Machine Intelligence 2

4.3 Self-Organising Maps

Prof. Dr. Klaus Obermayer

Fachgebiet Neuronale Informationsverarbeitung (NI)

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Self-Organising Maps

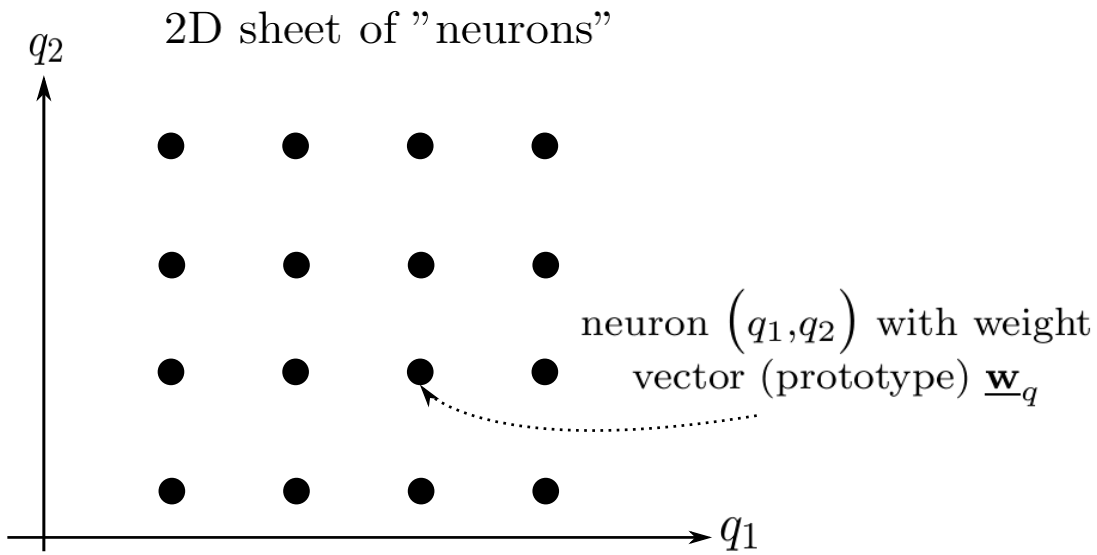
Self-organising maps (SOM)

- clustering & local embedding of vectorial data: $\underline{\mathbf{x}}^{(\alpha)}, \alpha = 1, \ldots, p$
- clustering of data based on similarity: squared Euclidean distance
- low-dimensional and **neighborhood preserving** representation for visualization

Model class

clustering with multidimensional cluster index $\underline{\mathbf{q}}$, arranged in a grid:

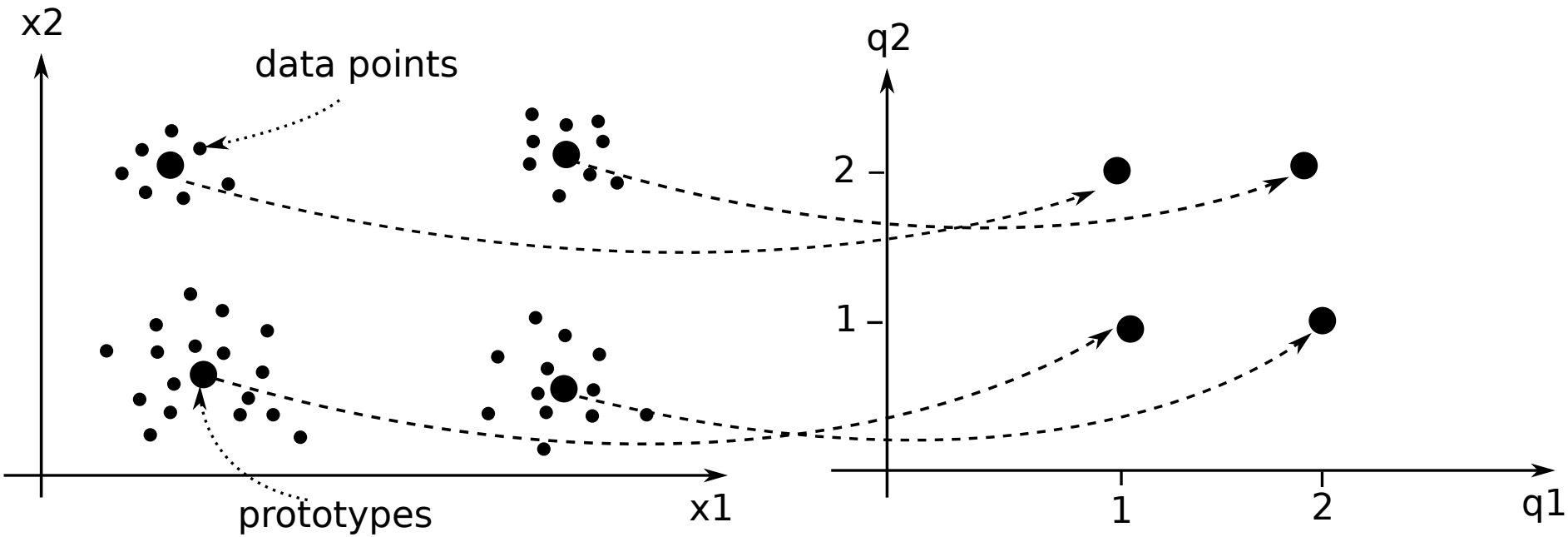
$$m_{\underline{\mathbf{q}}}^{(\alpha)} = \begin{cases} 1, & \text{if } \underline{\mathbf{q}} = \operatorname{argmin}_{\underline{\mathbf{r}}} \left| \underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{r}}} \right| \\ 0, & \text{else} \end{cases}$$



"Binary neurons" with position $\underline{\mathbf{q}} = (q_1, q_2)^T$ are assigned to prototypes $\underline{\mathbf{w}}_{\underline{\mathbf{q}}}$.

"Topographic" maps

Following algorithm's aim by self-organization:



(low-dim.) "map" of (high-dim.) data space for { visualization / dimension reduction / preprocessing for prediction

Algorithm 1: On-line learning for SOM

Initialization:

- choose no. M of partitions ("neurons")
- choose annealing schedule for ε and σ
- initialize M prototypes: $\underline{\mathbf{w}}_{\underline{\mathbf{q}}} = 1/p \sum_{\alpha} \underline{\mathbf{x}}^{(\alpha)} + \underline{\eta}$, $\underline{\eta}$ small noise vector

begin

choose a random data point $\underline{\mathbf{x}}^{(\alpha)}$

determine the closest prototype:

$$\underline{\mathbf{p}} = \underset{\underline{\mathbf{r}}}{\operatorname{argmin}} \left| \underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{r}}} \right|$$

change all prototypes $\underline{\mathbf{w}}_q$ according to:

$$\Delta \underline{\mathbf{w}}_{\underline{\mathbf{q}}} = \varepsilon \cdot h_{\underline{\mathbf{qp}}} \cdot \left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{q}}} \right) \qquad \text{for all } \underline{\mathbf{q}}$$

lower the learning rate ε and neighborhood width σ

end

Neighborhood function $h_{\underline{\mathbf{qp}}}$

$$\Delta \underline{\mathbf{w}}_{\underline{\mathbf{q}}} = \varepsilon \cdot h_{\underline{\mathbf{qp}}} \cdot \left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{q}}}^{\text{old}} \right) \qquad \text{for all q}$$

- $h_{\underline{\mathbf{qp}}}$ enforces similar learning steps for neighboring neurons
- common choice:

$$h_{\underline{\mathbf{qp}}} = \exp \left\{ - \frac{(\underline{\mathbf{q}} - \underline{\mathbf{p}})^2}{2\sigma^2} \right\}$$

- $\sigma = 0$: standard on-line K-means (only update $\underline{\mathbf{q}} = \underline{\mathbf{p}}$)

