Learning from examples in Neural Gas and Vector Quantization

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Abstract

The dynamics of training a neural gas for vector quantization in high dimensions is studied by means of methods from statistical physics. Prototype vectors for the representation of the data are updated either off-line from a given, fixed set of example data, or on-line from a sequence of single data. Here we concentrate on the latter case. For the on-line learning scenario, a description of the learning dynamics in terms of ordinary differential equations for a set of order parameters becomes exact in the limit of infinite-dimensional data. We explain the method, present first results and discuss possible extensions.

1. Introduction

- **Vector Quantization (VQ)**
  unsupervised identification of prototype vectors
  for the **representation** of data (e.g. clusters) by means of **distance-based competitive learning**, see, e.g. [1]
- **Neural Gas (NG)**
  representation of data by (many) prototypes
  determined by **rank based competitive learning** [2]
- **Self-Organizing Maps** (SOM)
  representation of data by a grid of prototypes
  competitive learning + **pre-defined topology** [3]

Aims:
– understand **typical properties** of VQ and NG
in terms of **model situations** with high-dim. data
– dynamics of on-line learning
– typical equilibrium properties of off-line training
– evaluate the **performance of training schemes**
– develop novel and **efficient algorithms**
– extensions to Self-Organizing Maps and similar systems

2. The Model

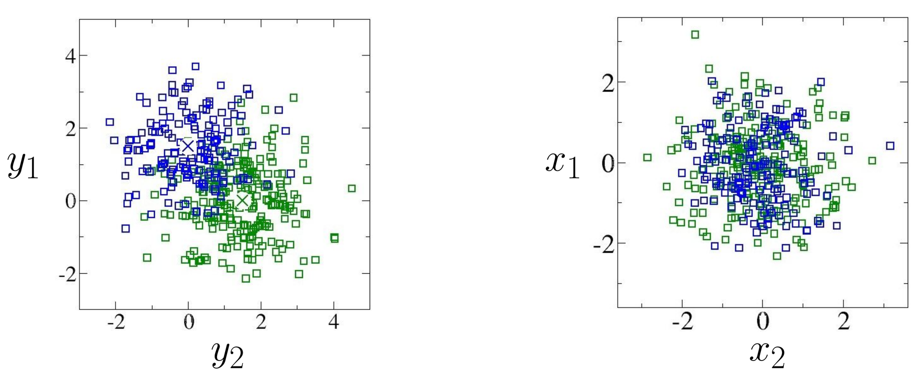
2.1 The example data

Independent random inputs $\vec{\xi}^\mu \in \mathbf{R}^N$, $\mu = 1, 2, \ldots P$,
drawn from a **mixture density** (index μ omitted)

$$P(\vec{\xi}) = \sum_{m=1}^{M} p_m P(\vec{\xi} \mid m) \text{ with } P(\vec{\xi} \mid m) = \frac{1}{(2\pi v_m)^{N/2}} \exp\left[-\frac{1}{2v_m}\left(\vec{\xi} - \ell\vec{B}_m\right)^2\right].$$

Mixture of Gaussians
spherical clusters with variance v_m, centered at $\ell\vec{B}_m$,
prior weights $\sum_m p_m = 1$

orthonormal vectors $\vec{B}_m \in \mathbf{R}^N$ with $\vec{B}_m \cdot \vec{B}_n = \delta_{m,n}$.
Note: $(\vec{B}_m)^2 = 1$, but $\left\langle (\vec{\xi})^2 \right\rangle_m = v_m N + \ell^2 \sim N$



Example: Monte Carlo data ($N = 200$) with $M = 2$, $v_1 = v_2 = 1$
left: *weak separation apparent in $y_m = \vec{B}_m \cdot \vec{\xi}$ centers marked by "×"*
right: *projections $x_k = \vec{w}_k \cdot \vec{\xi}$ on independent random $\vec{w}_k$ ($\vec{w}_k^2 = 1$)*

Notation: conditional averages $\langle \cdots \rangle_m$ over $P(\vec{\xi} \mid m)$

averages $\langle \cdots \rangle = \sum_{m=1}^{M} p_m \langle \cdots \rangle_m$ over the full $P(\vec{\xi})$

2.2 Training

Rank based training of prototypes

- initialize a **set of prototypes** $\left\{\vec{w}_k \in \mathbb{R}^N\right\}_{k=1}^{K}$
  e.g. random $\vec{w}_k(0) \approx 0$

