Multidimensional Data Visualization Investigation of Optimization-Based Visualization

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:

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



Experimental investigation of algorithms for MDS

The accuracy of fit evaluated via minimum of $S(\mathbf{x})$ depends on n and δ_{ij} , $i, j = 1, \ldots, n$. To reduce this undesirable impact, a relative error is used in the presentation of the results:

$$f(\mathbf{x}) = \sqrt{S(\mathbf{x}) / \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \delta_{ij}^{2}}.$$

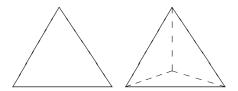
- Performance is measured using
 - Time and number of quadratic programming problems solved;
 - Mean $(\overline{f^*})$ and standard deviation (s.d. f^*) of global minimum estimates;
 - ▶ Best estimate of global minimum (f^*) and percentage of runs (perc) when the estimate differs from f^* by less than 10^{-4} .
- Various data sets.



Data set: vertices of the standard simplex

► The distances between any two vertices are equal. n = dim + 1.

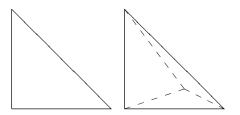
$$\Delta = \left(\begin{array}{cccccc} 0 & 1 & 1 & 1 & \cdots & 1 & 1 \\ 1 & 0 & 1 & 1 & & & 1 & 1 \\ 1 & 1 & 0 & 1 & & & 1 & 1 \\ 1 & 1 & 1 & 0 & & & 1 & 1 \\ \vdots & & & \ddots & & \vdots & \vdots \\ 1 & 1 & 1 & 1 & \cdots & 0 & 1 \\ 1 & 1 & 1 & 1 & \cdots & 1 & 0 \end{array}\right).$$



Data set: vertices of the unit simplex

$$v_{ij} = \begin{cases} 1, & i = j+1, \\ 0, & \text{otherwise,} \end{cases} | i = 1, \dots, n, j = 1, \dots, dim. \ n = \dim + 1.$$

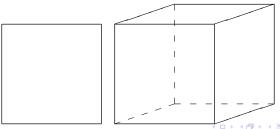
$$\Delta^1 = \left(\begin{array}{cccc} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & 2 & & 2 \\ 1 & 2 & 0 & & 2 \\ \vdots & & \ddots & \vdots \\ 1 & 2 & 2 & \cdots & 0 \end{array}\right), \; \Delta^2 = \left(\begin{array}{cccc} 0 & 1 & 1 & \cdots & 1 \\ 1 & 0 & \sqrt{2} & & \sqrt{2} \\ 1 & \sqrt{2} & 0 & & \sqrt{2} \\ \vdots & & \ddots & \vdots \\ 1 & \sqrt{2} & \sqrt{2} & \cdots & 0 \end{array}\right).$$



Data set: vertices of multidimensional cube

▶ The coordinates of *i*-th vertex of a dim-dimensional cube are equal either to 0 or to 1, and they are defined by binary code of i = 0, ..., n - 1. $n = 2^{\text{dim}}$.

$$\Delta^{1} = \begin{pmatrix} 0 & 1 & 1 & 2 & \cdots & n-1 & n \\ 1 & 0 & 2 & 1 & & n & n-1 \\ 1 & 2 & 0 & 1 & & n-2 & n-1 \\ 2 & 1 & 1 & 0 & & n-1 & n-2 \\ \vdots & & & \ddots & & \vdots \\ n-1 & n & n-2 & n-1 & & 0 & 1 \\ n & n-1 & n-1 & n-2 & \cdots & 1 & 0 \end{pmatrix}$$



Data set: error-perturbed distance data

► The data generated using uniformly distributed random points in *m*-dimensional space whose pairwise dissimilarities are computed by

$$\delta_{ij} = \sum_{k=1}^{m} \left| x_{ik}^{(e)} - x_{jk}^{(e)} \right|,$$

where $x_{ik}^{(e)} = x_{ik} + N(0, e(x_{ik}))$, and N(0, e) denotes the normally distributed random variable with mean zero and standard deviation e.

▶ Eight problems defined by all combinations of the parameters (n = 10, 20; m = 2, 3, e(x) = 0.15x, 0.3x) have been generated and they are referred as 'ghm'.

Empirical data sets

- A frequently used test problem for MDS algorithms is based on experimental testing of n = 10 soft drinks, where dissimilarities were measured by means of psychological experiment. This problem is referred as 'cola'.
- ► Another frequently used test problem is confusion data for (n = 36) Morse codes. This problem is referred as 'morsecodes'.

Pharmacological binding affinity data

- Binding affinity data is represented through a matrix, one dimension formed by different ligands tested in a series of experiments while the other represents different proteins.
- Receptor proteins can be from different types or subtypes, or from different species, or engineered mutants of these.
- Ligands can be natural neurotransmitters or pharmacological drugs, an agonist activates, an antagonist blocks the receptor.
- Dissimilarities are computed as distances between vectors of the log₁₀-transformed binding affinities.
 - Three human and five zebrafish α_2 -adrenoceptor proteins, and 20 ligands (Ruuskanen et al., 2005);
 - human, rat, guinea pig and pig proteins (Uhlen et al., 1998);
 - wild type and mutant proteins (Hwa et al., 1995).