Neighborhood function $h_{\underline{\mathbf{qp}}}$

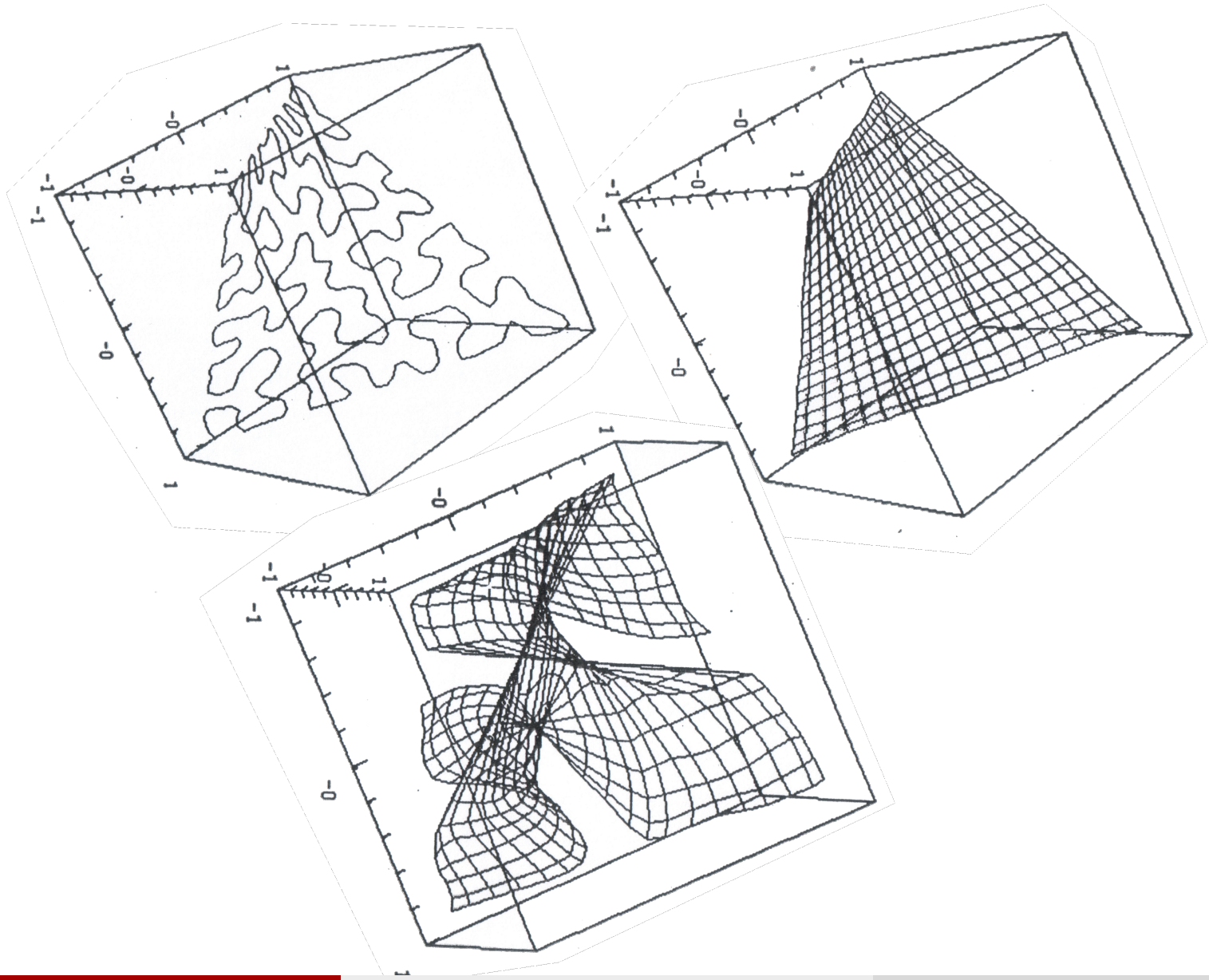
$$h_{\underline{\mathbf{qp}}} = \exp\left\{ - \frac{(\underline{\mathbf{q}} - \underline{\mathbf{p}})^2}{2\sigma^2} \right\}$$

σ annealing

- $\rightarrow$ start with large σ ($\rightsquigarrow$ neighborhood function convex over its support)
- $\rightarrow$ decrease linearly or exponentially (but "slow") during learning.
- $\rightarrow$ solution depends on final value of σ

- $\rightarrow$ $\sigma = 0$: minimum of the K-means clustering cost function but *"neighborhood preserving"*
- $\rightarrow$ σ small : better representation capabilities at the expense of a non-optimal clustering cost

2d manifold example



Measurements of Leptograpsus variegatus

Dead crabs loose their color and their sexual features –
$\Rightarrow$ Can we infer species & sex from the shell size and shape?

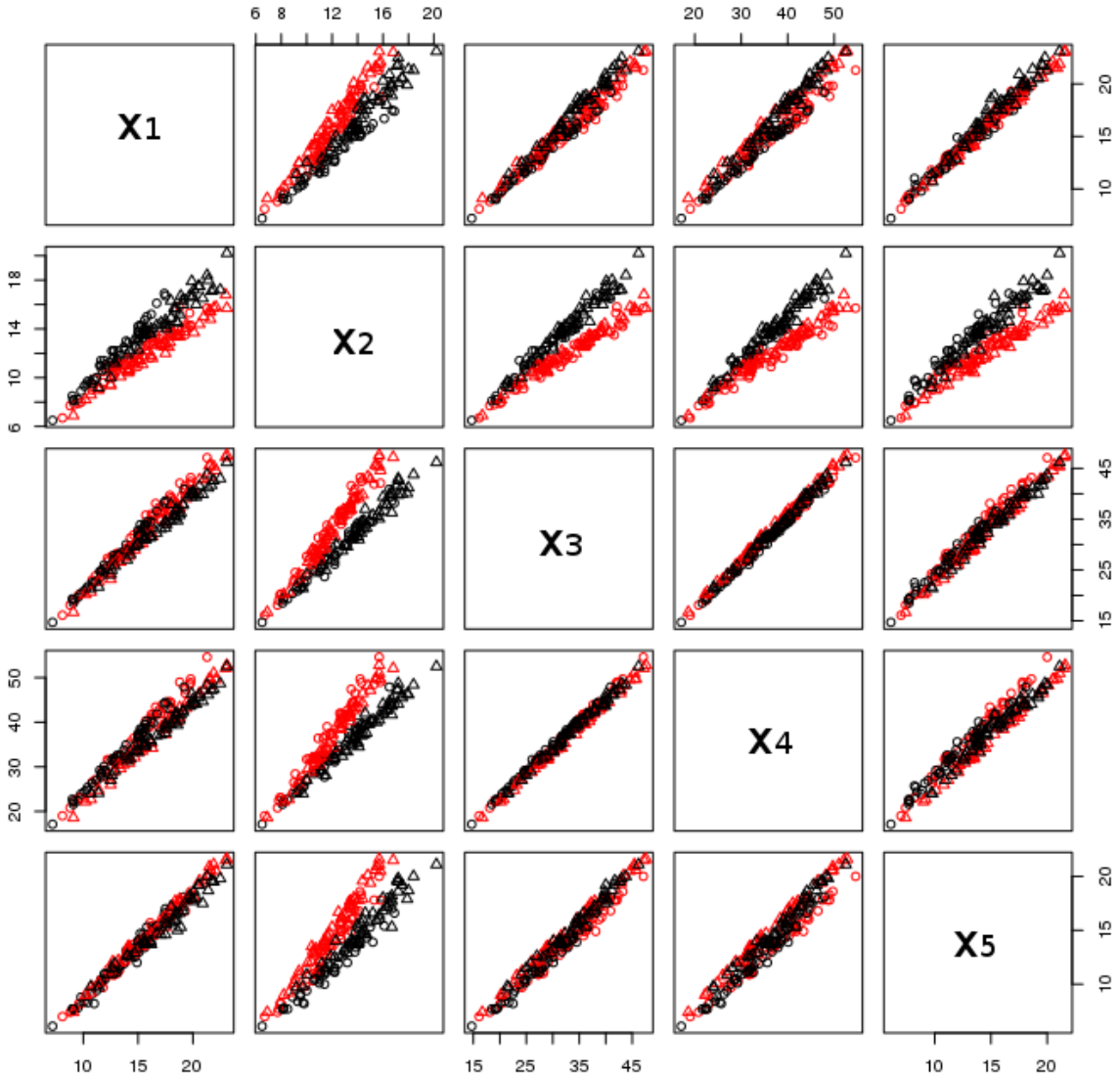
$$\text{crabs: L. variegatis} \left\{ \begin{array}{l} \text{orange} \\ \text{blue} \end{array} \right\} \begin{array}{l} \text{two (sub-)species} \\ \rightarrow \text{ male and female crabs} \end{array}$$

