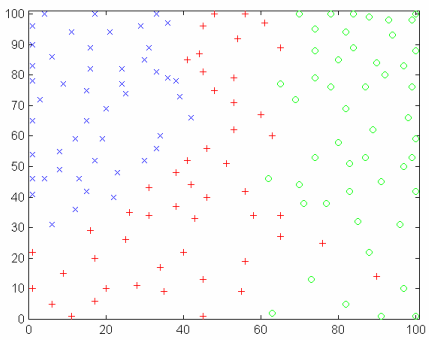
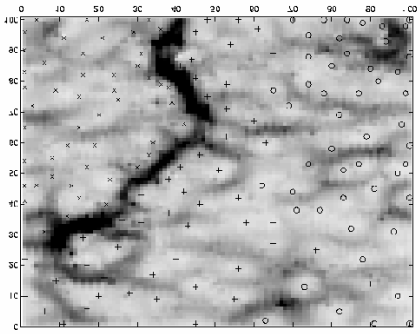
3. Self-Organising Maps

SOM: *Data visualisation & dimensionality reduction*





☺ *topology preserving mapping*

☺ *(discrete) mapping function*

☹ *non distance preserving*

☹ *boundary problems*

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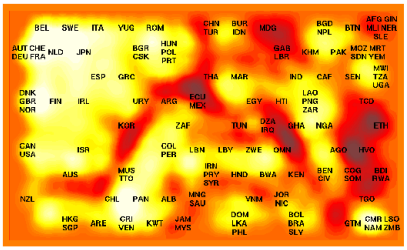
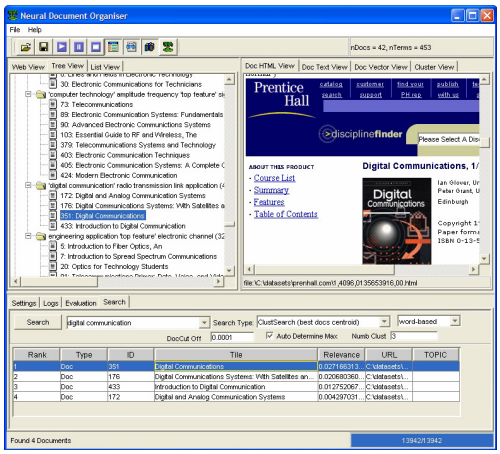
3. Self-Organising Maps

SOM: *Data visualisation & knowledge management*



courtesy of S. Kaski and T. Kohonen (1996)



Tree-View SOM
(Freeman and Yin 2004)

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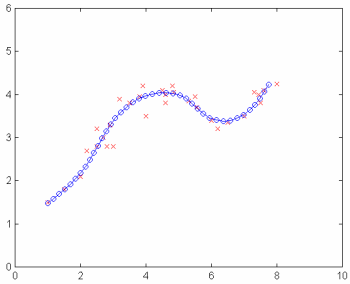
4. ViSOM & Principal Curve/Surface, MDS

ViSOM: *Visualisation induced SOM*
(Yin, 2001,2002)

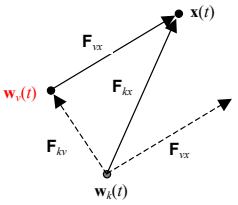
- To preserve distance/metric (**locally**) on the map
- To extrapolate smoothly

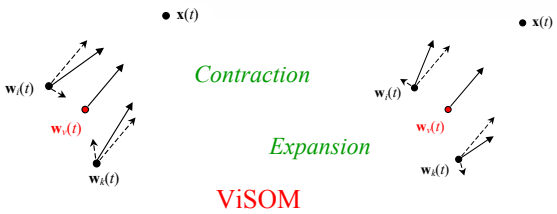


Principle

SOM update:

$$\mathbf{w}_k(t+1) = \mathbf{w}_k(t) + \alpha(t)\eta(v,k,t)[\mathbf{x}(t) - \mathbf{w}_k(t)]$$





ViSOM

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4. ViSOM & Principal Curve/Surface, MDS

