Differentiability of Functions of Distances

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Abstract

The stress loss function in metric multidimensional scaling is differentiable at local minima. In this note we generalize this result to more general functions of the distances.

Contents

Note: This is a working paper which will be expanded/updated frequently. All suggestions for improvement are welcome. The directory deleeuwpdx.net/pubfolders/distdiff has a pdf version, the bib file, and the complete Rmd file.

1 Introduction

In multidimensional scaling we minimize the stress measure proposed by Kruskal (1964a), Kruskal (1964b) and defined as

$$\sigma(x) = \sum_{k=1}^{m} w_k(\delta_k - \sqrt{x'A_k x})^2. \tag{1}$$

The w_k are known positive *weights*, the δ_k are known positive *dissimilarities*. The A_k are known positive semi-definite matrices. In multidimensional scaling the A_k are defined in such a way that the $x'A_k x$ are squared Euclidean distances between n points in $\mathbb{R}^p$, but this results in this note are valid for any positive semie-definite A_k.

Clearly stress is not differentiable at those x for which one or more of the $x'A_k x$ are zero. This can create problem for gradient-based algorithms, because the relevant derivatives may not exist and/or they may not vanish at stationary points.

It is shown, however, in De Leeuw (1984) that the directional derivative

$$\mathbf{D}\sigma(x, y) = \lim_{\epsilon \downarrow 0} \frac{\sigma(x + \epsilon y) - \sigma(x)}{\epsilon} \tag{2}$$

exists for all x and y. At a local minimum, i.e. an x for which $\mathbf{D}\sigma(x, y) \geq 0$ for each y, De Leeuw (1984), and more generally De Leeuw (2018), shows that $x'A_k x > 0$, which implies that stress is differentiable at local minima.

2 Results

We now generalize the result from De Leeuw (1984) to a much more general class of functions of the $\sqrt{x'A_kx}$.

Theorem 1: [Differentiability] Suppose $\sigma(x) = F(\sqrt{x'A_1x}, \cdots, \sqrt{x'A_mx})$ with F continuously differentiable and $\mathcal{D}_kF(z) < 0$ if $z_k = 0$. Then σ is differentiable at local minima, and at local minima $x'A_kx > 0$.

Proof:

For the $\sqrt{x'A_kx}$ we have

$$\sqrt{(x+\epsilon y)'A_k(x+\epsilon y)} = \sqrt{x'A_kx} + \epsilon \left\{ \begin{array}{ll} \frac{1}{\sqrt{x'A_kx}}x'A_ky & \text{if } x'A_kx > 0 \\ \sqrt{y'A_ky} & \text{if } x'A_kx = 0 \end{array} \right\} + o(\epsilon). \qquad (3)$$

Thus we find for the directional derivative of σ

$$\mathbf{D}\sigma(x,y) = \sum_{x'A_kx>0} \mathcal{D}_kF(\sqrt{x'A_1x}, \cdots, \sqrt{x'A_mx}) \frac{1}{\sqrt{x'A_kx}} x'A_ky +$$
$$\sum_{x'A_kx=0} \mathcal{D}_kF(\sqrt{x'A_1x}, \cdots, \sqrt{x'A_mx})\sqrt{y'A_ky}. \qquad (4)$$

If the assumption of the theorem is true there is an y such that the second term on the right in (4) is negative. If for that y the first term is positive we change y to $-y$. The first term becomes negative, the second term remains negative. Thus the derivative in the direction y is negative and x cannot be a local minimum. ∎

Corollary 1: [Separable] Suppose $\sigma(x) = \sum_{k=1}^m f_k(\sqrt{x'A_kx})$ with the f_k continuously differentiable and $Df_k(0) < 0$. Then σ is differentiable at local minima, and at local minima $x'A_kx > 0$.

Proof: In this case

$$\sum_{x'A_kx=0} \mathcal{D}_kF(\sqrt{x'A_1x}, \cdots, \sqrt{x'A_mx})\sqrt{y'A_ky} = \sum_{x'A_kx=0} Df_k(0)\sqrt{y'A_ky},$$

which can be made negative for some y. ∎

Corollary 2: [Least Squares] Suppose $\sigma(x) = \sum_{k=1}^m w_k(\delta_k - \phi(\sqrt{x'A_kx}))^2$ with ϕ continuously differentiable, $\phi(0) = 0$, and $\mathcal{D}\phi(0) > 0$. Then σ is differentiable at local minima, and at local minima $x'A_kx > 0$.

Proof: In this case

$$\sum_{x'A_kx=0} \mathcal{D}_kF(\sqrt{x'A_1x}, \cdots, \sqrt{x'A_mx})\sqrt{y'A_ky} = - \sum_{x'A_kx=0} w_k\delta_k\mathcal{D}\phi(0)\sqrt{y'A_ky},$$

which can be made negative for some y. ∎

Remark 1: [**RStress**] The result of corollary 2 can be applied to rStress (De Leeuw, Groenen, and Mair (2016)), defined as

$$\sigma_r(x) = \sum_{k=1}^{m} w_k(\delta_k - (\sqrt{x'A_kx})^r)^2$$

with $r > 0$. Thus $\phi(z) = z^r$ and $\mathcal{D}\phi(z) = rz^{r-1}$. But if $r < 1$ then ϕ is not differentiable at zero and our results do not apply. If $r > 1$ then $\mathcal{D}\phi(0) = 0$, rStress is differentiable everywhere, and again our results do not apply (although obviously if $r > 1$ then rStress is differentiable at local minima, even if $x'A_kx = 0$). The only rStress covered by our result is Kruskal's stress, with $r = 1$.

References

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