- *elementary features:*

$$\left. \begin{array}{ll} \text{frontal lobe size:} & x_1 \\ \text{rear width:} & x_2 \\ \text{carapace length:} & x_3 \\ \text{carapace width:} & x_4 \\ \text{body depth:} & x_5 \end{array} \right\} \text{5-dim. feature vector}$$

- *complex features:* linear combinations of elementary features
  $\Rightarrow$ directions in feature space which could identify color and/or sex.

The Leptograpsus data: scatter plot



sex

black: female

red: male

species

△ : orange

○ : blue

attributes

X_1: frontal lobe size (mm)

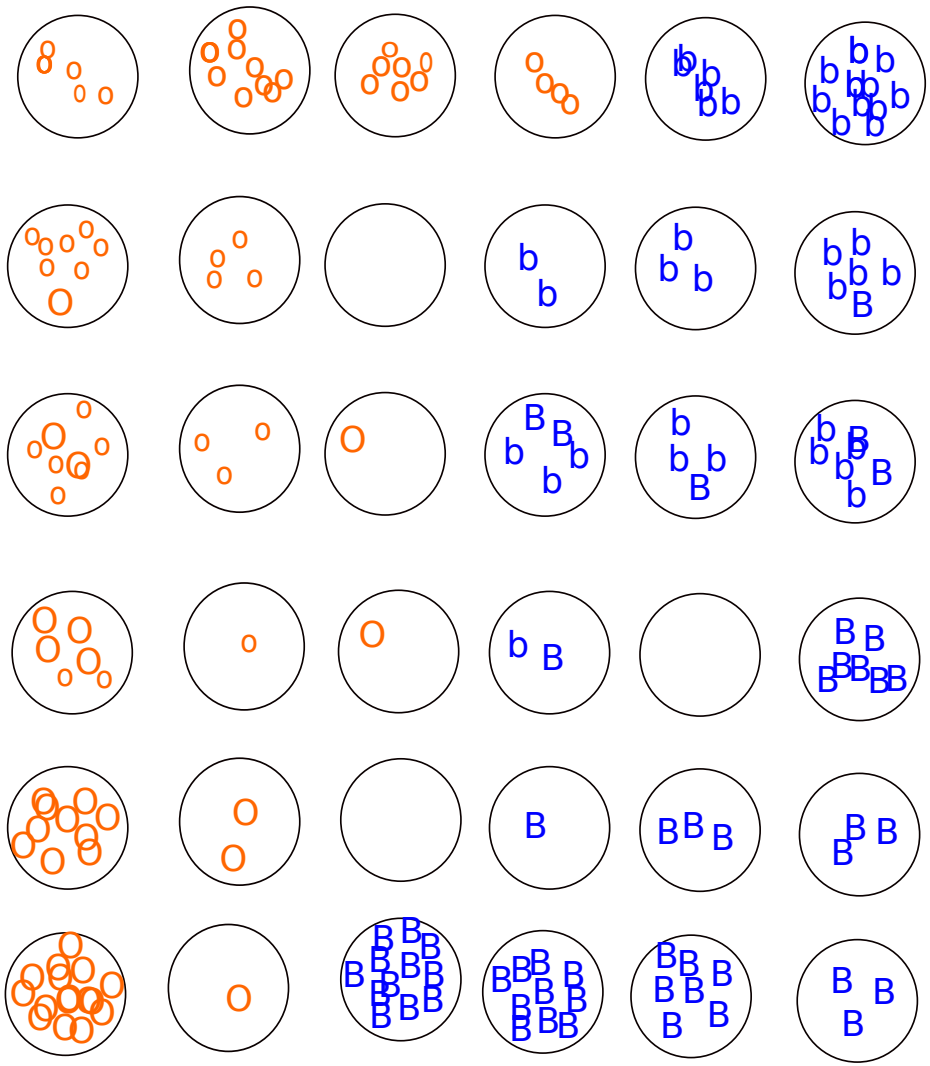
X_2: rear width (mm)

X_3: carapace length (mm)

X_4: carapace width (mm)

X_5: body depth (mm)

Leptograpsus example



capital letters -> male small letters -> female

attributes

X_1: frontal lobe size (mm)

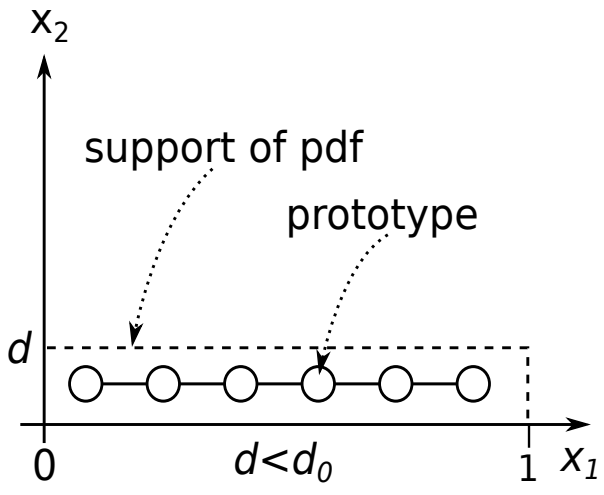
X_2: rear width (mm)

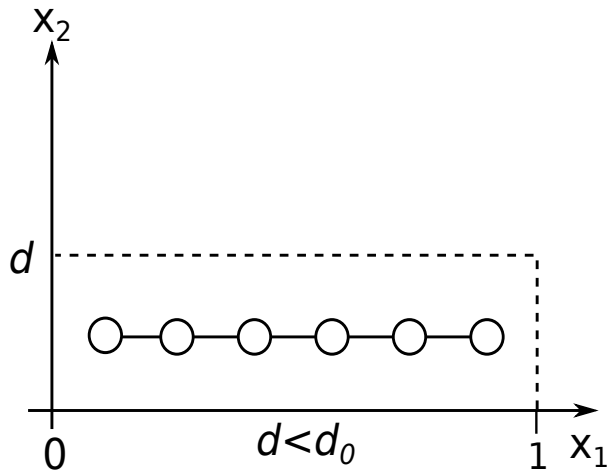
X_3: carapace length (mm)

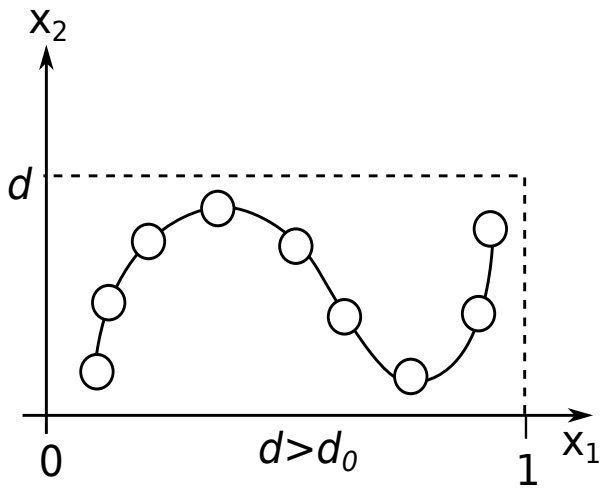
X_4: carapace width (mm)