Pharmacological data

| Ligand | $h\alpha_{2A}$ | $z\alpha_{2A}$ | $h\alpha_{2B}$ | $z\alpha_{2B}$ | $h\alpha_{2C}$ | $z\alpha_{2C}$ | $z\alpha_{2Da}$ | $z\alpha_{2Db}$ |
|-----------------------------------|----------------|----------------|----------------|----------------|----------------|----------------|-----------------|-----------------|
| Atipamezole | 1.6 | 13 | 1.5 | 5.0 | 4.3 | 2.1 | 5.1 | 6.9 |
| 2. Clonidine | 10 | 89 | 44 | 250 | 110 | 55 | 120 | 150 |
| Dexmedetomidine | 1.3 | 2.2 | 4.7 | 7.6 | 6.5 | 12 | 4.1 | 3.7 |
| Idazoxan | 17 | 85 | 24 | 40 | 17 | 17 | 52 | 94 |
| Oxymetazoline | 2.1 | 5.1 | 1100 | 1200 | 130 | 1300 | 1100 | 440 |
| 6. UK14,304 | 32 | 40 | 320 | 1200 | 190 | 700 | 260 | 280 |
| 7. L657.743 | 0.8 | 6.9 | 0.7 | 1.2 | 0.09 | 1.0 | 1.6 | 1.3 |
| 8. Rauwolscine | 1.9 | 1.0 | 1.1 | 1.4 | 0.2 | 0.5 | 2.3 | 2.3 |
| 9. Yohimbine | 5.9 | 5.2 | 7.5 | 9.3 | 4.6 | 3.4 | 6.4 | 4.0 |
| Chlorpromazine | 990 | 110 | 43 | 1.1 | 330 | 83 | 18 | 19 |
| 11. Clozapine | 32 | 3.3 | 12 | 9.3 | 2.1 | 3.2 | 12 | 24 |
| 12. ARC239 | 2100 | 1800 | 9.6 | 36 | 66 | 280 | 55 | 44 |
| 13. Prazosin | 1030 | 330 | 66 | 300 | 31 | 100 | 68 | 64 |
| Spiperone | 540 | 45 | 12 | 51 | 11 | 63 | 15 | 18 |
| Spiroxatrine | 320 | 150 | 2.4 | 93 | 3.1 | 35 | 11 | 11 |
| 16. WB-4101 | 5.4 | 11 | 60 | 51 | 1.9 | 19 | 31 | 16 |
| 17. 2-Amino-1- | 1300 | 5400 | 4200 | 9400 | 8100 | 5100 | 3700 | 4000 |
| phenylethanol | | | | | | | | |
| 18. Dopamine | 2000 | 790 | 6300 | 4400 | 1200 | 3900 | 1300 | 1700 |
| 19. (-)-Adrenaline | 150 | 140 | 710 | 910 | 130 | 1080 | 500 | 470 |
| 20. (–)-Noradrenaline | 110 | 260 | 680 | 647 | 250 | 580 | 380 | 510 |

Experimental testing of soft drinks

| Soft drinks | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|--------------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 1. Pepsi | 0 | 127 | 169 | 204 | 309 | 320 | 286 | 317 | 321 | 238 |
| 2. Coke | 127 | 0 | 143 | 235 | 318 | 322 | 256 | 318 | 318 | 231 |
| Classic Coke | 169 | 143 | 0 | 243 | 326 | 327 | 258 | 318 | 318 | 242 |
| Diet Pepsi | 204 | 235 | 243 | 0 | 285 | 288 | 259 | 312 | 317 | 194 |
| Diet Slice | 309 | 318 | 326 | 285 | 0 | 155 | 312 | 131 | 170 | 285 |
| 6. Diet 7-Up | 320 | 322 | 327 | 288 | 155 | 0 | 306 | 164 | 136 | 281 |
| 7. Dr Pepper | 286 | 256 | 258 | 259 | 312 | 306 | 0 | 300 | 295 | 256 |
| 8. Slice | 317 | 318 | 318 | 312 | 131 | 164 | 300 | 0 | 132 | 291 |
| 9. 7-Up | 321 | 318 | 318 | 317 | 170 | 136 | 295 | 132 | 0 | 297 |
| 10. Tab | 238 | 231 | 242 | 194 | 285 | 281 | 256 | 291 | 297 | 0 |

Diet 7-Up 7-UpSlice

Tab

Dr. Pepper

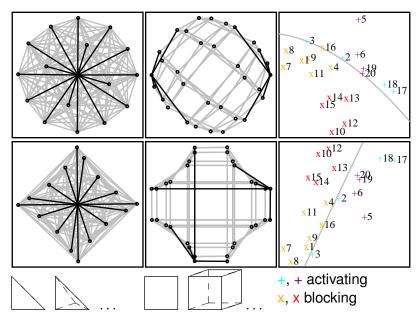
Coke Classic Cd&Psi Classic Coke
Coke
Pepsi

Diet Pepsi

Tab

Diet 7-Up
Diet Slice
Slice

MDS with Euclidean and city-block distances



The best known estimates of global minimum

| datasets | | n | min f^* , $m = 2$ | $\min f^*, m = 3$ |
|------------|----|----|---------------------|-------------------|
| standard | | 8 | 0.2825 | 0.1250 |
| simplices | | 12 | 0.3300 | 0.2013 |
| | | 16 | 0.3525 | 0.2321 |
| | | 20 | 0.3657 | 0.2508 |
| unit | | 8 | 0.2569 | 0.0992 |
| simplices | | 12 | 0.3167 | 0.1874 |
| | | 16 | 0.3439 | 0.2243 |
| | | 20 | 0.3595 | 0.2459 |
| cubes | | 8 | 0.2245 | 0.00 |
| | | 16 | 0.2965 | 0.1590 |
| | | 32 | 0.3313 | 0.2078 |
| | e% | | | |
| ghm | 15 | 10 | 0.1293 | 0.0906 |
| | 30 | 10 | 0.2711 | 0.1298 |
| | 15 | 20 | 0.1868 | 0.1610 |
| | 30 | 20 | 0.2966 | 0.2284 |
| cola | | 10 | 0.1647 | 0.0659 |
| morsecodes | 3 | 36 | 0.2944 | 0.1962 |