ViSOM: *Algorithm*

- *Grid structure and winner selection same to SOM*
- *Updating*

$$\Delta \mathbf{w}_k(t) = \alpha(t)\eta(v,k,t)\left([\mathbf{x}(t)-\mathbf{w}_v(t)]+[\mathbf{w}_v(t)-\mathbf{w}_k(t)]\frac{(d_{vk}-\Delta_{vk}\lambda)}{\Delta_{vk}\lambda}\right)$$

- *Refreshing*

At certain iterations (e.g. 20%), choosing a neuron randomly and using its weight as an alternative input.

$$\Delta \mathbf{w}_k = \mathbf{w}_k(t)+\alpha(t)\eta(v,k,t)\left([\mathbf{x}(t)-\mathbf{w}_v(t)]+[\xi+(1-\xi)(\frac{d_{vk}}{\Delta_{vk}\lambda}-1)][\mathbf{w}_v(t)-\mathbf{w}_k(t)]\right)$$

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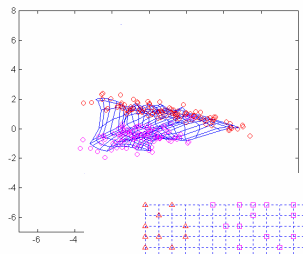
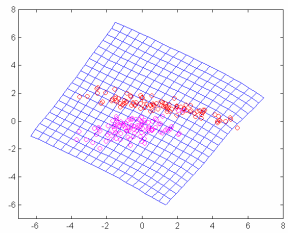
4. ViSOM & Principal Curve/Surface, MDS

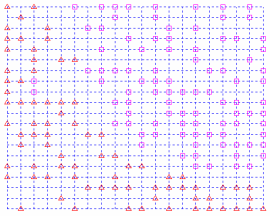
ViSOM: *Examples*

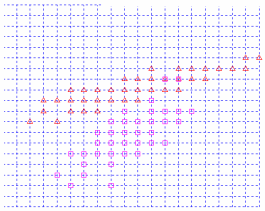


ViSOM



SOM





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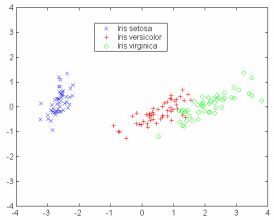
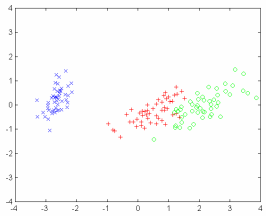
4. ViSOM & Principal Curve/Surface, MDS

ViSOM: *Examples*

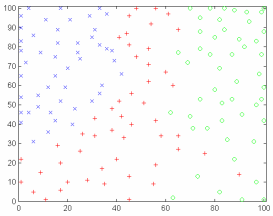
PCA

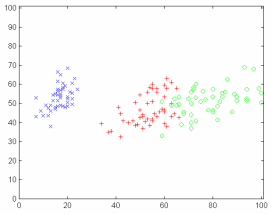




Sammon

SOM





ViSOM

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4. ViSOM & Principal Curve/Surface, MDS

