Interval MDS

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Contents

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 that add up to one. Note that some or all of the δ_k can be negative.

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. Now a little change of variables. Define $\gamma:=\alpha\delta_{\text{min}}+\beta$, and let $e_k:=\delta_k-\delta_{\text{min}}$. Note that $e_k\geq 0$ for all k.

The cone of vectors $\alpha\delta_k + \beta$ with $\alpha \geq 0$ and $\alpha\delta_k + \beta \geq 0$ is the same as the cone $\alpha e_k + \gamma$ with $\alpha \geq 0$ and $\gamma \geq 0$. Thus our original (unnormalized) problem is equivalent to minimization of

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

over $\alpha \geq 0$ and $\gamma \geq 0$, i.e. over the non-negative orthant. Of course the normalization condition becomes

$$\sum_{k=1}^{K} w_k(\alpha e_k + \gamma)^2 = 1. \tag{4}$$

2 Equations

So let's first consider the unnormalized problem of minimizing σ over $\alpha \geq 0$ and $\gamma \geq 0$.

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. at the origin.

Now, in a more compact notation,

$$\sigma(\alpha, \gamma) = \alpha^2[e^2] + \gamma^2 + [d^2] + 2\alpha\gamma[e] - 2\alpha[ed] - 2\gamma[d], \tag{5}$$

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 $[e]$ is zero all δ_k are equal, if $[d]$ is zero all d_k are zero. Just in case, if all e_k are zero then the optimum γ is $\gamma_0 = [d]$, while α_0 is arbitrary. The minimum is equal to $\sigma_0 = [d^2] - [d]^2$.

If the minimum is attained in the interior then the gradient must vanish at the minimum. The gradient vanishes at

$$\alpha_0 = \frac{[ed] - [e][d]}{[e^2] - [e]^2}, \tag{6}$$

$$\gamma_0 = [d] - \alpha_0[e]. \tag{7}$$

If $\alpha_0 \geq 0$ and $\gamma_0 \geq 0$ we are done and we have found the required minimum. The minimum value of σ is

$$\sigma_0 = [d^2] - [d]^2 - \frac{([ed] - [e][d])^2}{[e^2] - [e]^2}. \tag{8}$$

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 minimum on the line $\alpha = 0$ occurs at $\alpha_1 = 0$ and $\gamma_1 = [d]$, and is equal to

$$\sigma_1 = \sigma(\alpha_1, \gamma_1) = [d^2] - [d]^2. \tag{9}$$

Since $[d]$ is positive the point (α_1, γ_1) is in the non-negative orthant, and thus always feasible. From the normalization condition we find that the solution of the normalized problem on $\alpha = 0$ is the point $(0, 1)$.

The minimum on the line $\gamma = 0$ occurs at $\gamma_2 = 0$ and

$$\alpha_2 = \frac{[ed]}{[e^2]}, \tag{10}$$

and is equal to

$$\sigma_2 := \sigma(\alpha_2, 0) = [d^2] - \frac{[ed]^2}{[e^2]}. \tag{11}$$

Again $\alpha_2 \geq 0$ and thus (α_2, γ_2) is always feasible. the solution to the normalized problem on $\gamma = 0$ is the point $([e^2]^{-\frac{1}{2}}, 0)$.

Thus, summarizing, if (α_0, γ_0) is not feasible then the minimum of the unnormalized problem 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

```
#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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