SAMMON'S MAPPING AS SUBJECT OF HEURISTIC MINIMIZATION

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Abstract

Sammon's mapping is a nonlinear tool for optimum mapping between two metric spaces including Euclidean ones. The original data are transformed into 1D, 2D or 3D Euclidean space. The adequate objective function is continuous but non-smooth and non-convex with many local extremes. Thus, the global optimization heuristics play the role in finding of sub-optimum mapping. The paper is oriented to the role of parameters to the difficulty for optimization task and the quality of self-organization. The mapping and optimization routine are completely realized in the Matlab environment.

1 Mathematical background

Let **M** be non-empty finite set, **N** be non-empty set and $\langle \mathbf{M}, \mathrm{d} \rangle, \langle \mathbf{N}, \delta \rangle$ be two metric spaces with metrics $\mathrm{d} : \mathbf{M} \times \mathbf{M} \to \mathbf{R}_0^+$ or $\delta : \mathbf{N} \times \mathbf{N} \to \mathbf{R}_0^+$, respectively. In the special case of $\mathbf{N} = \mathbf{R}^n$ we can introduce Minkowski metrics for $p \geq 1$ as $\delta_p(\mathbf{x}, \mathbf{y}) = \left(\sum_{k=1}^{n} |x_k - y_k|^p \right)^{1/p}$. Euclidean metrics is then a special case for $p = 2$, Manhattan distance is a case of $p = 1$ and the maximum distance is a special case for $p \to \infty$ when $\delta_\infty(\mathbf{x}, \mathbf{y}) = \max_{1 \leq k \leq n} |x_k - y_k|$. The distances between elements of **M** are collected in matrix $\mathbf{D} = \{d_{i,j}\}_{i,j=1}^{m}$ where m is number of self-organized objects. The traditional Sammon's mapping[4] is a function $\mathrm{S} : M \to N$ which minimizes the objective function $\mathrm{F}(\mathbf{x}_1, \ldots, \mathbf{x}_m) = \sum_{i<j} \frac{\left(d_{i,j} - \delta_p(\mathbf{x}_i, \mathbf{x}_j)\right)^2}{d_{i,j}}$. The aim of optimum mapping is in plotting of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_m$ into 1D, 2D or 3D vector space, which enables to reconstruct relationships of objects from space **M** using another space $\mathbf{N} = \mathbf{R}^n$ where p = n = 2 in many applications.

The Sammon's mapping is similar to the minimization of sum of squares of absolute or relative differences of adequate distances. So, the original objective function was extended to the form

$$\Phi(\mathbf{x}_1, \ldots, \mathbf{x}_m) = \sum_{i<j} \left| \frac{d_{i,j} - \delta_p(\mathbf{x}_i, \mathbf{x}_j)}{d_{i,j}^q} \right|^r$$

where $p \in [1, \infty]$, $q \in [0,1]$, $r \in [1, \infty)$ are parameters of optimum mapping. The pure method of least squares is a case when $r = 2$, $q = 0$, the method of relative least squares is realizable for $r = 2$, $q = 1$ and Sammon's mapping corresponds with $r = 2$, $q = 1/2$. Thus Sammon's mapping is a compromise between absolute and relative method of least squares.

2 Optimization task

But alas, there are difficulties in the optimization of objective function F, which is only continuous but it is non-smooth and non-convex. The function has many local minima in the vector space $\mathbf{R}^{mn}$. That is why the global minimization has to be performed via heuristic approach. The competitive heuristics COMP1[3] with eight minimization strategies inside was used. One of them is based on deterministic reflection of simplex, four of them are representatives of random reflection, one strategy is a kind of evolutionary search and two of them are variants of differential evolution strategy. The individual competition heuristics are taken at random with the same probability in the first step. But the efficiency of them is immediately evaluated and the selection probabilities are modified for the next step until the stopping condition is satisfied. Heuristics COMP1 is recommended for difficult optimization tasks including Rosenbrock, Ackley, Rastrigin, Schwefel and Griewangk function minimization. It is supposed, the resulting coordinates of points are only sub-optimum ones.

3 Experimental part

The Matlab library for Sammon's mapping was created and tested on three examples:

- Seven equidistant points from $\mathbf{R}^1$ were mapped into $\mathbf{R}^2$
- Nineteen vertices of graph with hexagonal topology were mapped into $\mathbf{R}^2$
- Fourteen written words were mapped into $\mathbf{R}^2$ according to their Lehvenstein distance

The results are depicted on the Figs. 1 – 3 for $r = 2$, $q = ½$ in general. The value of p = 2 was used in the first example. The source codes of objective function and the optimization task are also included.