Reduced search space of problems exposing symmetries

- If exchange of some objects does not change dissimilarity data, exchange of points representing these objects does not change the value of *Stress* function.
- In continuous optimization: constrain sequence of first coordinate values of image points of symmetric objects.
- In combinatorial optimization: allow only some of permutations of first coordinate **p**₁.
- For geometric data sets
 - ▶ standard simplex: $x_{11} \le x_{21} \le ... \le x_{n1}$; $\mathbf{p}_1 = (1, 2, ..., n)$.
 - unit simplex: $x_{21} \le x_{31} \le ... \le x_{n1}$; $\mathbf{p}_1 = (I, 1, 2, ..., I 1, I + 1, ..., n)$.
 - ▶ hyper-cube: $x_{11} \le x_{i1}, i = 2, ...n; p_{11} = 1.$

Explicit enumeration: standard simplices

| | m = 1 | | m = 2 | | m = 3 | |
|----|---------------------|--------|----------------------|--------|----------------------|--------|
| n | t, s (NQP) | f* | t, s (NQP) | f* | t, s (NQP) | f* |
| 3 | 0.00 (3) | 0.3333 | 0.00 (6) | 0.00 | 0.00 (10) | 0.00 |
| 4 | 0.00 (12) | 0.4082 | 0.00 (78) | 0.00 | 0.01 (364) | 0.00 |
| 5 | 0.00 (60) | 0.4472 | 0.03 (1830) | 0.1907 | 1.79 (37820) | 0.00 |
| 6 | 0.00 (360) | 0.4714 | 1.71 (64980) | 0.2309 | 589.72 (7840920) | 0.00 |
| 7 | 0.03 (2520) | 0.4879 | 118.59 (3176460) | 0.2621 | (, | |
| 8 | 0.21 (20160) | 0.5000 | 10229.00 (203222880) | 0.2825 | | |
| 9 | 2.24 (181440) | 0.5092 | , | | | |
| 10 | 26.63 (1814400) | 0.5164 | | | | |
| 11 | 351.09 (19958400) | 0.5222 | | | | |
| 12 | 4702.00 (239500800) | 0.5270 | | | | |
| 3 | 0.00 (1) | 0.3333 | 0.00 (3) | 0.00 | 0.00 (6) | 0.00 |
| 4 | 0.00 (1) | 0.4082 | 0.00 (12) | 0.00 | 0.00 (78) | 0.00 |
| 5 | 0.00 (1) | 0.4472 | 0.00 (60) | 0.1907 | 0.09 (1830) | 0.00 |
| 6 | 0.00(1) | 0.4714 | 0.01 (360) | 0.2309 | 5.01 (64980) | 0.00 |
| 7 | 0.00 (1) | 0.4879 | 0.10 (2520) | 0.2621 | 379.88 (3176460) | 0.0945 |
| 8 | 0.00 (1) | 0.5000 | 1.01 (20160) | 0.2825 | 31681.00 (203222880) | 0.1250 |
| 9 | 0.00 (1) | 0.5092 | 11.89 (181440) | 0.2991 | | |
| 10 | 0.00 (1) | 0.5164 | 153.88 (1814400) | 0.3115 | | |
| 11 | 0.00 (1) | 0.5222 | 2121.56 (19958400) | 0.3217 | | |
| 12 | 0.00 (1) | 0.5270 | 31170.00 (239500800) | 0.3300 | | |

Explicit enumeration: unit simplices

| | m = 1 | | m = 2 | | m = 3 | |
|----|---------------------|--------|-----------------------|--------|----------------------|--------|
| n | t, s (NQP) | f* | t, s (NQP) | f* | t, s (NQP) | f^* |
| 3 | 0.00 (3) | 0.00 | 0.00 (6) | 0.00 | 0.00 (10) | 0.00 |
| 4 | 0.00 (12) | 0.3651 | 0.00 (78) | 0.00 | 0.01 (364) | 0.00 |
| 5 | 0.00 (60) | 0.4140 | 0.04 (1830) | 0.00 | 2.02 (37820) | 0.00 |
| 6 | 0.01 (360) | 0.4554 | 2.05 (64980) | 0.1869 | 661.11 (7840920) | 0.00 |
| 7 | 0.02 (2520) | 0.4745 | 137.12 (3176460) | 0.2247 | | |
| 8 | 0.23 (20160) | 0.4917 | 11662.00 (203222880) | 0.2569 | | |
| 9 | 2.51 (181440) | 0.5018 | | | | |
| 10 | 29.78 (1814400) | 0.5113 | | | | |
| 11 | 378.45 (19958400) | 0.5176 | | | | |
| 12 | 5265.00 (239500800) | 0.5236 | | | | |
| 3 | 0.00 (2) | 0.00 | 0.00 (4) | 0.00 | 0.00 (7) | 0.00 |
| 4 | 0.00 (2) | 0.3651 | 0.00 (18) | 0.00 | 0.01 (99) | 0.00 |
| 5 | 0.00(3) | 0.4140 | 0.01 (108) | 0.00 | 0.14 (2574) | 0.00 |
| 6 | 0.00(3) | 0.4554 | 0.02 (720) | 0.1869 | 8.49 (101160) | 0.00 |
| 7 | 0.00 (4) | 0.4745 | 0.25 (5760) | 0.2247 | 695.19 (5446080) | 0.00 |
| 8 | 0.00 (4) | 0.4917 | 2.90 (50400) | 0.2569 | 66686.00 (381049200) | 0.0992 |
| 9 | 0.00 (5) | 0.5018 | 37.16 (504000) | 0.2759 | | |
| 10 | 0.00 (5) | 0.5113 | 560.84 (5443200) | 0.2936 | | |
| 11 | 0.00 (6) | 0.5176 | 7813.00 (65318400) | 0.3058 | | |
| 12 | 0.00 (6) | 0.5236 | 122360.00 (838252800) | 0.3167 | | |

