Multidimensional scaling as a tool for smoothing over complex spatial regions

David Lawrence Miller

Mathematical Sciences
University of Bath

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Outline

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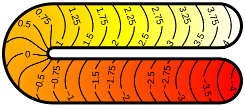
Smoothing in 2 dimensions

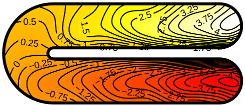
- Have some geographical region and wish to find out something about the biological population in it.
- Response is eg. animal distribution, wish to predict based on (x, y) and other covariates eg. habitat, size, sex, etc.
- This problem is relatively easy if the domain is simple.

Leakage (or, “whales don’t live in glaciers”)

- Smoothing of complex domains makes this a lot more difficult.
- Problem of leakage.
- Wrong metric.
- Euclidean distance doesn’t always make sense.



(modified) Ramsay test function



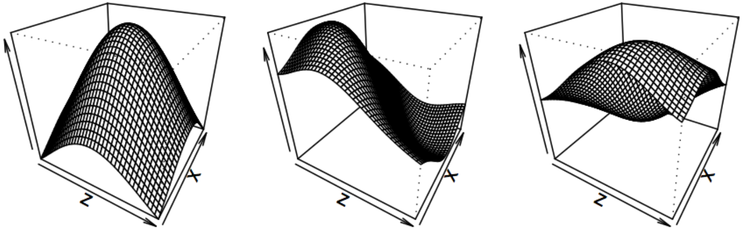
Thin plate spline fit

Smoothing with penalties

- Do smoothing with splines in an additive model framework.
- Take some linear combination of (known) basis functions.
- Penalize based on integral of second squared derivative:

$$\int\int_{\Omega}\left(\left(\frac{\partial^2 f(x,y)}{\partial x^2}\right)^2 + 2\left(\frac{\partial^2 f(x,y)}{\partial x \partial y}\right)^2 + \left(\frac{\partial^2 f(x,y)}{\partial y^2}\right)^2\right)\mathrm{d}x\mathrm{d}y.$$

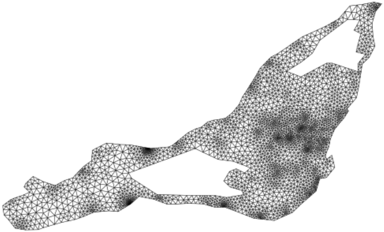
- Here using thin plate regression splines (eg Wood (2003)).

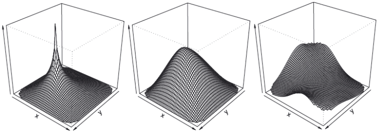


Proposed solutions to leakage problems

Two categories: PDE boundary condition based, within-area distance based.

- PDEs:
  - FELSPLINE (Ramsay, 2002).
  - Soap film smoothers (Wood *et al*, 2008).
- Within-area distance
  - Within-area distance (Wang and Ranalli, 2007).



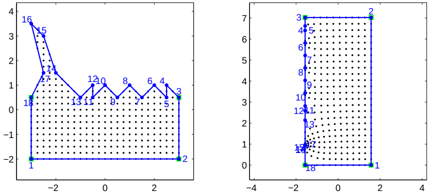


“The Third Way”

- Domain morphing.
- Takes into account within-area distance.
- Gives a known domain that is easier to smooth over.
- Potentially less computationally intensive.
- Eilers (2006) proposes Schwarz-Christoffel transform.

However:

- Don’t maintain isotropy - distribution of points odd.
- Not clear what this does to the smoothness penalty - artefacts, penalty issues.



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Multidimensional scaling and within-area distances

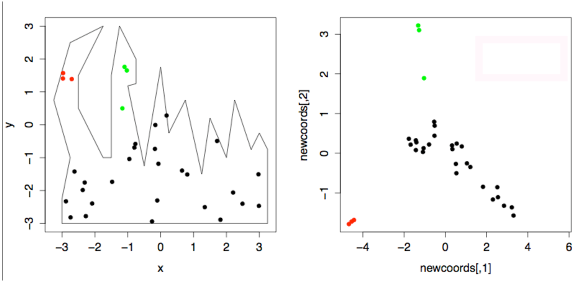
- Idea: use MDS to to arrange points in the domain according to their distance within the domain.