4 Conclusions

Generalized form of Sammon's mapping produces objective function which was subject of minimization. The COMP1 heuristics was used for global minimization of non-convex and non-smooth function. The experimental results with less than 20 patterns in 2D space with $p = r = 2$, $q = ½$ are looking like very optimistic. But the heuristics is very expensive in time for more than 50 patterns. The mapping and optimization routine were completely realized in the Matlab environment.

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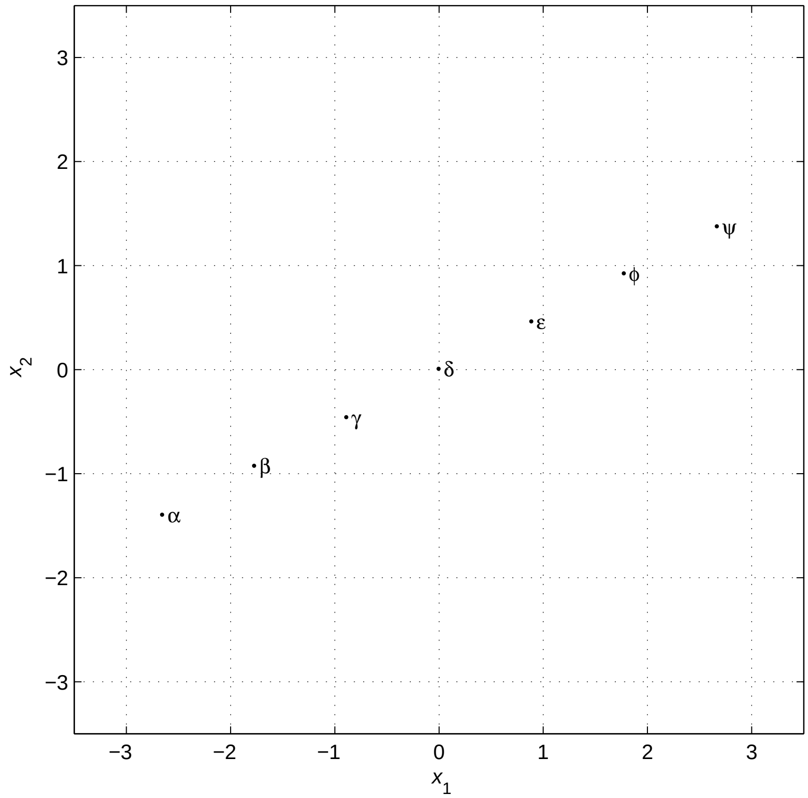