Explicit enumeration: hyper-cubes

| | m = 1 | | m = 2 | m = 2 | | |
|-----|--------------|--------|----------------------|--------|------------|-------|
| n | t, s (NQP) | f* | t, s (NQP) | f* | t, s (NQP) | f^* |
| 4 | 0.00 (12) | 0.4082 | 0.00 (78) | 0.00 | 0.02 (364) | 0.00 |
| 8 | 0.24 (20160) | 0.4787 | 12572.00 (203222880) | 0.2245 | | |
| 4 | 0.00 (6) | 0.4082 | 0.00 (57) | 0.00 | 0.01 (308) | 0.00 |
| _ 8 | 0.06 (5040) | 0.4787 | 5483.00 (88908120) | 0.2245 | | |

Explicit enumeration on SUN Fire E15k parallel computer: simplices, n = 7, m = 2

| | | standard simplex | | | unit simplex | |
|----|--------------|------------------|-------|--------------|--------------|-------|
| р | <i>t</i> , s | s_p | e_p | <i>t</i> , s | s_p | e_p |
| 1 | 1037 | 1.00 | 1.00 | 1299 | 1.00 | 1.00 |
| 2 | 518 | 2.00 | 1.00 | 650 | 2.00 | 1.00 |
| 3 | 349 | 2.97 | 0.99 | 438 | 2.97 | 0.99 |
| 4 | 261 | 3.97 | 0.99 | 327 | 3.97 | 0.99 |
| 5 | 210 | 4.95 | 0.99 | 262 | 4.95 | 0.99 |
| 6 | 175 | 5.91 | 0.98 | 219 | 5.93 | 0.99 |
| 7 | 151 | 6.88 | 0.98 | 188 | 6.89 | 0.98 |
| 8 | 134 | 7.73 | 0.97 | 168 | 7.75 | 0.97 |
| 9 | 118 | 8.80 | 0.98 | 147 | 8.85 | 0.98 |
| 10 | 107 | 9.71 | 0.97 | 134 | 9.66 | 0.97 |
| 11 | 97 | 10.72 | 0.97 | 120 | 10.78 | 0.98 |
| 12 | 90 | 11.58 | 0.96 | 111 | 11.69 | 0.97 |
| 13 | 82 | 12.62 | 0.97 | 102 | 12.68 | 0.98 |
| 14 | 77 | 13.54 | 0.97 | 95 | 13.62 | 0.97 |
| 15 | 72 | 14.39 | 0.96 | 89 | 14.55 | 0.97 |
| 16 | 67 | 15.44 | 0.97 | 84 | 15.54 | 0.97 |
| 17 | 64 | 16.12 | 0.95 | 79 | 16.47 | 0.97 |
| 18 | 60 | 17.23 | 0.96 | 76 | 17.18 | 0.95 |
| 19 | 58 | 17.90 | 0.94 | 72 | 18.03 | 0.95 |
| 20 | 55 | 18.95 | 0.95 | 68 | 19.17 | 0.96 |
| 21 | 52 | 19.96 | 0.95 | 65 | 19.96 | 0.95 |
| 22 | 49 | 20.95 | 0.95 | 62 | 20.85 | 0.95 |
| 23 | 48 | 21.81 | 0.95 | 59 | 22.06 | 0.96 |
| 24 | 46 | 22.50 | 0.94 | 57 | 22.60 | 0.94 |

Worst case results of branch and bound: simplices, m = 1

| | n | f* | Enumeration: t, s (NQPP) | Branch and bound: t, s (NQPP) |
|-----------|----|--------|--------------------------|-------------------------------|
| standard | 3 | 0.3333 | 0.00 (3) | 0.00 (3) |
| simplices | 4 | 0.4082 | 0.00 (12) | 0.00 (14) |
| | 5 | 0.4472 | 0.00 (60) | 0.00 (73) |
| | 6 | 0.4714 | 0.01 (360) | 0.01 (432) |
| | 7 | 0.4879 | 0.02 (2520) | 0.05 (2951) |
| | 8 | 0.5000 | 0.21 (20160) | 0.24 (23110) |
| | 9 | 0.5092 | 2.22 (181440) | 2.47 (204549) |
| | 10 | 0.5164 | 27.39 (1814400) | 28.33 (2018948) |
| | 11 | 0.5222 | 334.30 (19958400) | 361.60 (21977347) |
| | 12 | 0.5270 | 4687.0 (239500800) | 4970.0 (261478146) |
| | 13 | 0.5311 | 68762 (3113510400) | 73714 (3374988545) |
| unit | 3 | 0.00 | 0.00 (3) | 0.00 (3) |
| simplices | 4 | 0.3651 | 0.00 (12) | 0.00 (14) |
| | 5 | 0.4140 | 0.00 (60) | 0.00 (73) |
| | 6 | 0.4554 | 0.00 (360) | 0.01 (432) |
| | 7 | 0.4745 | 0.04 (2520) | 0.03 (2951) |
| | 8 | 0.4917 | 0.24 (20160) | 0.32 (23110) |
| | 9 | 0.5018 | 2.48 (181440) | 2.77 (204549) |
| | 10 | 0.5113 | 33.16 (1814400) | 31.67 (2018948) |
| | 11 | 0.5176 | 372.59 (19958400) | 404.64 (21977347) |
| | 12 | 0.5236 | 5208.0 (239500800) | 5545.0 (261478146) |
| | 13 | 0.5279 | 78579 (3113510400) | 86436 (3374988545) |