X_5: body depth (mm)

Dimension reducing mappings







Semantic maps

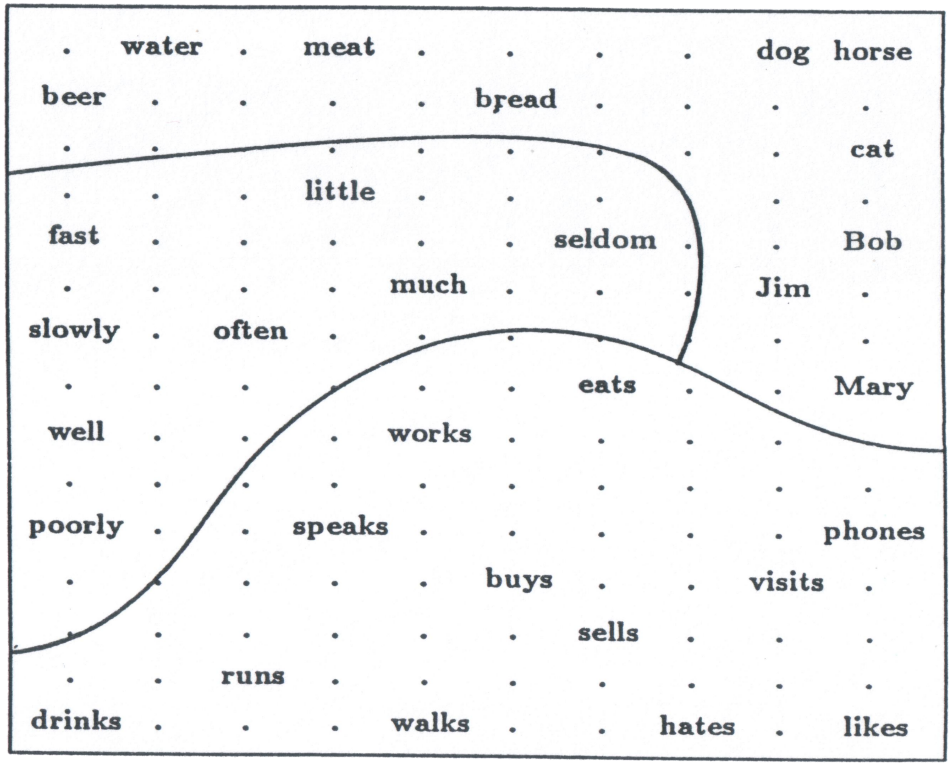
Abstract Data: Verbal Statements

Bob/Jim/Mary	1
horse/dog/cat	2
beer/water	3
meat/bread	4
runs/walks	5
works/speaks	6
visits/phones	7
buys/sells	8
likes/hates	9
drinks/eats	10
much/little	11
fast/slowly	12
often/seldom	13
well/poorly	14

Sentence Patterns:

1-5-12	1-9-2	2-5-14
1-5-13	1-9-3	2-9-1
1-5-14	1-9-4	2-9-2
1-6-12	1-10-3	2-9-3
1-6-13	1-11-4	2-9-4
1-6-14	1-10-12	2-10-3
1-6-15	1-10-13	2-10-12
1-7-14	1-10-14	2-10-13
1-8-12	1-11-12	2-10-14
1-8-2	1-11-13	1-11-4
1-8-3	1-11-14	1-11-12
1-8-4	2-5-12	2-11-13
1-9-1	2-5-13	2-11-14

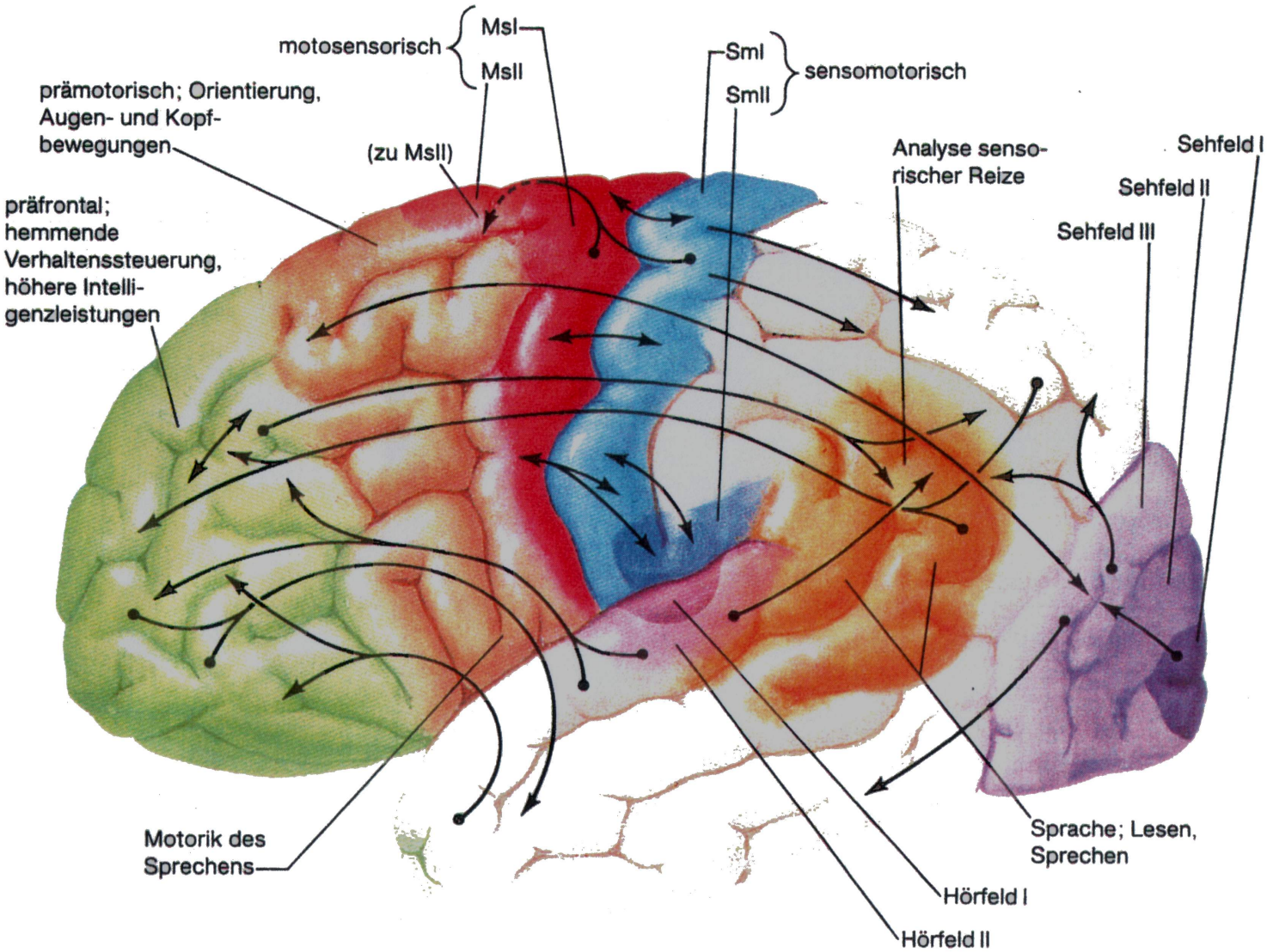
Mary likes meat
Jim speaks well
Mary likes Jim
Jim eats often
Mary buys meat
dog drinks fast
horse hates meat
Jim eats seldom
Bob buys meat
cat walks slowly
Jim eats bread
cat hates Jim
Bob sells beer
(etc.)