ViSOM: *Examples*

Ranking table of UK universities

- source: The Sunday Times, 18 September 2000

Ranking	*University*	*F1*	*F2*	*F3*	*F4*	*F5*	*F6*	*F7*	***Total***
1	Cambridge	241	182	247	97	88	100	50	**1005**
2	Oxford	214	175	244	97	81	100	30	**941**
3	LSE	200	175	233	97	68	100	50	**923**
4	Imperial	203	154	232	98	67	100	10	**864**
5	York	206	143	208	94	63	76	60	**850**
6	UCL	172	152	210	95	71	100	30	**830**
7	St Andrews	139	131	194	96	73	91	100	**824**
8	Warwick	153	155	215	97	69	86	20	**795**
9	Bath	132	142	211	97	66	83	60	**791**
9	Nottingham	176	125	218	96	74	72	30	**791**
11	Bristol	145	131	218	96	75	94	20	**779**
11	Durham	163	132	207	91	64	72	50	**779**
11	Edinburg	106	145	218	96	74	100	40	**779**
14	Lancaster	156	144	186	95	62	63	50	**756**
15	UMIST	135	144	188	97	58	100	30	**752**
16	Birmingham	146	127	204	96	67	87	20	**747**
17	Loughborough	162	115	177	95	57	66	60	**732**
18	Southampton	143	124	180	93	55	71	50	**716**
19	King's College	135	126	204	96	63	100	-10	**714**
20	Newcastle	134	117	193	97	60	87	20	**708**
21	Manchester	125	134	198	96	66	98	-10	**707**
22	Leeds	122	127	199	97	61	74	20	**700**
23	Sheffield	143	125	213	97	61	72	-20	**691**
24	East Anglia	125	127	176	96	63	60	40	**687**
24	Leicester	125	120	183	94	52	93	20	**687**

F1:Research
F2:Teaching
F3:A-levels
F4:Employment
F5:S/S ratio
F6:1st/2:1s
F7:Dropout rate

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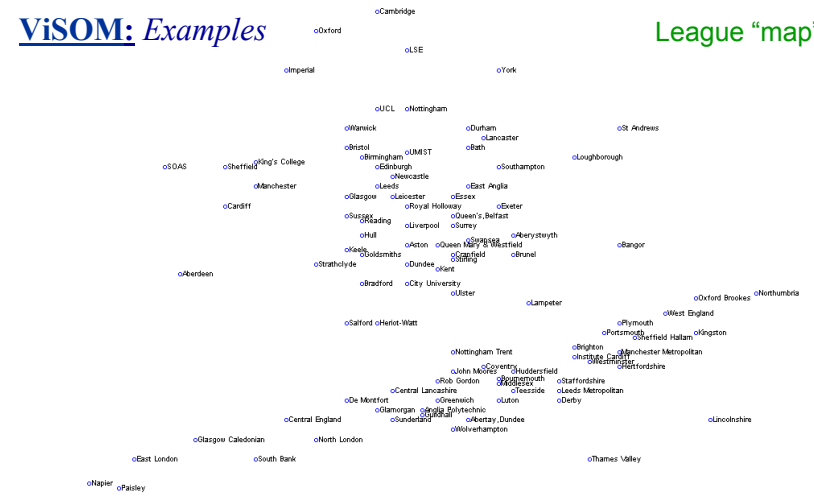
4. ViSOM & Principal Curve/Surface, MDS

ViSOM: *Examples*

League "map"



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4. ViSOM & Principal Curve/Surface, MDS

ViSOM: *A discrete principal curve/surface (Yin, 2002)*

Projection:

$$\rho_f(\mathbf{x}) = \sup_{\rho\in\Lambda}\{\rho : \|\mathbf{x} - f(\rho)\| = \inf_{\vartheta}\|\mathbf{x} - f(\vartheta)\|$$

Expectation:

$$f(\rho) = E[\mathbf{X} \mid \rho_f(\mathbf{X}) = \rho]$$

Kernel smoothing:

$$F(\rho) = \frac{\sum_i^S \mathbf{x}_i \kappa(\rho, \rho_i)}{\sum_i^S \kappa(\rho, \rho_i)}$$

SOM/ViSOM smoothing:

$$\mathbf{w}_k = \frac{\sum_i^S \mathbf{x}_i h(k,i)}{\sum_i^S h(k,i)}$$

SOM: $\|k\text{-}i\| \neq \|\mathbf{w}_k\text{-}\mathbf{w}_i\|$

ViSOM: $\|k\text{-}i\| \approx \|\mathbf{w}_k\text{-}\mathbf{w}_i\|$

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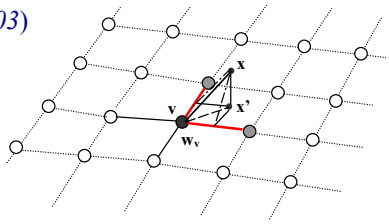
4. ViSOM & Principal Curve/Surface, MDS