Scheme:

- First need to find the within-area distances.
- Perform MDS on the matrix of within-area distances.
- Find the new configuration of the points.
- Smooth over the new points.

Multidimensional scaling refresher

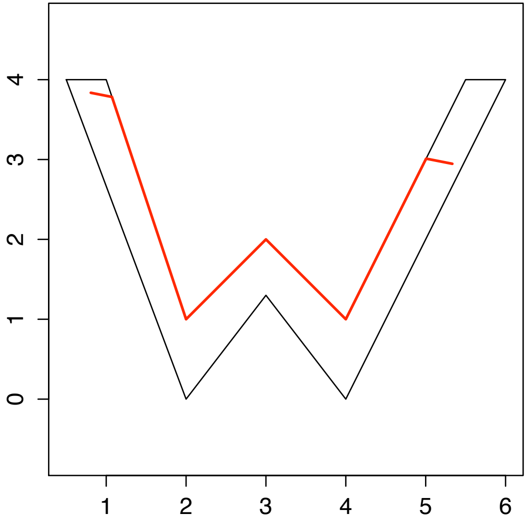
- Use double centred matrix of between point distances, D, using the eigen-decomposition of DD^T we can find new points.
- Finds a configuration of points such that Euclidean distance between points in new arrangement is approximately the same as distance in the domain.
- New points can be added into the MDS configuration via Gower's interpolation (Gower, 1968)



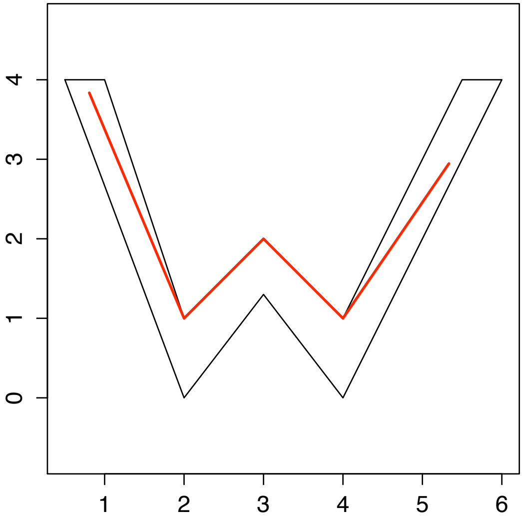
A “new” algorithm for finding within-area distances

- Algorithm “bounces” around inside the polygon.
- Initial path is just the path around the edge, then iterate over two steps: *delete* and *alter*.
- Delete (iterating over all nodes):
  - If we can shorten the path by simply deleting a node, do that.
- Alter (iterating over all nodes):
  - If we can find a shorter sub-path by bouncing off the other “side” of the polygon, do that.