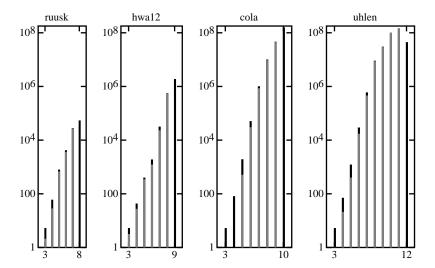
Pessimistic results of branch and bound: simplices, m > 1

| | m | n | f* | Enumeration: t, s (NQPP) | Branch and bound: t, s (NQPP) |
|-----------|---|---|--------|--------------------------|-------------------------------|
| standard | 2 | 4 | 0.00 | 0.01 (78) | 0.00 (63) |
| simplices | 2 | 5 | 0.1907 | 0.05 (1830) | 0.03 (1322) |
| • | 2 | 6 | 0.2309 | 1.73 (64980) | 0.85 (27255) |
| | 2 | 7 | 0.2621 | 113.77 (3176460) | 59.61 (1655631) |
| | 2 | 8 | 0.2825 | 10183 (203222880) | 5107.0 (102073658) |
| | 2 | 9 | 0.2991 | | 502844 (3574743410) |
| | 3 | 4 | 0.00 | 0.02 (364) | 0.01 (133) |
| | 3 | 5 | 0.00 | 1.79 (37820) | 1.12 (23017) |
| | 3 | 6 | 0.00 | 580.87 (7840920) | 25.49 (335771) |
| | 3 | 7 | 0.0945 | 301860 (2670344040) | 11111 (92710201) |
| unit | 2 | 4 | 0.00 | 0.00 (78) | 0.00 (73) |
| simplices | 2 | 5 | 0.00 | 0.05 (1830) | 0.03 (662) |
| | 2 | 6 | 0.1869 | 2.02 (64980) | 0.51 (16076) |
| | 2 | 7 | 0.2247 | 133.28 (3176460) | 17.65 (422940) |
| | 2 | 8 | 0.2569 | 11631 (203222880) | 1675.0 (29943080) |
| | 2 | 9 | 0.2759 | | 134281 (1905072549) |
| | 3 | 4 | 0.00 | 0.02 (364) | 0.02 (313) |
| | 3 | 5 | 0.00 | 2.02 (37820) | 0.49 (9837) |
| | 3 | 6 | 0.00 | 653.91 (7840920) | 46.67 (578691) |
| | 3 | 7 | 0.00 | 334788 (2670344040) | 2652.0 (20674563) |

Realistic results of branch and bound: cubes and empirical datasets

| | m | n | f* | Enumeration: t, s (NQPP) | Branch and bound: t, s (NQPP) |
|-------|-------|----|--------|---------------------------------------|-------------------------------|
| cubes | 1 | 4 | 0.4082 | 0.00 (12) | 0.00 (14) |
| | 1 | 8 | 0.4787 | 0.23 (20160) | 0.12 (11260) |
| | 2 | 4 | 0.00 | 0.00 (78) | 0.00 (73) |
| | 2 | 8 | 0.2245 | 12518 (203222880) | 124.68 (2157090) |
| | 3 | 4 | 0.00 | 0.02 (364) | 0.02 (353) |
| | 3 | 8 | 0.00 | | 6189 (35216122) |
| ruusk | usk 1 | 8 | 0.2975 | 0.25 (20160) | 0.02 (665) |
| | 2 | 8 | 0.1096 | 12183 (203222880) | 3.85 (82617) |
| | 3 | 8 | 0.0188 | | 838.68 (6381457) |
| hwa12 | 1 | 9 | 0.0107 | 3.06 (181440) | 0.02 (2217) |
| | 2 | 9 | 0.00 | , , , | 203.25 (2344833) |
| cola | 1 | 10 | 0.3688 | 27.47 (1814400) | 1.46 (65642) |
| | 2 | 10 | 0.1647 | | 14136 (163235214) |
| uhlen | 1 | 12 | 0.2112 | 6413.0 (239500800) | 0.62 (36559) |
| | 2 | 12 | 0.0825 | · · · · · · · · · · · · · · · · · · · | 35951 (312924750) |
| hwa21 | 1 | 12 | 0.1790 | 6648.0 (239500800) | 1.49 (71748) |

Histograms of levels of solutions



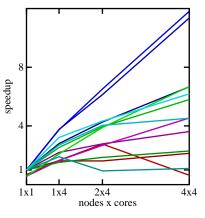
Results of parallel algorithm

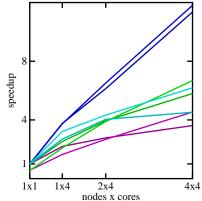
| _ | 1 | 1 × 1 | 1 | I × 4 | | 2 × 4 | | 4 × 4 |
|---|--------|-----------|--------|-------------|-------------|------------|--------|------------|
| 1 | t, s | NQP | t, s | NQP | t, s | NQP | t, s | NQP |
| 0 | 2.28 | 82617 | | ruusk1, n | = 8, m = 2 | | | |
| 4 | 2.28 | 83630 | 1.41 | 180637 | 1.41 | 288547 | 1.07 | 475328 |
| 5 | 3.36 | 142800 | 1.38 | 191839 | 0.83 | 240849 | 3.56 | 302056 |
| 0 | 479.41 | 6381457 | | ruusk1, n | = 8, m = 3 | 1 | | |
| 4 | 479.69 | 6403810 | 218.62 | 10085145 | 172.68 | 14201943 | 132.61 | 21415601 |
| 5 | 840.87 | 13887913 | 291.15 | 16040461 | 179.02 | 18143183 | 105.64 | 20847563 |
| 0 | 120.95 | 2344833 | | hwa12, n : | = 9, m = 2 | | | |
| 4 | 120.84 | 2346237 | 79.52 | 5138135 | 64.96 | 6986355 | 52.61 | 10742968 |
| 5 | 121.89 | 2407591 | 47.64 | 3135785 | 30.55 | 3699097 | 20.79 | 5014227 |
| 6 | 216.78 | 5488888 | 57.66 | 5565997 | 30.95 | 5842364 | 18.04 | 6199196 |
| 7 | | | | | | | 612.00 | 208871963 |
| 0 | 9032 | 204022569 | | cola, n = | 10, m = 2 | | | |
| 4 | 9011 | 204022487 | 3212 | 229324265 | 2108 | 270022713 | 1349 | 326420931 |
| 5 | 8991 | 204037437 | 2391 | 212954615 | 1466 | 226026528 | 792 | 244647590 |
| 6 | 8999 | 206189960 | 2405 | 212379122 | 1380 | 224377631 | 761 | 241643940 |
| 7 | 15189 | 396725753 | 4607 | 410841540 | 2700 | 433396504 | 1388 | 438645561 |
| 0 | 20515 | 312924750 | | uhlen1, n = | = 12, m = 2 | 2 | | |
| 4 | 20494 | 312925348 | 10754 | 556642796 | 21847 | 1278648079 | 18532 | 2149661364 |
| 5 | 20428 | 312960596 | 7579 | 386113225 | 5054 | 508285836 | 4516 | 751368922 |
| 6 | 20522 | 315503838 | 6360 | 363849948 | 4721 | 461364157 | 3302 | 570468417 |
| 7 | 27674 | 506947703 | 17241 | 947746934 | 47190 | 2370684051 | 28521 | 3044562204 |