ViSOM Extensions:

° *Resolution Enhancement by **Local Linear Projection -LLP** (Yin, 2003)*

$$\mathbf{LLP}_{x,y} = \max_{v'_{x,y}=v_{x,y}\pm 1}\{[\frac{(\mathbf{x}-\mathbf{w_v})\bullet(\mathbf{w_v}-\mathbf{w_{v'}})}{\|\mathbf{w_v}-\mathbf{w_{v'}}\|^2}],\ 0\}$$

$$\mathbf{x}' = \arg\max_{\mathbf{c}}[(\mathbf{x}-\mathbf{w_c})] + \mathbf{LLP}(\mathbf{x},\mathbf{v})$$



° *Incremental or growing ViSOM - **gViSOM** (Yin, 2007)*

Start with a small map (**rectangular** or **hexagonal**); add rows/columns or polygons to the sides or vertices where activities are high; etc.

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4. ViSOM & Principal Curve/Surface, MDS

ViSOM Extensions:

° *PRSOM (Wu&Chow, TNN 2005)= STVQ (Graeple, et al. 1997)+ViSOM*

$$w_j(t+1) = w_j(t)+\varepsilon(t)p'_j(x(t))\left[\sum_{i=1}^{N} p_i(x(t))([x(t)-w_i(t)] + \gamma[w_i(t)-w_j(t)]\left(\frac{d_{ij}^2-\lambda\Delta_{ij}^2}{\lambda\Delta_{ij}^2+I_{ij}}\right)\right].$$

$$E = F_{vq}+\gamma F_{reg} = \frac{1}{2}\sum_{t=1}^{M}\left\|\sum_{j=1}^{N} p_j(x(t))[x(t)-w_j]\right\|^2 + \frac{\gamma}{8}\sum_{t=1}^{M}\sum_{j=1}^{N}\sum_{m=1}^{N} p_j(x(t))p_m(x(t))\frac{(d_{jm}^2-\lambda\Delta_{jm}^2)^2}{(\lambda\Delta_{jm}^2+I_{jm})}$$

° *Neural Gas ViSOM (Estévez & Figueroa, NN 2006)*

° *Other extensions are readily applicable, e.g. hierarchical, growing, etc..*

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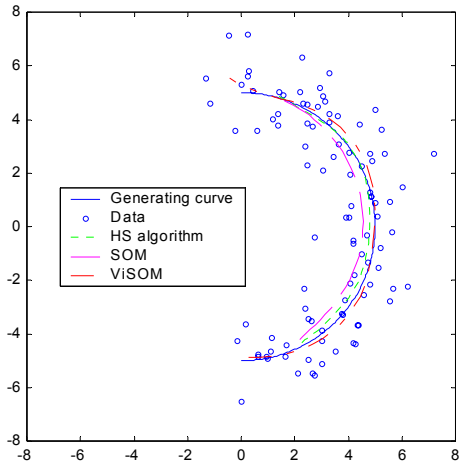
4. ViSOM & Principal Curve/Surface, MDS



Yin (2002)

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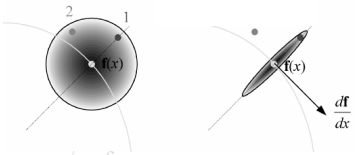
4. ViSOM & Principal Curve/Surface, MDS

Other PC/S algorithms:

- **SOM** has been related to PC/S and termed discrete PC/S by *Ritter, Martinetz & Schulten in 1992*. However, the differences are:
  - Projection onto nodes instead of curve/surface
  - Smoothing is governed by indexes in the map space, not the input space

$$\mathbf{w}_k = \frac{\sum_i^S \mathbf{x}_i h(k,i)}{\sum_i^S h(k,i)} \qquad F(\rho) = \frac{\sum_i^S \mathbf{x}_i \kappa(\rho,\rho_i)}{\sum_i^S \kappa(\rho,\rho_i)}$$



SOM: $||k-i|| \neq ||\mathbf{w}_k - \mathbf{w}_i|| = ||\rho - \rho_i||$

ViSOM: $||k-i|| \approx ||\mathbf{w}_k - \mathbf{w}_i||$

More importantly for the SOM, one cannot get the curve/surface at any point other than the nodes, even with interpolations.