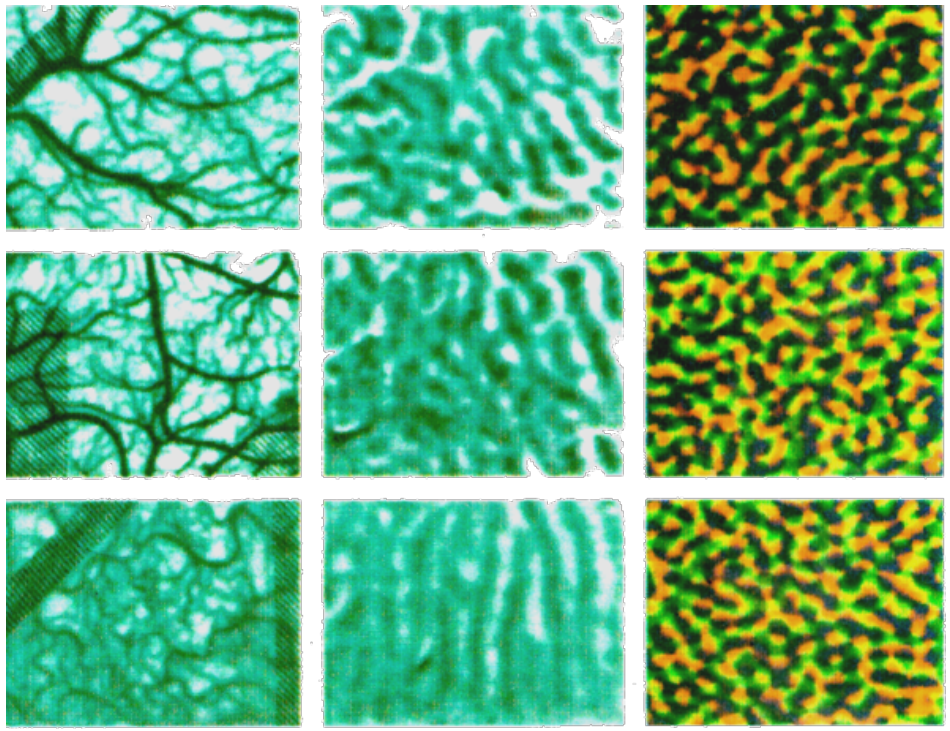
$$\begin{bmatrix} \vec{v}_s \\ \vec{v}_c \end{bmatrix} = \begin{bmatrix} \vec{0} \\ \vec{v}_c \end{bmatrix} + \begin{bmatrix} \vec{v}_s \\ \vec{0} \end{bmatrix}$$

Ritter & Kohnen 1989

Orientation & ocular dominance maps

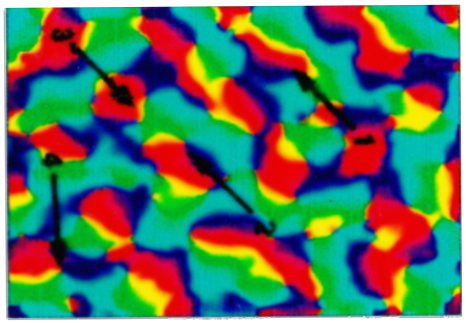


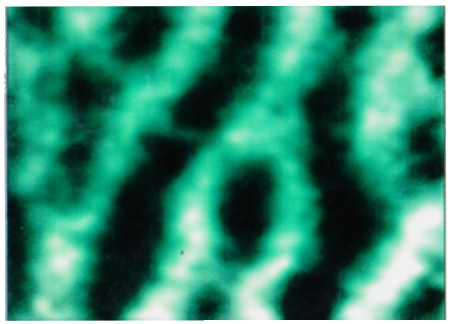
Orientation & ocular dominance maps



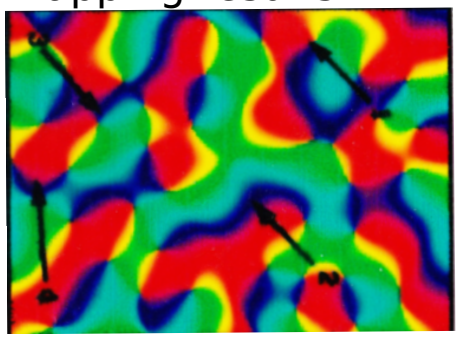
Orientation & ocular dominance maps

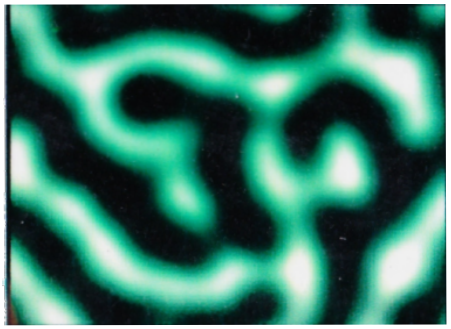
experimental data:





mapping results:





5d feature vector

position: $x, y \in [0, d]$

orientation preference & specificity:

$r\cos(2\phi),\ \phi \in [0, \pi[$

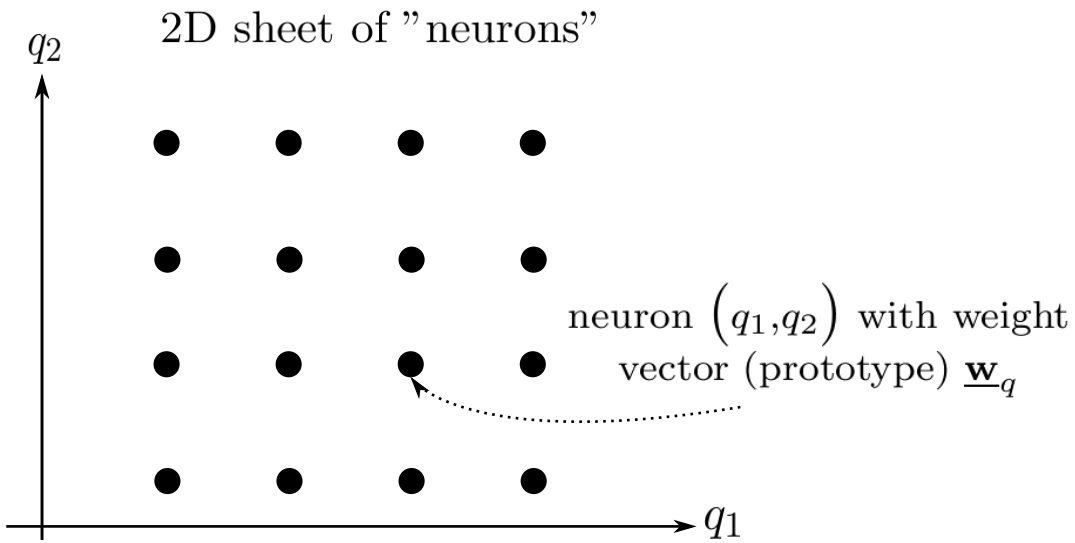
$r\sin(2\phi),\ \phi \in [0, \pi[$

ocular dominance: $z \in \{-1, 1\}$

Self-organizing maps for pairwise data

- distance matrix $\underline{\mathbf{D}}$ specifying the distances or 'dissimilarities' $d_{\alpha\alpha'}$ between p "objects" $\alpha = 1, \ldots, p$
- set of M clusters (partitions) $\underline{\mathbf{q}}$ with a geometrical structure (e.g. 1-d line or 2-d grid).
- binary assignment variables (normalized):

$$m_{\underline{\mathbf{q}}}^{(\alpha)} = \begin{cases} 1, & \text{if object } \alpha \text{ belongs to cluster } \underline{\mathbf{q}} \\ 0, & \text{else} \end{cases}$$



	1	2	3		p
1	0	1.7	0.99		3.0
2	1.7	0	0.3	...	0.1
3	0.9	0.3	0		0.2
⋮		⋮		⋱	⋮
p	3.0	0.1	0.2	...	0

relational representation "pairwise data"