Speedup

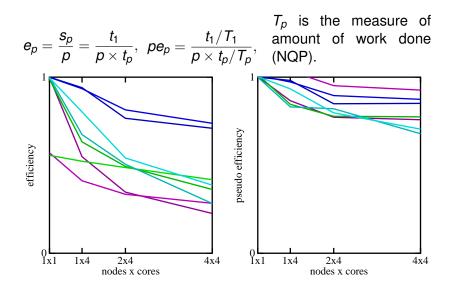
$$s_p = rac{t_1}{t_p},$$

 t_p is the time used by the algorithm implemented on p cores, t_1 is the shortest time on one process.

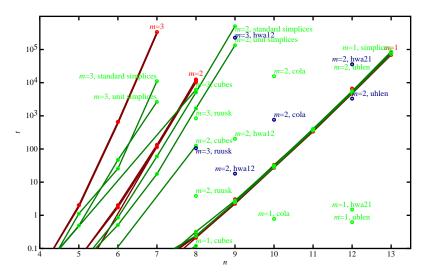




Efficiency of parallelization



Results of explicit enumeration and branch and bound



Random search, multistart and evolutionary algorithms: m = 2, $t_c = 10$ s

| datasets | | | random | search | multis | tart | evolutio | onary |
|-----------|-----|----|---------------|---------|-----------|-----------------|---------------|---------|
| | | n | f* | s.d. f* | <u>f*</u> | s.d. <i>f</i> * | f* | s.d. f* |
| standard | | 8 | 0.2825 | 0.0000 | 0.2825 | 0.0000 | 0.2825 | 0.0000 |
| simplices | 3 | 12 | 0.3326 | 0.0008 | 0.3310 | 0.0004 | 0.3301 | 0.0002 |
| | | 16 | 0.3575 | 0.0009 | 0.3550 | 0.0005 | 0.3530 | 0.0004 |
| | | 20 | 0.3720 | 0.0011 | 0.3686 | 0.0004 | 0.3663 | 0.0003 |
| unit | | 8 | 0.2569 | 0.0000 | 0.2569 | 0.0000 | 0.2569 | 0.0000 |
| simplices | 3 | 12 | 0.3218 | 0.0015 | 0.3168 | 0.0002 | 0.3167 | 0.0000 |
| | | 16 | 0.3527 | 0.0016 | 0.3463 | 0.0006 | 0.3440 | 0.0002 |
| | | 20 | 0.3701 | 0.0019 | 0.3627 | 0.0005 | 0.3597 | 0.0002 |
| cubes | | 8 | 0.2304 | 0.0091 | 0.2245 | 0.0000 | 0.2245 | 0.0000 |
| | | 16 | 0.3857 | 0.0095 | 0.3012 | 0.0021 | 0.2966 | 0.0002 |
| | | 32 | 0.4753 | 0.0056 | 0.3508 | 0.0060 | 0.3346 | 0.0021 |
| | e% | | | | | | | |
| ghm | 15 | 10 | 0.1695 | 0.0083 | 0.1293 | 0.0000 | 0.1293 | 0.0000 |
| | 30 | 10 | 0.3084 | 0.0084 | 0.2711 | 0.0000 | 0.2711 | 0.0000 |
| | 15 | 20 | 0.3708 | 0.0166 | 0.1872 | 0.0005 | 0.1868 | 0.0000 |
| | 30 | 20 | 0.4282 | 0.0085 | 0.3034 | 0.0025 | 0.2967 | 0.0005 |
| cola | | 10 | 0.1983 | 0.0074 | 0.1667 | 0.0012 | 0.1648 | 0.0003 |
| morseco | des | 36 | 0.4073 | 0.0040 | 0.3329 | 0.0063 | 0.3125 | 0.0048 |