1) present a **single example vector** $\vec{\xi}^\mu$

2) evaluate the (squared) **distances** $d(k,\mu) = \left(\vec{\xi}^\mu - \vec{w}_k\right)^2$
sort: $d(j(1),\mu) \geq d(j(2),\mu) \geq \ldots \geq d(j(K),\mu)$
here: $r(j)$ is the **rank** of prototype j w.r.t. $\vec{\xi}^\mu$
$j(r)$ is the index of the prototype with rank r

3) update all prototypes
$$\vec{w}_k(t+1) = \vec{w}_k(t) + \frac{\eta}{N} f(r(k)) \left(\vec{\xi}^\mu - \vec{w}_k(t)\right)$$

– **learning rate** η controls the step size
– update is **towards the data**
– **rank function** $f(r)$ defines the magnitude:

- $f(r) = e^{-r/\sigma}$ rank based Neural Gas as in [2]
- $f(r) = \begin{cases} 1 & \text{if } r = 1 \\ 0 & \text{else} \end{cases}$ (Winner-Takes-All)
- $f(r) = K - r$ linear rank function $(K - 1 \geq f(r) \geq 0)$
  considered in the following

associated cost function quantization error

$$H(\{w_k\}) = \sum_\mu \sum_k f(r(k)) \left(\vec{\xi}^\mu - \vec{w}_k\right)^2$$

3. The analysis

training from a sequence of **independent examples** ($t \equiv \mu$),
consider **macroscopic overlaps as order parameters**

$$R_{km}(\mu) = \vec{w}_k(\mu) \cdot \vec{B}_m \quad \text{and} \quad Q_{jk}(\mu) = \vec{w}_j(\mu) \cdot \vec{w}_k(\mu)$$
$$\text{for} \quad k = 1, 2, \ldots, K, \quad \text{and} \quad m = 1, 2, \ldots, M.$$

training algorithm $\rightarrow KM + K(K+1)$ recursion relations

$$\frac{R_{km}(\mu) - R_{km}(\mu-1)}{1/N} = \eta f(r(k)) \left(y_m^\mu - R_{km}(\mu-1)\right)$$
$$\frac{Q_{kl}(\mu) - Q_{kl}(\mu-1)}{1/N} = \eta f(r(k)) \left(x_k^\mu - Q_{kl}(\mu-1)\right) + \eta f(r(l)) \left(x_l^\mu - Q_{kl}(\mu-1)\right) + \eta^2 f(r(k)) f(r(l)) + \mathcal{O}\left(\frac{1}{N}\right)$$

with $x_k^\mu = \vec{w}_k(\mu-1) \cdot \vec{\xi}^\mu$ and $y_m^\mu = \vec{B}_m \cdot \vec{\xi}^\mu$

Central Limit Theorem $\rightarrow$ **Gaussian** $P(\{x_k^\mu\}, \{y_m^\mu\})$ given by

$$\langle x_k^\mu \rangle_m = \ell R_{km}(\mu-1), \quad \langle y_m^\mu \rangle_n = \ell \delta_{mn}, \quad \langle x_k^\mu x_l^\mu \rangle_m - \langle x_k^\mu \rangle_m \langle x_l^\mu \rangle_m = v_m Q_{kl}(\mu-1)$$
$$\langle x_k^\mu y_n^\mu \rangle_m - \langle x_k^\mu \rangle_m \langle y_n^\mu \rangle_m = R_{kn}^{\mu-1}, \quad \langle y_m^\mu y_n^\mu \rangle_q - \left\langle y_m^\mu \right\rangle_q \left\langle y_n^\mu \right\rangle_q = v_q \delta_{mn}.$$

thermodynamic limit $N \rightarrow \infty$:

- **averages over latest example** $\rightarrow$ r.h.s. as functions of overlaps
- $\rightarrow$ **coupled ODEs** in *continuous time* $\alpha = \mu/N$.
- $\{R_{km}, Q_{kl}\}$ **self–averaging** w.r.t. random examples, e.g. [6]
  fluctuations vanish in the limit $N \rightarrow \infty$