Cost function & model selection

$$E_{\left[\left\{m_{\underline{\mathbf{q}}}^{(\alpha)}\right\}\right]} = \frac{1}{p}\sum_{\underline{\mathbf{r}}} \frac{\sum_{\alpha,\alpha'}\left(\sum_{\underline{\mathbf{q}}} h_{\underline{\mathbf{r}}\underline{\mathbf{q}}} m_{\underline{\mathbf{q}}}^{(\alpha)}\right)\left(\sum_{\underline{\mathbf{q}}} h_{\underline{\mathbf{r}}\underline{\mathbf{q}}} m_{\underline{\mathbf{q}}}^{(\alpha')}\right) d_{\alpha\alpha'}}{\sum_{\alpha}\left(\sum_{\underline{\mathbf{q}}} h_{\underline{\mathbf{r}}\underline{\mathbf{q}}} m_{\underline{\mathbf{q}}}^{(\alpha)}\right)} \stackrel{!}{=} \min$$

- $m_q^{(\alpha)} \rightarrow \sum_{\underline{\mathbf{q}}} h_{\underline{\mathbf{r}}\underline{\mathbf{q}}} m_{\underline{\mathbf{q}}}^{(\alpha)}$
- "neighboring" clusters (w.r.t. $h_{\underline{\mathbf{r}}\underline{\mathbf{q}}}$) contribute to the total average distance
- "neighborhood preserving maps" induce lower cost

Algorithm 2: SOM for pairwise data (mean-field approximation)

Initialization:

- choose no. M of partitions, initial (β_0) and final (β_f) noise parameters, annealing factor η, width σ of neighborhood function $h_{\underline{\mathbf{sq}}}$, tolerance θ
- initialize mean-fields $e_{\underline{\mathbf{q}}}^{(\alpha)}$: random numbers $\in [0,1]$

$\beta \leftarrow \beta_0$

while $\beta < \beta_f$ **do** annealing

  repeat EM

    compute assignment probabilities $\left\langle m_{\underline{\mathbf{q}}}^{(\alpha)} \right\rangle_Q = \frac{\exp\left\{-\beta\left(e_{\underline{\mathbf{q}}}^{(\alpha)}\right)_{\text{old}}\right\}}{\sum_{\underline{\mathbf{r}}} \exp\left\{-\beta\left(e_{\underline{\mathbf{r}}}^{(\alpha)}\right)_{\text{old}}\right\}} \quad \forall \underline{\mathbf{q}}, \alpha$

    compute new mean-fields

$$\left(e_{\underline{\mathbf{q}}}^{(\alpha)}\right)_{\text{new}} = \frac{1}{p} \sum_{\underline{\mathbf{s}}} h_{\underline{\mathbf{sq}}} \left[\frac{1}{\sum_{\gamma} \left(\sum_{\underline{\mathbf{r}}} h_{\underline{\mathbf{sr}}} \left\langle m_{\underline{\mathbf{r}}}^{(\gamma)} \right\rangle_Q \right)} \sum_{\delta} \left(\sum_{\underline{\mathbf{r}}} h_{\underline{\mathbf{sr}}} \left\langle m_{\underline{\mathbf{r}}}^{(\delta)} \right\rangle_Q \right] \right.$$

$$\left. \cdot \left\{ d_{\delta\alpha} - \frac{1}{2} \frac{1}{\sum_{\gamma} \left(\sum_{\underline{\mathbf{r}}} h_{\underline{\mathbf{sr}}} \left\langle m_{\underline{\mathbf{r}}}^{(\gamma)} \right\rangle_Q \right)} \sum_{\varepsilon} \left(\sum_{\underline{\mathbf{r}}} h_{\underline{\mathbf{sr}}} \left\langle m_{\underline{\mathbf{r}}}^{(\varepsilon)} \right\rangle_Q \right) d_{\varepsilon\delta} \right\} \right] \quad \forall \underline{\mathbf{q}}, \alpha$$

  until $\left| \left(e_{\underline{\mathbf{q}}}^{(\alpha)}\right)_{\text{new}} - \left(e_{\underline{\mathbf{q}}}^{(\alpha)}\right)_{\text{old}} \right| < \theta \quad \forall \underline{\mathbf{q}}, \alpha$

  $\beta \leftarrow \eta\beta$

end

Comments

- replacing $h_{\underline{\mathbf{sp}}}$ by $\delta_{\underline{\mathbf{sp}}}$ recovers standard pairwise clustering
- "Kohonen-approximation": replace $h_{\underline{\mathbf{sp}}}$ by $\delta_{\underline{\mathbf{sp}}}$ for the neighborhood function (only) at $\circledast$ in algorithm 2
  - $\rightarrow$ reduction of computational cost
  - $\rightarrow$ visualization properties remain
  - $\rightarrow$ original algorithm suggested by T. Kohonen is recovered for squared Euclidean distances $d_{\alpha\alpha'}$ and $\beta \rightarrow \infty$
- no need for σ annealing

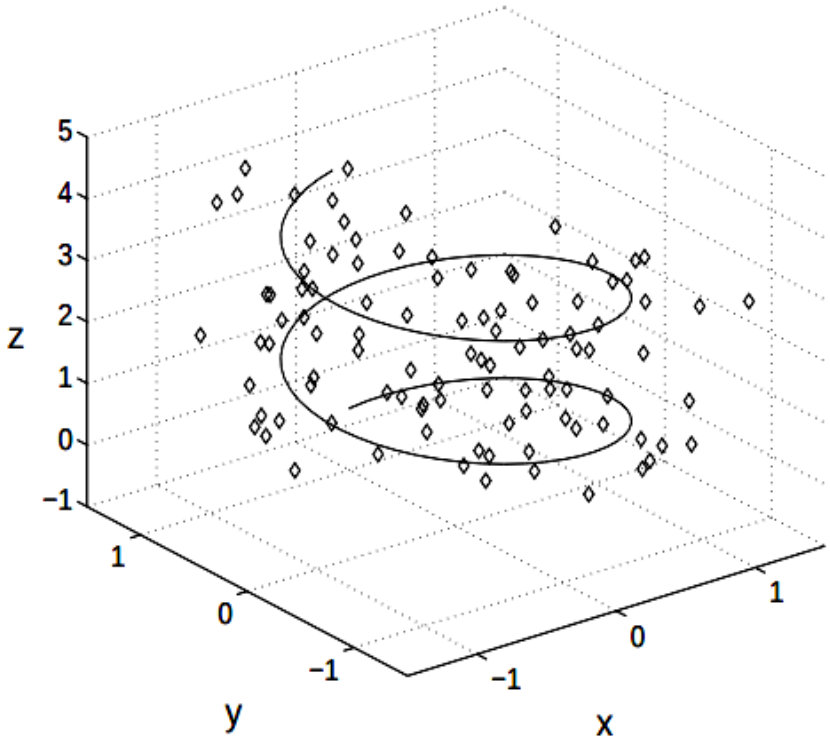
Toy example: noisy spiral

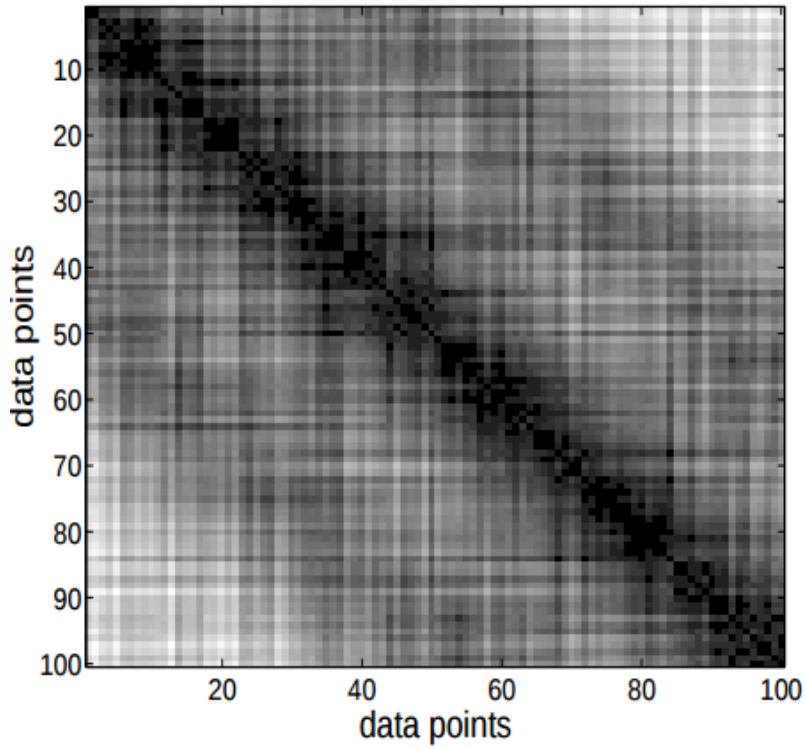
1000 data points:

$$x = \sin\theta + \eta_x$$
$$y = \cos\theta + \eta_y$$
$$z = \frac{\theta}{\pi} + \eta_z$$