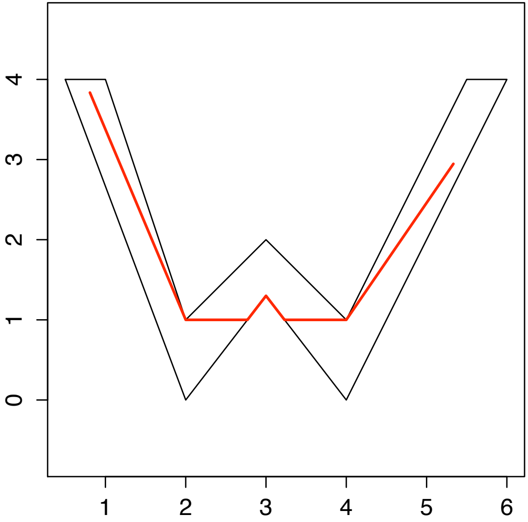
Finding the path - 1



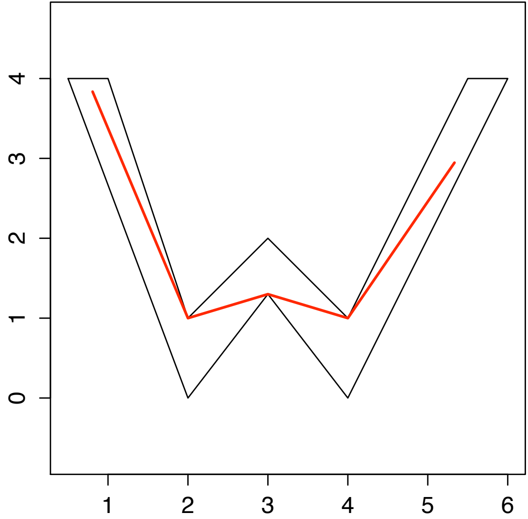
Finding the path - 2



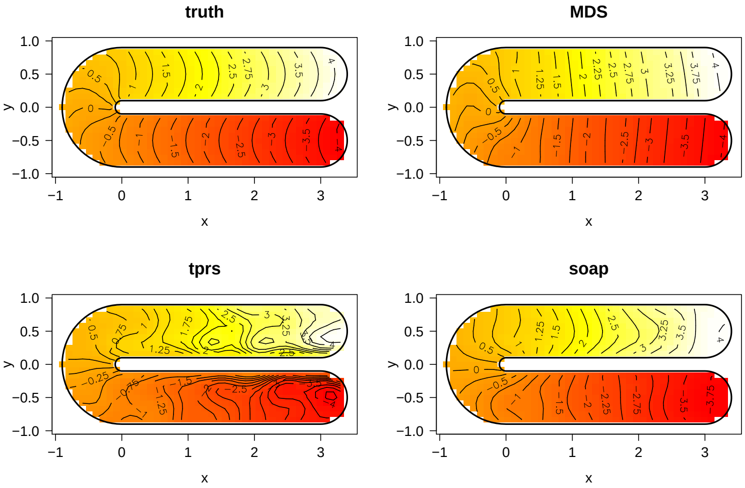
Finding the path - 3



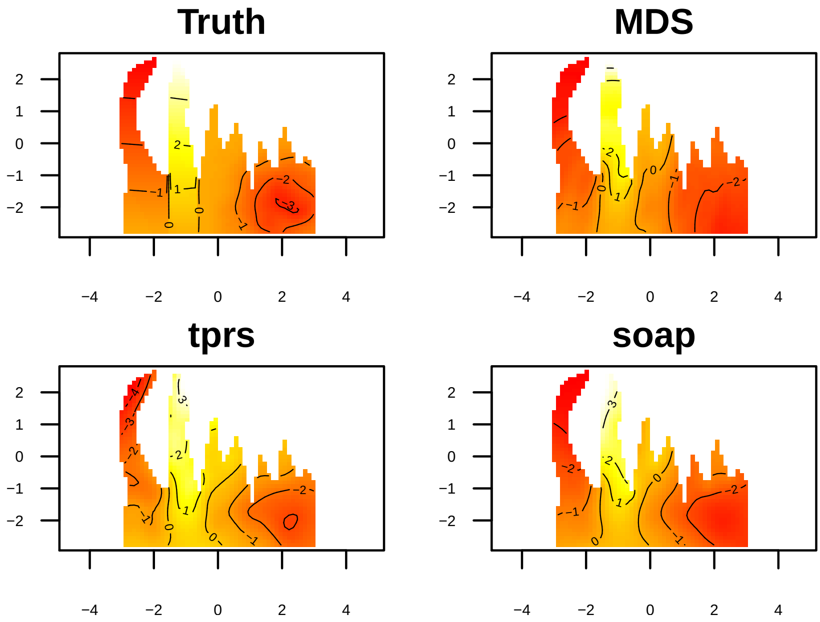
Finding the path - 4



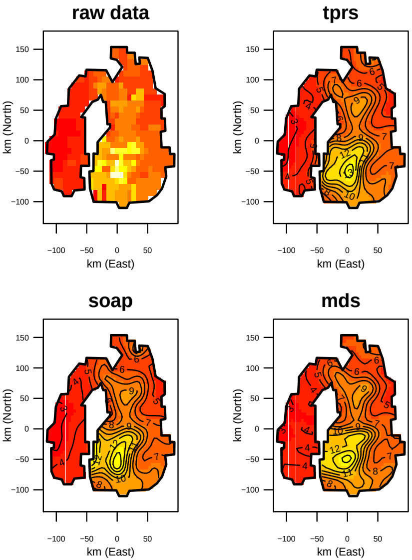
Ramsay simulations



A different domain

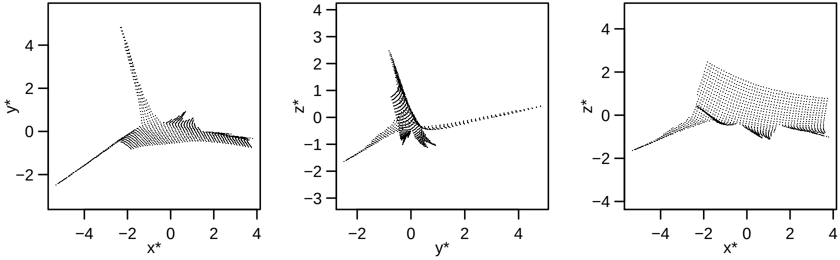


The Aral sea


raw data
tprs
soap
mds
km (North)
km (East)
150
100
50
0
−50
−100
−100
−50
0
50

So, it looks good, but...

- Computationally costly to find the within-area distances. (Esp. prediction.)
- Comparative in MSE terms to the soap film smoother.
- Artefacts.
- Taking a *m*-D projection of *n*-D space.



