Interval MDS

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1 Problem

In the transformation phase of interval MDS we want to minimize

$$\sigma(\alpha,\beta):=\sum_{k=1}^K w_k(\alpha\delta_k+\beta-d_k)^2 \tag{1}$$

over the inequality constraints $\alpha\geq 0$ and $\alpha\delta_k+\beta\geq 0$ and the normalization constraint

$$\sum_{k=1}^K w_k(\alpha\delta_k+\beta)^2=1. \tag{2}$$

The w_k in definition (1) are non-negative weights. We assume, without loss of generality, that they add up to one.

The theory of normalized cone regression (De Leeuw (1975), Bauschke, Bui, and Wang (2018), De Leeuw (2019)) shows that we can ignore the normalization constraint and impose only the inequality constraints. We find the solution to the normalized problem by normalizing the solution of the unnormalized problem.

The inequality constraints are obviously equivalent to $\alpha\geq 0$ and $\alpha\delta_{\text{min}}+\beta\geq 0$, with δ_{min} the smallest of the δ_k. If $\gamma:=\alpha\delta_{\text{min}}+\beta$, and $e_k:=\delta_k-\delta_{\text{min}}$ then

$$\sigma(\alpha,\beta)=\sum_{k=1}^K w_k(\alpha\delta_k+\beta-d_k)^2=\sum_{k=1}^K w_k(\alpha e_k+\gamma-d_k)^2:=\sigma(\alpha,\gamma), \tag{3}$$

and we minimize σ over $\alpha \geq 0$ and $\gamma \geq 0$, i.e. over the non-negative orthant. Note that $e_k \geq 0$ for all k.

2 Equations

We start with the trivial observation that the minimum of any function over the non-negative orthant in two-dimensional space is attained either in the interior, i.e. the positive orthant, or on one of the two rays emanating from the origin along the axes, or at the intersection of these rays, i.e. the origin.

Now, in a more compact notation,

$$\sigma(\alpha, \gamma) = \alpha^2[e^2] + \gamma^2 + [d^2] + 2\alpha\gamma[e] - 2\alpha[ed] - 2\gamma[d], \tag{4}$$

where the square brackets indicate weighted means. We also assume that the MDS problem is non-trivial, by which we mean in this context that both $[e]$ and $[d]$ are positive.

If the minimum is attained in the interior then the gradient must vanish at the minimum. Suppose not all e_k are equal to zero (i.e. not all δ_k are equal). The gradient vanishes at

$$\alpha_0 = \frac{[ed] - [e][d]}{[e^2] - [e]^2}, \tag{5}$$

$$\gamma_0 = [d] - \alpha_0[e]. \tag{6}$$

If $\alpha_0 \geq 0$ and $\gamma_0 \geq 0$ we are done. We have found the required minimum at α_0 and $\beta_0 = \gamma_0 - \alpha_0\delta_{\text{min}}$.

If (α_0, γ_0) is not in the non-negative orthant, the minimum either occurs on the line $\alpha = 0$ or on the line $\gamma = 0$, or at their intersection (the origin).

The minimum on the line $\alpha = 0$ occurs at $\gamma_1 = [d]$ and is equal to

$$\sigma_1 = \sigma(0, \gamma_1) = [d^2] - [d]^2. \tag{7}$$

Since $[d]$ is positive in MDS the point $(\alpha_1 = 0, \gamma_1)$ is in the non-negative orthant, and thus always feasible. Also $\beta_1 = \gamma_1$ and thus $\alpha_1\delta_k + \beta_1 = [d]$.

The minimum on the line $\gamma = 0$ occurs at

$$\alpha_2 = \frac{[ed]}{[e^2]}, \tag{8}$$

and is equal to

$$\sigma_2 := \sigma(\alpha_2, 0) = [d^2] - \frac{[ed]^2}{[e^2]}. \tag{9}$$

Again $\alpha_2 \geq 0$ and thus $(\alpha_2, \gamma_2 = 0$ is always feasible. Also $\gamma_2 = 0$ means that $\beta_2 = -\alpha_2\delta_{\text{min}}$ and $\alpha_2\delta_k + \beta_2 = \alpha_2 e_k$.

Thus, summarizing, if (α_0, γ_0) is not feasible then the minimum is at (α_1, β_1) if $\sigma_1 < \sigma_2$ and at (α_2, β_2) if $\sigma_2 < \sigma_1$. There is C code (for the unweighted case of the smacof project) in the appendix.

3 Appendix: Code

```c
#include <math.h>
#include <stdlib.h>
#define MIN(x, y) (((x) < (y)) ? (x) : (y))
#define SQUARE(x) ((x) * (x))

void smacofUnweightedInterval(const unsigned n, const double (*delta)[n][n],
                              const double (*dmat)[n][n],
                              double (*dhat)[n][n]) {
    double deltamin = INFINITY;
    for (unsigned i = 0; i < n; i++) {
        for (unsigned j = 0; j < n; j++) {
            deltamin = MIN(deltamin, (*delta)[i][j]);
        }
    }
    double sed = 0.0, see = 0.0, se = 0.0, sd = 0.0, sdd = 0.0,
           dm = (double)(n * (n - 1) / 2);
    for (unsigned j = 0; j < (n - 1); j++) {
        for (unsigned i = (j + 1); i < n; i++) {
            double eij = (*delta)[i][j] - deltamin;
            double dij = (*dmat)[i][j];
            se += eij;
            sd += dij;
            sed += eij * dij;
            see += SQUARE(eij);
            sdd += SQUARE(dij);
        }
    }
    se /= dm;
    sd /= dm;
    sed /= dm;
    see /= dm;
    sdd /= dm;
    double alpha = (sed - se * sd) / (see - SQUARE(se));
    double gamma = (sd - alpha * se);
    if ((alpha < 0.0) || (gamma < 0.0)) {
        double s1 = sdd - SQUARE(sed) / see;
        double s2 = sdd - SQUARE(sd);
        if (s1 <= s2) {
            alpha = 0.0;
            gamma = sd;
        } else {
            alpha = sed / see;
```

```
            gamma = 0.0;
        }
    }
    double beta = gamma - alpha * deltamin;
    for (unsigned j = 0; j < (n - 1); j++) {
        for (unsigned i = (j + 1); i < n; i++) {
            (*dhat)[i][j] = alpha * (*delta)[i][j] + beta;
            (*dhat)[j][i] = (*dhat)[i][j];
        }
    }
    return;
}
```

References

Bauschke, H. H., M. N. Bui, and X. Wang. 2018. "Projecting onto the Intersection of a Cone and a Sphere." *SIAM Journal on Optimization* 28: 2158–88.

De Leeuw, J. 1975. "A Normalized Cone Regression Approach to Alternating Least Squares Algorithms." Department of Data Theory FSW/RUL.

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