Differentiability of rStress at a Local Minimum

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Note: This is a working paper which will be expanded/updated frequently. The directory deleeuwpdx.net/pubfolders/rstressdiff has a pdf copy of this article and the complete Rmd file.

1 Problem

We study differentiability of the multidimensional scaling loss function rStress ((**deleeuw_E_16a?**)), defined as

$$\sigma_r(x) := \sum_{i=1}^{n} w_i(\delta_i - (x'A_ix)^r)^2 \tag{1}$$

for some $r > 0$. Here the w_i are positive weights and the δ_i are positive dissimilarities. The matrices A_i are positive semi-definite, and the quantities $x'A_ix$ are squared distances.

Clearly if $x'A_ix > 0$ for all i the loss function is differentiable. De Leeuw (1984) proves directional differentiability for $r = \frac{1}{2}$ and he shows that at a local minimum we generally have $x'A_ix > 0$. We investigate if and how this results generalizes to σ_r.

2 Directional Derivatives

Define the directional derivative

$$d\sigma_r(x,y) := \lim_{\epsilon\downarrow 0}\frac{\sigma_r(x+\epsilon y)-\sigma_r(x)}{\epsilon}.$$

For our computations we need

$$\begin{aligned}I_+(x) &:= \{i \mid x'A_ix > 0\},\\ I_0(x) &:= \{i \mid x'A_ix = 0\}.\end{aligned}$$

Then

$$\begin{aligned}\frac{\sigma_r(x+\epsilon y)-\sigma_r(x)}{\epsilon} &= -4r\sum_{i\in I_+} w_i(\delta_i-(x'A_ix)^r)(x'A_ix)^{r-1}y'A_ix\\ &\qquad - 2\epsilon^{2r-1}\sum_{i\in I_0} w_i\delta_i(y'A_iy)^r + \epsilon^{4r-1}\sum_{i\in I_0} w_i(y'A_iy)^{2r} + \frac{o(\epsilon)}{\epsilon},\end{aligned}$$

and thus

$$d\sigma_r(x,y) = \begin{cases}-4r\sum_{i=1}^n w_i(\delta_i-(x'A_ix)^r)(x'A_ix)^{r-1}y'A_ix & \text{if } r>\frac{1}{2},\\ -4r\sum_{i\in I_+} w_i(\delta_i-(x'A_ix)^r)(x'A_ix)^{r-1}y'A_ix - 2\sum_{i\in I_0} w_i\delta_i(y'A_iy)^r & \text{if } r=\frac{1}{2},\\ +\infty & \text{if } r<\frac{1}{2}.\end{cases}$$

3 Results

From our computations we derive the following results.

Theorem 1: If $r > \frac{1}{2}$ then σ_r is differentiable at x. If σ_r has a local minimum at x then

$$\sum_{i=1}^n w_i\delta_i(x'A_ix)^{r-1}A_ix = \sum_{i=1}^n w_i(x'A_ix)^{2r-1}A_ix.$$

Theorem 2: If $r = \frac{1}{2}$ then σ_r is directionally differentiable at x in every direction y. If σ_r has a local minimum at x then

$$\sum_{i\in I_+(x)} w_i\delta_i(x'A_ix)^{r-1}A_ix = \sum_{i\in I_+(x)} w_i(x'A_ix)^{2r-1}A_ix.$$

and $I_0(x) = \emptyset$.

Theorem 3: If $r < \frac{1}{2}$ then σ_r is directionally differentiable only in those directions y with $y'A_iy = 0$ for all $i \in I_0(x)$.

Thus for $r = \frac{1}{2}$ we have non-zero distances and differentiability at local minima, for $r > \frac{1}{2}$ it is quite possible that local minima with zero distances exist, and for $r > \frac{1}{2}$ rStress is not even directionally differentiable at points with zero distances.

4 Local Maximum

We can also generalize a result of De Leeuw (1993) to rStress.

Theorem 4: σ_r has a local maximum at x if and only if $x = 0$.

Proof: If $x = 0$ then

$$\sigma_r(x + \epsilon y) - \sigma_r(x) = -2\epsilon^{2r}\left\{\sum_{i=1}^n w_i\delta_i(y'Ay)^r - \frac{1}{2}\epsilon^{2r}\sum_{i=1}^n w_i(y'A_iy)^{2r}\right\}.$$

It follows that if

$$\frac{1}{2}\epsilon^{2r} \leq \frac{\sum_{i=1}^n w_i\delta_i(y'Ay)^r}{\sum_{i=1}^n w_i(y'A_iy)^{2r}}$$

we have $\sigma(x + \epsilon y) - \sigma(x) \leq 0$. So, although σ_r may not even directionally differentiable at $x = 0$, it does decrease in all directions and is thus a local minimum.

Converse, suppose σ_r has a local maximum at $x \neq 0$. Then

$$\sigma_r(\epsilon x) = \sum_{i=1}^n w_i\delta_i^2 - 2\theta\sum_{i=1}^n w_i\delta_i(x'Ax)^r + \theta^2\sum_{i=1}^n w_i(x'A_ix)^{2r},$$

with $\theta := \epsilon^{2r}$. Thus σ_r is a convex quadratic in θ and it cannot have a local maximum on the ray through x. **QED** $$

#NEWS

001 01/14/16 – First upload

002 01/15/16 – Added local maximum result

003 02/08/16 – Corrected some typos

#References

De Leeuw, J. 1984. "Differentiability of Kruskal's Stress at a Local Minimum." *Psychometrika* 49: 111–13.

———. 1993. "Fitting Distances by Least Squares." Preprint Series 130. Los Angeles, CA: UCLA Department of Statistics.