Evolutionary algorithm: m = 2, $t_c = 10$ s, $n_p = 60$

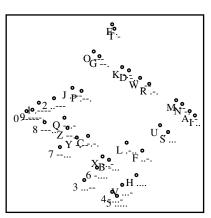
| | | | $N_{init} = 60$ | | N _{init} = | 100 | $N_{init} = 100$ | | |
|------------|----|----|------------------|---------|---------------------|---------|------------------|---------|--|
| datasets | | | $p_{mut} = 0.00$ | | p _{mut} = | 0.00 | $p_{mut} = 0.01$ | | |
| | | n | <u>f*</u> | s.d. f* | <u>f*</u> | s.d. f* | <u>f*</u> | s.d. f* | |
| standard | | 8 | 0.2825 | 0.0000 | 0.2825 | 0.0000 | 0.2825 | 0.0000 | |
| simplices | | 12 | 0.3301 | 0.0002 | 0.3300 | 0.0002 | 0.3300 | 0.0001 | |
| | | 16 | 0.3530 | 0.0004 | 0.3529 | 0.0004 | 0.3527 | 0.0003 | |
| | | 20 | 0.3663 | 0.0003 | 0.3661 | 0.0002 | 0.3661 | 0.0003 | |
| unit | | 8 | 0.2569 | 0.0000 | 0.2569 | 0.0000 | 0.2569 | 0.0000 | |
| simplices | | 12 | 0.3167 | 0.0000 | 0.3167 | 0.0000 | 0.3167 | 0.0000 | |
| | | 16 | 0.3440 | 0.0002 | 0.3440 | 0.0001 | 0.3440 | 0.0001 | |
| | | 20 | 0.3597 | 0.0002 | 0.3596 | 0.0002 | 0.3596 | 0.0002 | |
| cubes | | 8 | 0.2245 | 0.0000 | 0.2245 | 0.0000 | 0.2245 | 0.0000 | |
| | | 16 | 0.2966 | 0.0002 | 0.2966 | 0.0002 | 0.2966 | 0.0001 | |
| | | 32 | 0.3346 | 0.0021 | 0.3354 | 0.0029 | 0.3355 | 0.0028 | |
| | e% | | | | | | | | |
| ghm | 15 | 10 | 0.1293 | 0.0000 | 0.1293 | 0.0000 | 0.1293 | 0.0000 | |
| | 30 | 10 | 0.2711 | 0.0000 | 0.2711 | 0.0000 | 0.2711 | 0.0000 | |
| | 15 | 20 | 0.1868 | 0.0000 | 0.1868 | 0.0000 | 0.1868 | 0.0000 | |
| | 30 | 20 | 0.2967 | 0.0005 | 0.2968 | 0.0008 | 0.2970 | 0.0012 | |
| cola | | 10 | 0.1648 | 0.0003 | 0.1651 | 0.0006 | 0.1651 | 0.0006 | |
| morsecodes | | 36 | 0.3125 | 0.0048 | 0.3061 | 0.0027 | 0.3057 | 0.0028 | |

Evolutionary algorithm and distance smoothing

| dataset | S | | | evolutiona | ry algorithm | distance smoothing | | |
|--------------------|----|----|--------|------------------|-----------------|--------------------|-----------------|--|
| <i>e</i> % | | n | m | $\overline{f^*}$ | s.d. <i>f</i> * | $\overline{f^*}$ | s.d. <i>f</i> * | |
| ghm | 15 | 10 | 2 | 0.1293 | 0.0000 | 0.1457 | 0.0150 | |
| 30 15 | | 10 | 2 | 0.2711 | 0.0000 | 0.2878 | 0.0113 | |
| | | 20 | 2 | 0.1868 | 0.0000 | 0.2071 | 0.0130 | |
| | 30 | 20 | 2 | 0.2970 | 0.0012 | 0.3093 | 0.0076 | |
| cola 10 | | 10 | 2 | 0.1651 | 0.0006 | 0.1823 | 0.0136 | |
| morsecodes | | 36 | 2 | 0.3057 | 0.0028 | 0.3106 | 0.0966 | |
| ghm 15 30 15 | | 10 | 3 | 0.0906 | 0.0000 | 0.1116 | 0.0146 | |
| | | 10 | 3 | 0.1298 | 0.0000 | 0.1486 | 0.0086 | |
| | | 20 | 3 | 0.1629 | 0.0016 | 0.1761 | 0.0065 | |
| 30 | | 20 | 3 | 0.2394 | 0.0031 | 0.2454 | 0.0063 | |
| cola 10 | | 3 | 0.0673 | 0.0013 | 0.0914 | 0.0087 | | |
| morsecodes 36 | | 3 | 0.2231 | 0.0055 | 0.2045 | 0.0062 | | |

Comparison of evolutionary algorithm with simulated annealing: morsecodes, m = 2

| min $\mathcal{S}^*/2$ | max $\mathcal{S}^*/2$ | time (s) | | | | | | |
|------------------------|-----------------------|----------|--|--|--|--|--|--|
| evolutionary algorithm | | | | | | | | |
| 153.5395 | 154.5550 | 1000 | | | | | | |
| 153.1380 | 154.0815 | 2000 | | | | | | |
| 153.0355 | 153.9175 | 10000 | | | | | | |
| simulated annealing | | | | | | | | |
| 153.2583 | 155.2006 | 1142 | | | | | | |
| 153.2411 | 155.5416 | 2309 | | | | | | |