$\theta \in [0, 4\pi]; \qquad \eta \backsim \mathcal{N}_{(0,0.3)}$

Euclidean squared distance

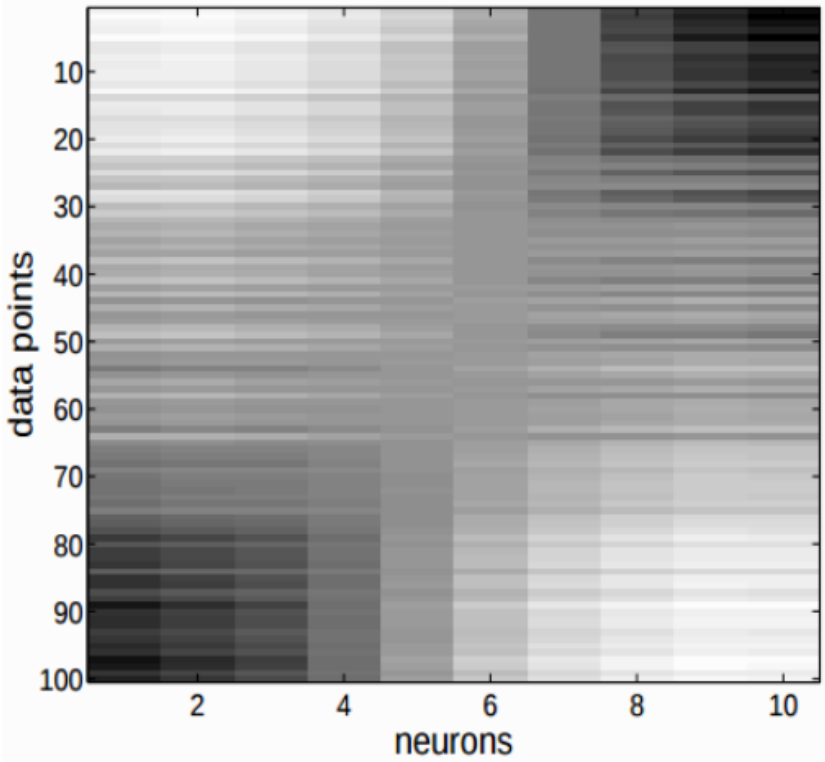




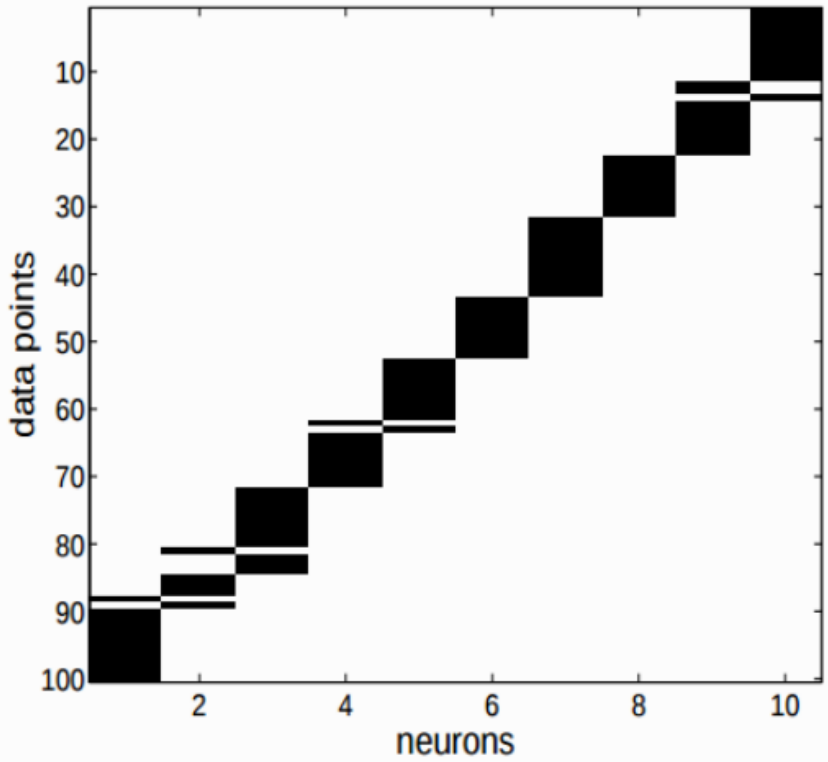
Toy example: noisy spiral

- 10 neurons in 1D
- Gaussian neighborhood function, $\sigma = 0.5$

β=0.8



β=186.21

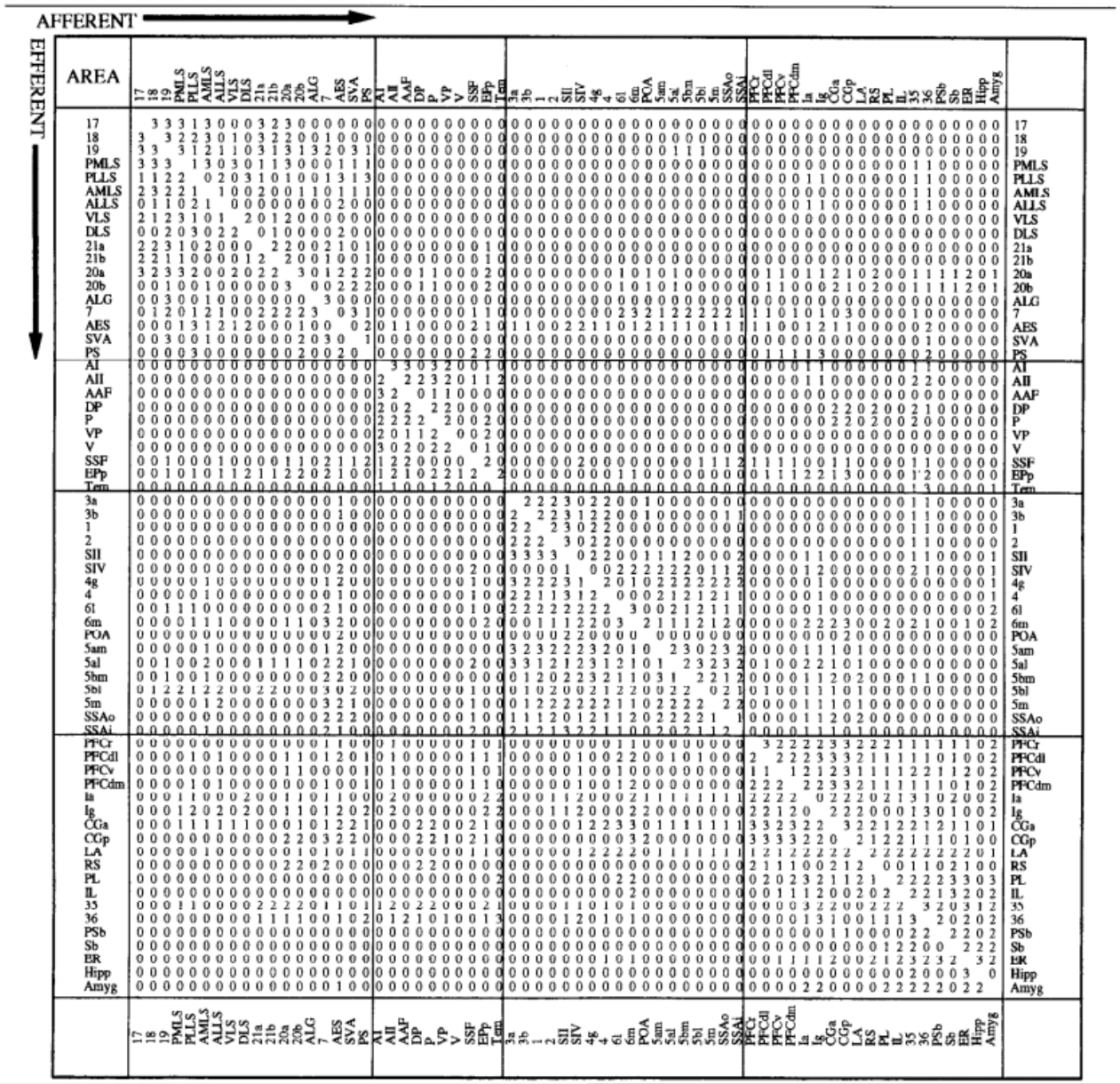


Mapping cat's cerebral cortex

Preprocessing:

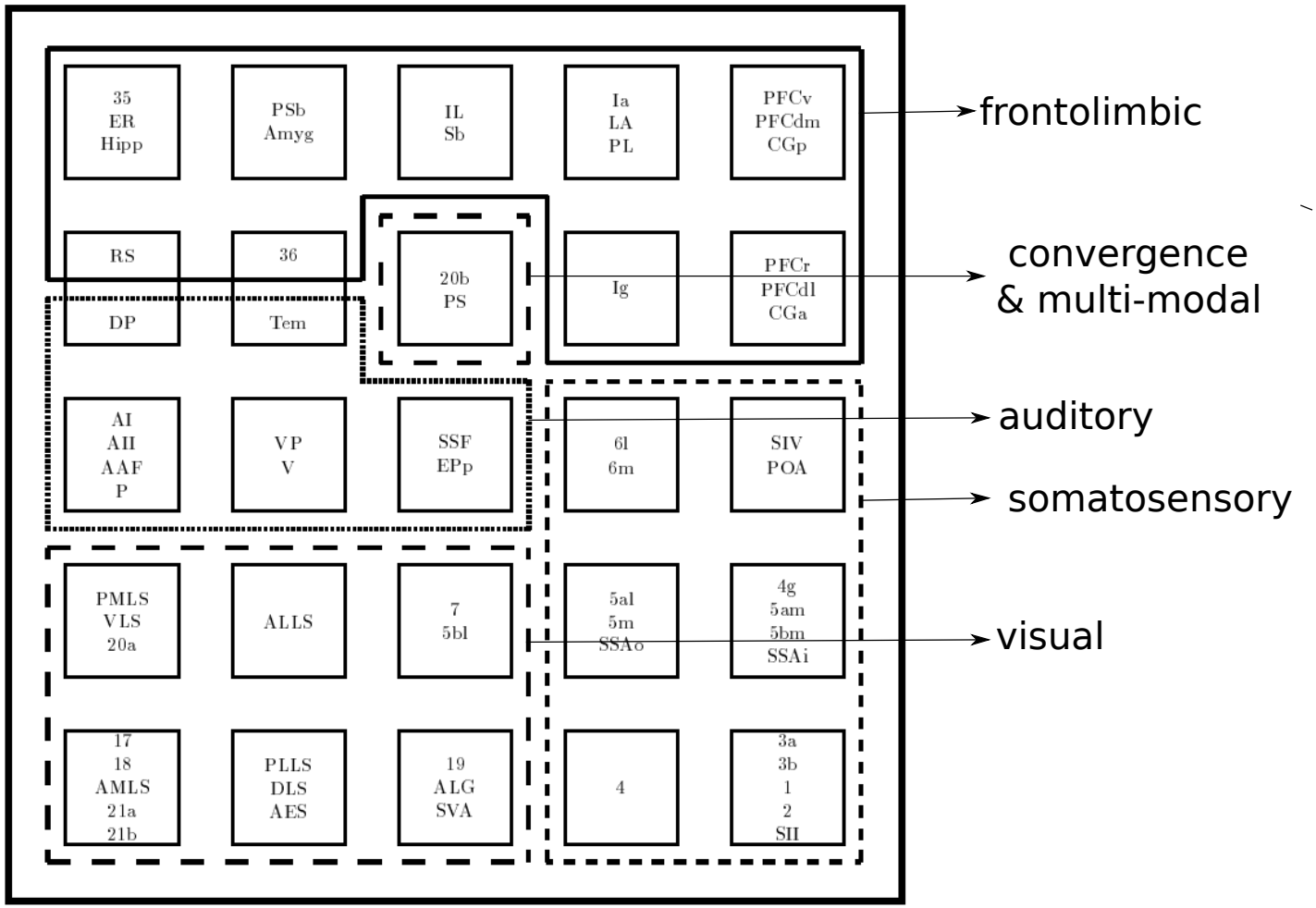
$d_{(l,l')} \leftarrow 4 - d_{(l,l')}$

diagonal: $d_{(l,l)} = 0$



Mapping cat's cerebral cortex

"Kohonen"-map:
5x5 neurons,
Gaussian
neighborhood
$\delta_n = 0.4$



Squared Euclidean distances

$$d_{\alpha\alpha'} = \frac{1}{2}\left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{x}}^{(\alpha')}\right)^2$$

cost function:

$$E_{\left[\left\{m_{\underline{\mathbf{q}}}^{(\alpha)}\right\}\right]} = \frac{1}{p}\sum_{\underline{\mathbf{q}},\alpha}\left(\sum_{\underline{\mathbf{p}}} h_{\underline{\mathbf{qp}}} m_{\underline{\mathbf{p}}}^{(\alpha)}\right)\left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_q\right)^2 = \frac{1}{p}\sum_{\underline{\mathbf{p}}\alpha} m_{\underline{\mathbf{p}}}^{(\alpha)} \sum_{\underline{\mathbf{q}}} h_{\underline{\mathbf{qp}}}\left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{q}}}\right)^2$$

