Multidimensional Data Visualization Dimensionality of Embedding Space

Multidimensional scaling (MDS) is a difficult global optimization problem

- ► The points representing objects should be found whose inter-point distances fit the given dissimilarities.
- ► The problem is reduced to minimization of a fitness criterion, e.g. so called *Stress* function

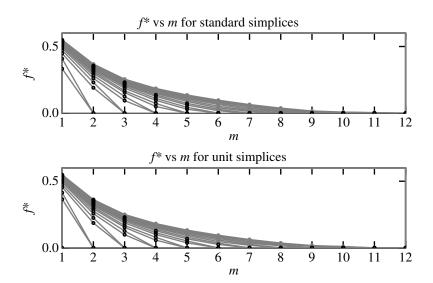
$$S(\mathbf{x}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \left(d\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right) - \delta_{ij} \right)^{2}.$$

- ► Although *Stress* function seems rather simple, it normally has many local minima.
- ▶ The problem is high dimensional: $\mathbf{x} \in \mathbb{R}^N$ and the number of variables is equal to $N = n \times m$.
- Non-differentiability normally cannot be ignored. Minkowski distances:

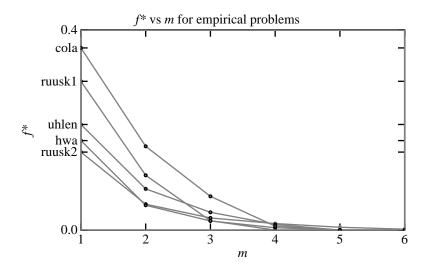
$$d_r(\mathbf{x}_i,\mathbf{x}_j) = \left(\sum_{k=1}^m |x_{ik} - x_{jk}|^r\right)^{1/r}.$$



On dimensionality of embedding space



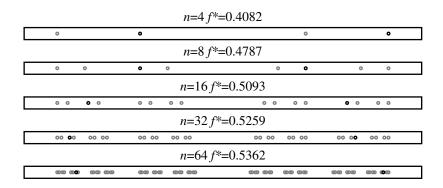
On dimensionality of embedding space



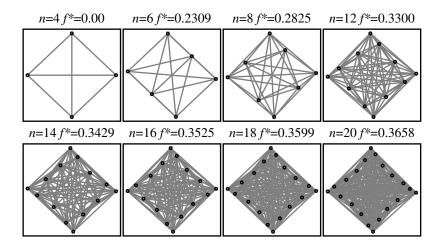
Images of simplices, m = 1

	n=4 j	f*=0.40	082		$n=4 f^*=0.3651$
•	۰		•	•	0 0 0
	n=5 j	f*=0.44	72	n=5 f*=0.414	
•	0	•	•	•	0 0 0 0
n=6 f*=0.4714					n=6 f*=0.4554
•	0 0	•	•	•	0 0 0 0 0
$n=7 f^*=0.488$					$n=7 f^*=0.4745$
•	0 0	•	0 0	0	0 0 0 0 0 0
$n=11 f^*=0.5222$					$n=11 f^*=0.5176$
0 0	0 0 0	0 0	0 0 0	• •	0 0 0 0 0 0 0 0 0 0
$n=15 f^*=0.5375$					n=15 f*=0.5352
0 0	0 0 0 0		000	0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0
n=19 f*=0.5461					n=19 f*=0.5447
000		0000		0 0	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0

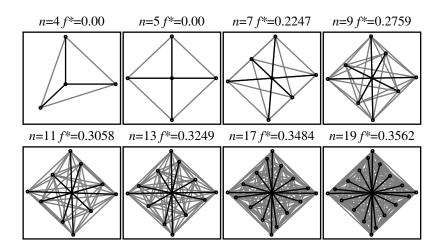
Images of cubes, m = 1



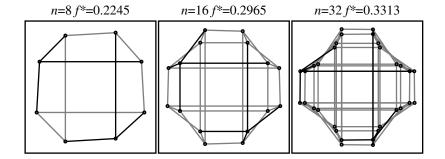
Images of standard simplices, m = 2



Images of unit simplices, m = 2



Images of cubes, m = 2



Images of empirical data, m = 2

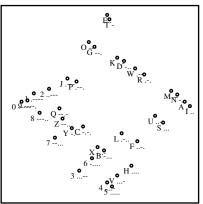
'cola'

Classic Coke Coke Pepsi

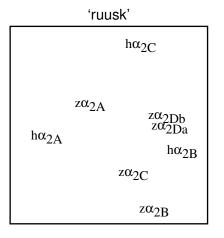
Diet Pepsi Dr. Pepper Tab

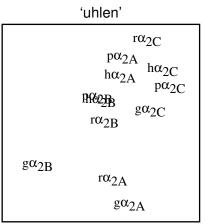
Diet 7-Up
7-Up
Diet Slice
Slice

'morseodes'

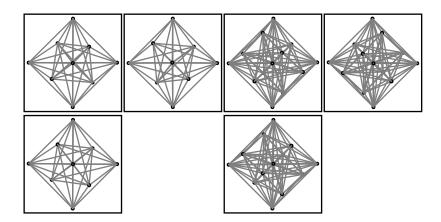


Images of pharmacological data, m = 2

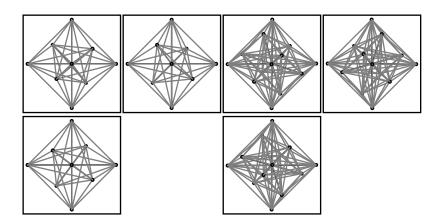




Images of standard simplices, m = 3



Images of unit simplices, m = 3



Images of cubes, m = 3

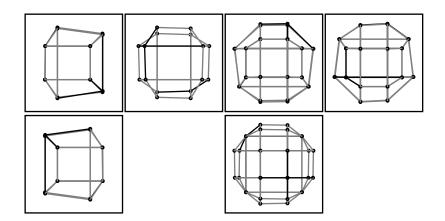


Image of the properties of human and zebrafish α_2 -adrenoceptors, m=3

∘hα _{2A}	•hα _{2A}
•zα _{2A} •hα _{2C} •zδh(2B ⁺¹²)h •zα _{2B}	•202 _A •ha _{2C} •202 _C •202 _B •202 _B
*7α2Λ *7αβαλ *7αβα *1αβ *1αβ *1αβ *1αβ *1αβ *1αβ *1αβ *	n=8 f*=0.0188 •hα _{2A} •zα _{2A} •zα _{2A} •hα _{2C} •zα _{2Db} •zα _{2B} •zα _{2B} •zα _{2B}

Image of the properties of 20 ligands binding human and zebrafish α_2 -adrenoceptors, m=3

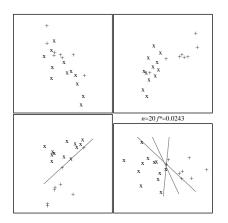


Image of the properties of human, rat, guinea pig and pig α_2 -adrenoceptors, m=3

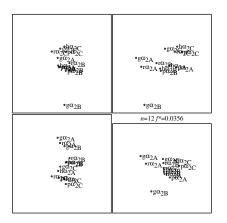


Image of the properties of wild type and mutant α_1 -adrenoceptors, m=3