Analytical evaluation possible with the following simplifications

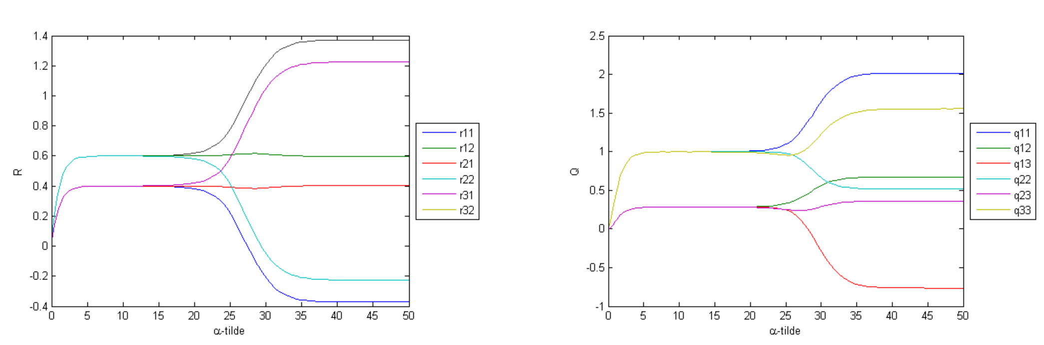
- **limit of small learning rates** $\rightarrow$ neglect term $\propto \eta^2$
  $\eta \rightarrow 0$, $\alpha \rightarrow \infty$, such that $\tilde{\alpha} = \eta\alpha = \mathcal{O}(1)$
- **linear rank function**
  note: rank can be obtained from pair-wise comparison
  $r(k) = \sum_{j \neq k} \Theta\left[d(k,\mu) - d(j,\mu)\right]$ with $\Theta(x) = \begin{cases} 1 & \text{for } x \geq 0 \\ 0 & \text{else} \end{cases}$

numerical integration of ODE, from initial $R_{km}(0), Q_{kl}(0)$
$\rightarrow$ **learning curves** $R_{km}(\tilde{\alpha}), Q_{kl}(\tilde{\alpha})$
$\rightarrow$ **typical dynamics of learning** in high dimensions
fixed point analysis,...

4. First results

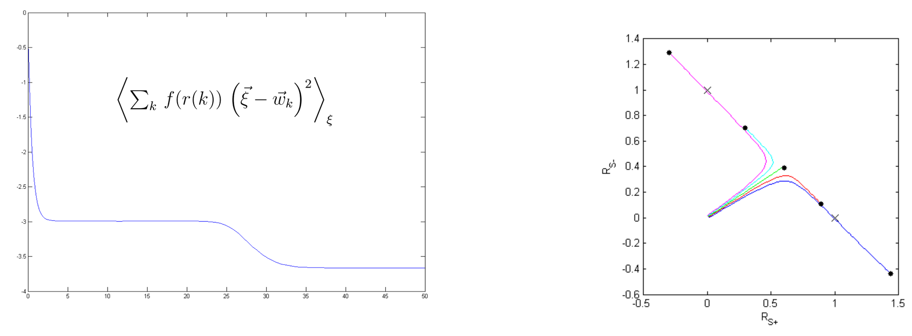
4.1 Learning curves

Example situation
data from two clusters, $p_1 = 0.6, p_2 = 0.4$, variances $v_1 = v_2 = 1$,
separation $\ell = 1$, 3 prototype vectors
evolution of R_{jm}, Q_{ij}:



intial phase: **unspecialized units** in the space $\perp \{B_j\}_{m=1}^{M}$.
asymptotic configuration: lowest quantization error

Left: evolution of the average (weighted) **quantization error**

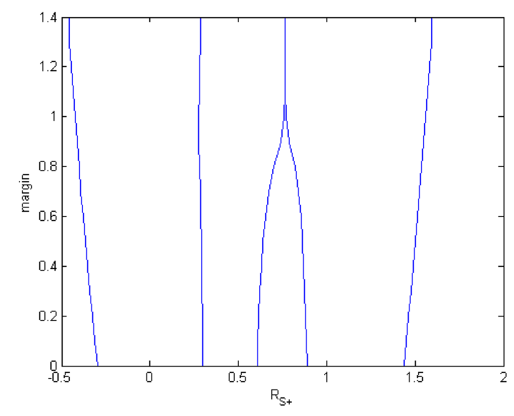


Right: trajectory of **5 prototypes**, projected into the $B_{1,2}$-plane

4.2 Modified rank evaluation

NG rank function $f(r) \propto e^{-r/\sigma}$:
system approaches *Winner-Takes-All* behavior for $\sigma \rightarrow 0$

Modified rank function:
similar effect by introduction of a *margin* c
$f(\hat{r}(j)) = \sum_{j \neq k} \Theta\left[d_j - d_k - c\right]$ (count only *clear wins*)



margin vs. $\alpha \rightarrow \infty$ asymptotic configuration

- few prototypes and/or small margin:
  all prototype along connection of clusters
- many prototypes and/or large margin:
  projections of several $\vec{w}_i$ merge
  actual position differs in the space $\perp$ to $\left\{\vec{B}_m\right\}$

5. Outlook

- detailed fixed point analysis
  (repulsive/attractive configurations, plateaus in the learning curves)
- investigation of the *magnification factor* of NG
  (*density* of prototypes vs. density of the data)
- optimized training schedules: learning rate, margins
- analysis of *batch Neural Gas* algorithms

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