GTM (generative topographic mapping) and **PPS** (probabilistic principal surface) are parametrised SOMs with GTM using spherical and PPS oriented Gaussians for the nodes.

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4. ViSOM & Principal Curve/Surface, MDS

SOM, ViSOM & MDS:

- **MDS cost function:**

$$\min \sum_{i,j} (d_{ij} - D_{ij})^2 = \min \sum_{i,j} (d_{ij}^2 + D_{ij}^2 - 2 d_{ij} D_{ij}) = \min \sum_{i,j} (-2 d_{ij} D_{ij})$$

- **SOMs cost function (sample cost of Voronoi region *i*):**

$$\min \sum_j \eta(i,j) \left\| \mathbf{x} - \mathbf{w}_j \right\|^2 = \min \sum_j f(\| i - j \|) \left\| \bar{\mathbf{x}}_i - \bar{\mathbf{x}}_j \right\|^2$$

$$\min = \sum_j f(D_{ij}) d_{ij}^{\ 2} \approx \min \sum_j -(D_{ij} d_{ij})^2$$

- SOM: $D_{ij} = \| i - j \|^2$
- ViSOM: $D_{ij} = \| i - j \| \cong \| \mathbf{w}_i - \mathbf{w}_j \|$

- SOM is a qualitative (nonmetric) MDS.
- ViSOM is a metric MDS.

C Measure
(Goodhill&Sejnowski, 1997)

$$C = \sum_i \sum_j F(i,j) G[M(i), M(j)]$$

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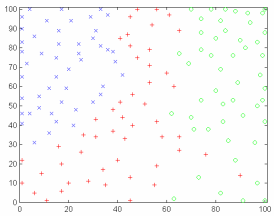
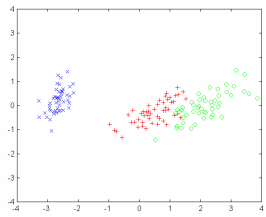
4. ViSOM Examples

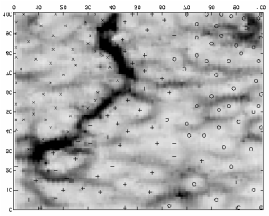
Iris:



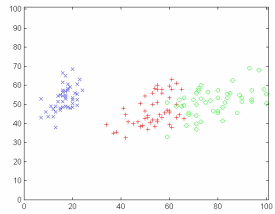
Sammon metric MDS



SOM



ViSOM (λ=0.075)



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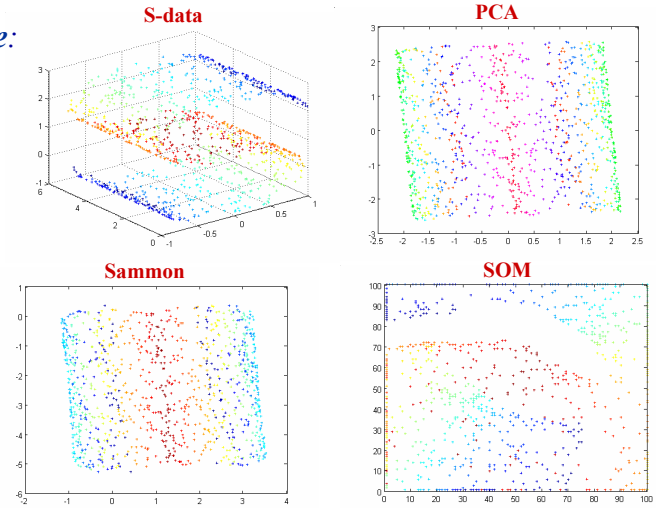
4. ViSOM Examples

S-curve:



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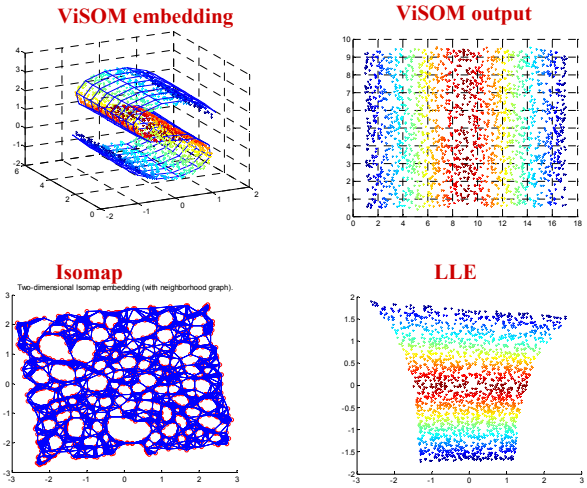
4. ViSOM Examples

S-curve:

Yin (2007)



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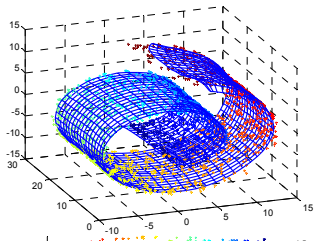
4. ViSOM Examples

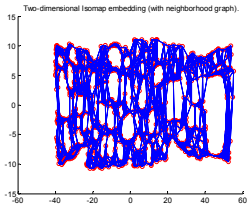
Swissroll:

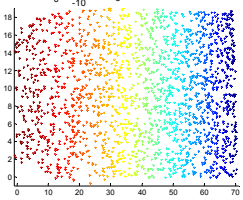
Yin (2007)

Swissroll data & gViSOM embedding(final size 18x70, λ=1.5)



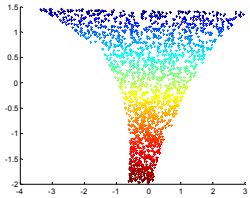
Isomap





gViSOM with LLP

LLE



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5. Kernel SOM & Mixture Model

Kernel SOM: *Background*

- Kernel method has become popular.

$$\phi : X \to F, \qquad \mathbf{x} \mapsto \phi(\mathbf{x})$$

$$\kappa : X \times X \in \Re, \qquad \kappa(\mathbf{x};\mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle$$

- PCA

$$\mathbf{Cq} = \lambda \mathbf{q}, \qquad \mathbf{C} = \frac{1}{n}\sum_i \mathbf{x}_i \mathbf{x}_i^T, \quad \mathbf{q} = \sum_i \alpha_i \mathbf{x}_i,$$

- Kernel PCA

$$\mathbf{K}\boldsymbol{\alpha} = \lambda \boldsymbol{\alpha}, \qquad K_{ij} := \langle \phi(\mathbf{x}_i), \phi(\mathbf{x}_j) \rangle, \qquad \boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots\ldots \alpha_n]^T,$$

$$\mathbf{q} = \sum_i \alpha_i \phi(\mathbf{x}_i), \qquad \langle \phi(\mathbf{x}_k), \mathbf{q} \rangle = \sum_i \alpha_i \kappa(\mathbf{x}_k, \mathbf{x}_i),$$

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5. Kernel SOM & Mixture Model

KM-Kernel SOM (*MacDonald & Fyfe, 2000*):

$$\phi : \mathbf{x} \to F \qquad \mathbf{x} \mapsto \phi(\mathbf{x}), \qquad \mathbf{m}_i = \sum_n \alpha_{i,n}\phi(\mathbf{x}_n),$$

$$\|\phi(\mathbf{x}) - \mathbf{m}_i\|^2 = \|\phi(\mathbf{x}) - \sum_n \alpha_{i,n}\phi(\mathbf{x}_n)\|^2$$

$$= \kappa(\mathbf{x},\mathbf{x}) - 2\sum_n \alpha_{i,n}\kappa(\mathbf{x},\mathbf{x}_n) + \sum_{n,m} \alpha_{i,n}\alpha_{i,m}\kappa(\mathbf{x}_n,\mathbf{x}_m)$$