Evolutionary algorithm on SUN Fire E15k: unit simplices, m = 2, $t_c = 10$ s

| | | 1 proce | essor | 8 processors | | | | | |
|----|--------|---------|--------|--------------|--------|--------|--------|------|--|
| n | f*min | f*mean | f*max | perc | f*min | f*mean | f* | perc | |
| 6 | 0.1869 | 0.1869 | 0.1869 | 100 | 0.1869 | 0.1869 | 0.1869 | 100 | |
| 7 | 0.2247 | 0.2247 | 0.2247 | 100 | 0.2247 | 0.2247 | 0.2247 | 100 | |
| 8 | 0.2569 | 0.2569 | 0.2569 | 100 | 0.2569 | 0.2569 | 0.2569 | 100 | |
| 9 | 0.2759 | 0.2759 | 0.2759 | 100 | 0.2759 | 0.2759 | 0.2759 | 100 | |
| 10 | 0.2936 | 0.2936 | 0.2936 | 100 | 0.2936 | 0.2936 | 0.2936 | 100 | |
| 11 | 0.3058 | 0.3058 | 0.3058 | 100 | 0.3058 | 0.3058 | 0.3058 | 100 | |
| 12 | 0.3167 | 0.3167 | 0.3167 | 100 | 0.3167 | 0.3167 | 0.3167 | 100 | |
| 13 | 0.3249 | 0.3249 | 0.3249 | 100 | 0.3249 | 0.3249 | 0.3249 | 100 | |
| 14 | 0.3325 | 0.3325 | 0.3330 | 93 | 0.3325 | 0.3325 | 0.3325 | 100 | |
| 15 | 0.3384 | 0.3386 | 0.3391 | 70 | 0.3384 | 0.3384 | 0.3384 | 100 | |
| 16 | 0.3439 | 0.3443 | 0.3448 | 25 | 0.3439 | 0.3439 | 0.3443 | 94 | |
| 17 | 0.3484 | 0.3490 | 0.3497 | 8 | 0.3484 | 0.3486 | 0.3490 | 56 | |
| 18 | 0.3526 | 0.3532 | 0.3538 | 3 | 0.3526 | 0.3529 | 0.3531 | 17 | |
| 19 | 0.3562 | 0.3568 | 0.3575 | 2 | 0.3562 | 0.3565 | 0.3568 | 5 | |
| 20 | 0.3597 | 0.3602 | 0.3607 | 4 | 0.3595 | 0.3599 | 0.3602 | 2 | |
| 21 | 0.3625 | 0.3630 | 0.3636 | 4 | 0.3623 | 0.3627 | 0.3631 | 2 | |

Evolutionary algorithm on SUN Fire E15k: $t_c = 30 \text{s}/p$

| | p = 1 | | p = 4 | | p = 8 | | p = 12 | | p = 16 | |
|----|--------|--------|-------|--------|------------|---------|-------------------|--------|--------|--------|
| n | perc · | f* | perc | f* | perc | f* | perc [°] | f* | perc | f* |
| | | | | S | tandard si | mplices | | | | |
| 5 | 100 | 0.1907 | 100 | 0.1907 | 100 | 0.1907 | 100 | 0.1907 | 100 | 0.1907 |
| 6 | 100 | 0.2309 | 100 | 0.2309 | 100 | 0.2309 | 100 | 0.2309 | 100 | 0.2309 |
| 7 | 100 | 0.2621 | 100 | 0.2621 | 100 | 0.2621 | 100 | 0.2621 | 100 | 0.262 |
| 8 | 100 | 0.2825 | 100 | 0.2825 | 100 | 0.2825 | 100 | 0.2825 | 100 | 0.282 |
| 9 | 100 | 0.2991 | 100 | 0.2991 | 100 | 0.2991 | 100 | 0.2991 | 100 | 0.2991 |
| 10 | 99 | 0.3115 | 100 | 0.3115 | 100 | 0.3115 | 100 | 0.3115 | 100 | 0.3115 |
| 11 | 95 | 0.3217 | 100 | 0.3217 | 100 | 0.3217 | 100 | 0.3217 | 100 | 0.3217 |
| 12 | 79 | 0.3300 | 100 | 0.3300 | 100 | 0.3300 | 100 | 0.3300 | 98 | 0.3300 |
| 13 | 60 | 0.3371 | 95 | 0.3371 | 86 | 0.3371 | 52 | 0.3371 | 29 | 0.337 |
| 14 | 45 | 0.3429 | 87 | 0.3429 | 34 | 0.3429 | 6 | 0.3429 | 1 | 0.3429 |
| 15 | 35 | 0.3481 | 20 | 0.3481 | 2 | 0.3481 | 1 | 0.3481 | 1 | 0.348 |
| 16 | 26 | 0.3525 | 7 | 0.3525 | 1 | 0.3527 | 1 | 0.3527 | 1 | 0.352 |
| | | | | | unit simp | lices | | | | |
| 6 | 100 | 0.1869 | 100 | 0.1869 | 100 | 0.1869 | 100 | 0.1869 | 100 | 0.1869 |
| 7 | 100 | 0.2247 | 100 | 0.2247 | 100 | 0.2247 | 100 | 0.2247 | 100 | 0.224 |
| 8 | 100 | 0.2569 | 100 | 0.2569 | 100 | 0.2569 | 100 | 0.2569 | 100 | 0.2569 |
| 9 | 100 | 0.2759 | 100 | 0.2759 | 100 | 0.2759 | 100 | 0.2759 | 100 | 0.2759 |
| 10 | 100 | 0.2936 | 100 | 0.2936 | 100 | 0.2936 | 100 | 0.2936 | 100 | 0.293 |
| 11 | 100 | 0.3058 | 100 | 0.3058 | 100 | 0.3058 | 100 | 0.3058 | 100 | 0.305 |
| 12 | 100 | 0.3167 | 100 | 0.3167 | 100 | 0.3167 | 100 | 0.3167 | 100 | 0.316 |
| 13 | 91 | 0.3249 | 100 | 0.3249 | 100 | 0.3249 | 77 | 0.3249 | 62 | 0.324 |
| 14 | 92 | 0.3325 | 100 | 0.3325 | 49 | 0.3325 | 20 | 0.3325 | 13 | 0.332 |
| 15 | 69 | 0.3384 | 61 | 0.3384 | 4 | 0.3384 | 3 | 0.3384 | 2 | 0.338 |
| 16 | 64 | 0.3439 | 8 | 0.3439 | 1 | 0.3439 | 1 | 0.3443 | 3 | 0.3443 |
| | | | | | cube | | | | | |
| 8 | 100 | 0.2245 | 100 | 0.2245 | 100 | 0.2245 | 100 | 0.2245 | 100 | 0.224 |
| 16 | 35 | 0.2965 | 1 | 0.2965 | 1 | 0.2965 | 1 | 0.2974 | 1 | 0.3009 |