Fig.1.: Sammon's mapping of linear case

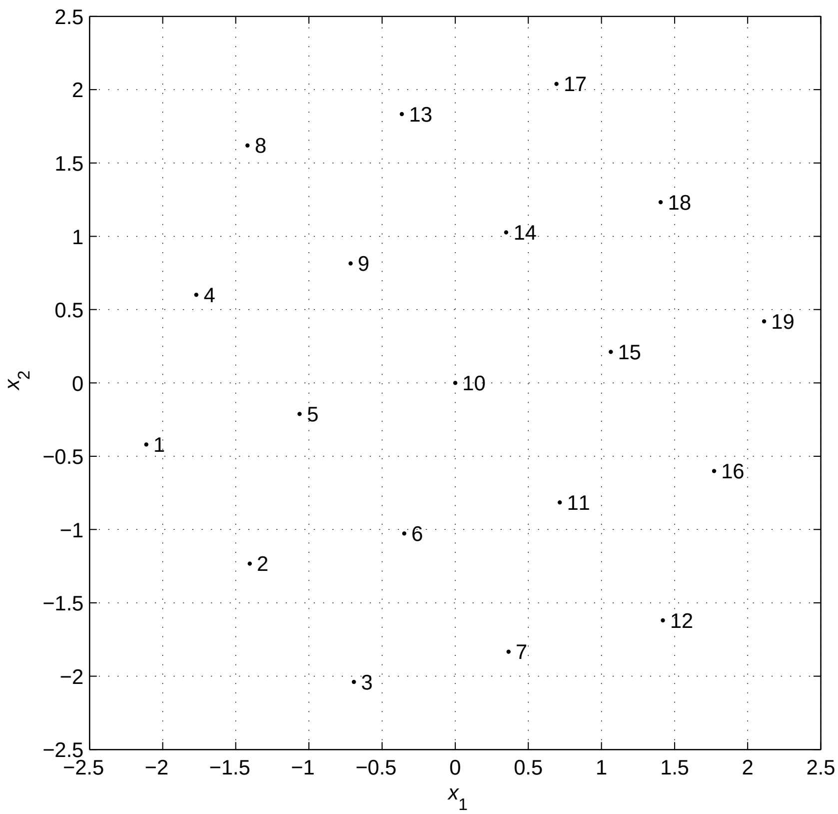

Fig.2.: Sammon's mapping of graph vertices (hexagonal topology)

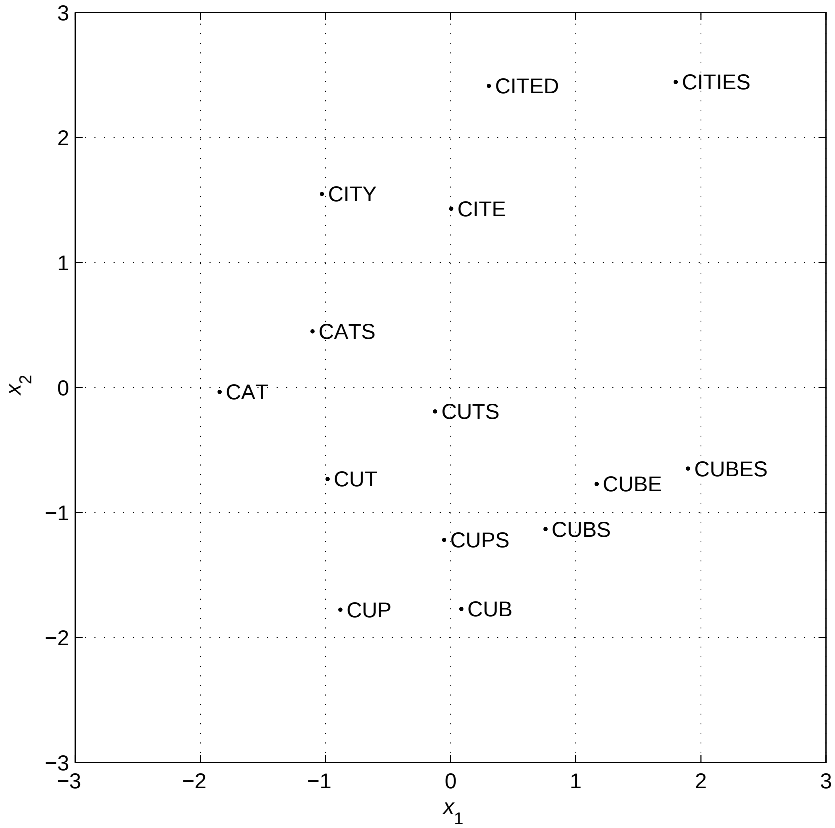

Fig.3.: Sammon's mapping of written words

Appendix 1: Objective function

```
function f=SAMMONOBJ(x)
global samm_d
global samm_m
global samm_n
global samm_p
global samm_q
global samm_r

x=reshape(x,[samm_m samm_n]);
f=0;
for i=1:samm_m-1
    for j=i+1:samm_m
        delta=norm(x(i,:)-x(j,:),samm_p);
        d=samm_d(i,j);
        f=f+(abs(d-delta)/d^samm_q)^samm_r;
    end
end
```

Appendix 2: Optimization task

```
function [xopt,fopt]=SAMMONMAP(d,n,p,q,r)
global samm_d
global samm_m
global samm_n
global samm_p
global samm_q
global samm_r

m=length(d);
samm_d=d;samm_m=m;samm_n=n;samm_p=p;samm_q=q;samm_r=r;
dmax=max(max(d));
upp=dmax*ones(1,m*n);
low=-upp;
 [x_star,fn_star,result_type,func_evals,success, nrst, cni]=...
    gcrs_c1_8('SAMMONOBJ', low, upp, 10*length(upp), 1e-10, 20000, 0,0, 10)
xopt=reshape(x_star,[m n]);
xopt=xopt-ones(m,1)*mean(xopt);
fopt=fn_star;
```