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t) + \Lambda[\phi(\mathbf{x}) - \mathbf{m}_i(t)], \qquad \Lambda = \frac{\zeta_{i(\mathbf{x}),j}}{\sum_{n=1}^{t+1}\zeta_{i,n}}$$

$$\alpha_{i,n}(t+1) = \begin{cases} \alpha_{i,n}(t)(1-\Lambda), & \text{for } n \neq t+1 \\ \zeta, & \text{for } n = t+1 \end{cases}$$

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5. Kernel SOM & Mixture Model

GD-Kernel SOM (*Andras 2002; Pan et al. 2004*):

$$v = \arg\min_i \|\mathbf{x} - \mathbf{m}_i\|^2 \qquad v = \arg\min_i \|\phi(\mathbf{x}) - \phi(\mathbf{m}_i)\|^2$$

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t) + \alpha(t)h(v(\mathbf{x}),i)\nabla J(\mathbf{x},\mathbf{m}_i)$$

$$J(\mathbf{x},\mathbf{m}_i) = \|\phi(\mathbf{x}) - \phi(\mathbf{m}_i)\|^2 = \kappa(\mathbf{x},\mathbf{x}) + \kappa(\mathbf{m}_i,\mathbf{m}_i) - 2\kappa(\mathbf{x},\mathbf{m}_i)$$

$$\nabla J(\mathbf{x},\mathbf{m}_i) = \frac{\partial\kappa(\mathbf{m}_i,\mathbf{m}_i)}{\partial\mathbf{m}_i} - 2\frac{\partial\kappa(\mathbf{x},\mathbf{m}_i)}{\partial\mathbf{m}_i}$$

$$v = \arg\min_i J(\mathbf{x},\mathbf{m}_i) = \arg\min_i[-2\kappa(\mathbf{x},\mathbf{m}_i)] = \arg\min_i[-\exp(-\frac{\|\mathbf{x}-\mathbf{m}_i\|^2}{2\sigma^2})]$$

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t) + \alpha(t)h(v(\mathbf{x}),i)\frac{1}{2\sigma^2}\exp(-\frac{\|\mathbf{x}-\mathbf{m}_i\|^2}{2\sigma^2})(\mathbf{x}-\mathbf{m}_i)$$

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5. Kernel SOM & Mixture Model

Kernel SOM: *An application*

Table: *Classification errors on UCI colon cancer dataset. M, A and V denote the minimum distance, average distance and majority voting methods to label the nodes. (Lau, Yin & Hubbard 2006)*

Kernel	*Type I Kernel SOM*			*Type II Kernel SOM*			*SOM*		
	M	A	V	M	A	V	M	A	V
Gaussian	5.6	5.8	5.6	5.3	5.3	5.7	4.3	7.0	3.8
Cauchy	5.5	5.6	5.5	5.5	5.5	4.8			
Log	4.6	4.6	4.6	5.2	5.2	4.6			

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5. Kernel SOM & Mixture Model

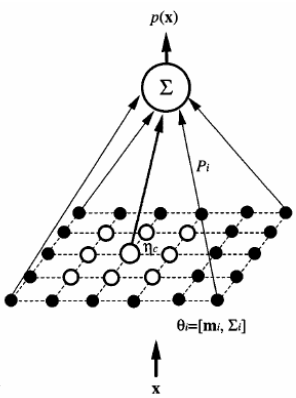
Mixture Model:

$$p(\mathbf{x}\,|\,\Theta) = \sum_{i=1}^{K} p_i(\mathbf{x}\,|\,\theta_i)P_i$$

Kullback-Leibner divergence:

$$\mathbf{I} = -\int \log\frac{\hat{p}(\mathbf{x})}{p(\mathbf{x})}p(\mathbf{x})d\mathbf{x}$$

$$\frac{\partial \mathbf{I}}{\partial \theta_i} = -\int [\frac{1}{\hat{p}(\mathbf{x}\,|\,\hat{\Theta})}\frac{\partial \hat{p}(\mathbf{x}\,|\,\hat{\Theta})}{\partial \theta_i}]p(\mathbf{x})d\mathbf{x}$$