$$\underline{\mathbf{w}}_{\underline{\mathbf{q}}} = \frac{\sum_{\alpha'}\left(\sum_{\underline{\mathbf{p}}} h_{\underline{\mathbf{qp}}} m_{\underline{\mathbf{p}}}^{(\alpha')}\right)\underline{\mathbf{x}}^{(\alpha')}}{\sum_{\alpha'}\left(\sum_{\underline{\mathbf{p}}} h_{\underline{\mathbf{qp}}} m_{\underline{\mathbf{p}}}^{(\alpha')}\right)}$$

$\underline{\mathbf{w}}_{\underline{\mathbf{q}}}$: center of mass of all data which belongs to cluster weighted by the neighborhood function $h_{\underline{\mathbf{qp}}}$

On-line minimization of E^T

Algorithm 3: Online learning for SOM with Euclidean distances

Initialization of prototypes

Select learning step ε

begin

choose a random data point $\underline{\mathbf{x}}^{(\alpha)}$

assign data point to the prototype with minimum assignment cost

$$\underline{\mathbf{p}} = \underset{\underline{\mathbf{r}}}{\operatorname{argmin}} \sum_{\underline{\mathbf{q}}} \underbrace{h_{\underline{\mathbf{r}}\underline{\mathbf{q}}}}_{\circledast} \left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{q}}}^{\text{old}}\right)^2$$

change all prototypes according to

$$\Delta \underline{\mathbf{w}}_{\underline{\mathbf{q}}} = \varepsilon h_{\underline{\mathbf{p}}\underline{\mathbf{q}}} \cdot \left(\underline{\mathbf{x}}^{(\alpha)} - \underline{\mathbf{w}}_{\underline{\mathbf{q}}}\right) \text{ for all } \underline{\mathbf{q}}$$

end