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5. Kernel SOM & Mixture Model

Self Organising Mixture Network: (*Yin & Allinson, 2001*)

$$\hat{\theta}_i(t+1) = \hat{\theta}_i(t) + \alpha(t)h(v(\mathbf{x}),i)[\frac{1}{\hat{p}(\mathbf{x}\,|\,\hat{\Theta})}\frac{\partial \hat{p}(\mathbf{x}\,|\,\hat{\Theta})}{\partial \theta_i}]$$

$$= \hat{\theta}_i(t) + \alpha(t)h(v(\mathbf{x}),i)[\frac{\hat{P}_i(t)}{\sum_j \hat{P}_i(t)\hat{p}_j(\mathbf{x}\,|\,\theta_j)}\frac{\partial \hat{p}_i(\mathbf{x}\,|\,\hat{\theta}_i)}{\partial \theta_i}]$$

$$\hat{P}_i(t+1) = \hat{P}_i(t) + \alpha(t)[\frac{\hat{p}_i(\mathbf{x}\,|\,\hat{\theta}_i)\hat{P}_i(t)}{\hat{p}(\mathbf{x}\,|\,\hat{\Theta})} - \hat{P}_i(t)] = \hat{P}_i(t) - \alpha(t)h(v(\mathbf{x}),i)[\hat{P}(i\,|\,\mathbf{x}) - \hat{P}_i(t)]$$

$$v = \arg\max_i \{\hat{P}(i\,|\,\mathbf{x}) = \frac{\hat{P}_i\hat{p}_i(\mathbf{x}\,|\,\hat{\theta}_i)}{\hat{p}(\mathbf{x}\,|\,\hat{\Theta})}\}$$

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5. Kernel SOM & Mixture Model

Self Organising Mixture Network:

Homoscedastic case

$$v = \arg\max_i \frac{\hat{p}_i(\mathbf{x}\,|\,\theta_i)}{\sum_j \hat{p}_i(\mathbf{x}\,|\,\theta_j)}$$

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t) + \alpha(t)h(v(\mathbf{x}),i)\frac{1}{\sum_j p_j(\mathbf{x}\,|\,\theta_j)}\frac{\partial p_i(\mathbf{x}\,|\,\theta_i)}{\partial \mathbf{m}_i}$$

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5. Kernel SOM & Mixture Model

Self Organising Mixture Network:

Homoscedastic and Gaussian case

$$v = \arg\max_i [\exp(-\frac{\|\mathbf{x}-\mathbf{m}_i\|^2}{2\sigma^2})]$$

$$\mathbf{m}_i(t+1) = \mathbf{m}_i(t) + \alpha(t)h(v(\mathbf{x}),i)\frac{1}{2\sigma^2}\frac{1}{\sum_j p_j(\mathbf{x}\,|\,\theta_j)}\exp(-\frac{\|\mathbf{x}-\mathbf{m}_i\|^2}{2\sigma^2})(\mathbf{x}-\mathbf{m}_i)$$

The same as those of Kernel SOM !!

(*Yin, Neural Networks, 19: 780-784, 2006*)

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Summary

- Objective functions of many mappings, such as *MDS*, *LLE*, *Isomap*, *eigenmap* and *ViSOM* are closely linked, but a *good algorithm or implementation* is the key.
- Converting problems (e.g. in *eigenmap or spectral clustering*) into a linear one is an advantage, in terms of uniqueness and stability of the solution.
- *SOM* is a useful tool for data clustering, *relational* visualisation (*nonmetric* scaling) and management. *ViSOM* is particularly suited for *direct visualisation* and is a *metric* preserving *nonlinear manifold*. *gViSOM* is an effective algorithm.
- *SOM* is linked to *mixture model* and kernel method.