Can we get around the squashing?

- 3-D projection does better, but can we keep going? (Nullspace gets BIG!)
- For anisotropic smoothing, Wood (2000) suggests:

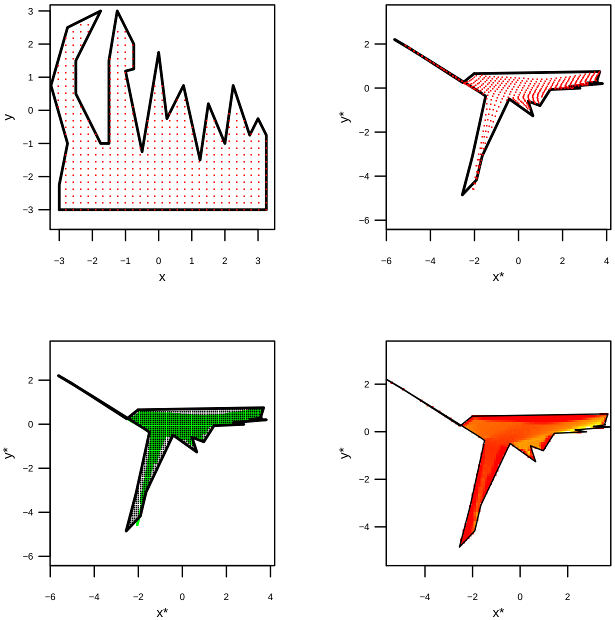
$$\int\int_\Omega \left(\frac{\partial^2 f(x,y)}{\partial x^2}\right)^2 + 2k\left(\frac{\partial^2 f(x,y)}{\partial x \partial y}\right)^2 + k^3\left(\frac{\partial^2 f(x,y)}{\partial y^2}\right)^2 \mathrm{d}x\mathrm{d}y.$$

- $\mathcal{L}^*(x,y)$, a function of point density in the new space.
- Adjust penalty:

$$\int\int_\Omega \mathcal{L}^*(x,y)\left(\left(\frac{\partial^2 f(x,y)}{\partial x^2}\right)^2 + \left(\frac{\partial^2 f(x,y)}{\partial x \partial y}\right)^2 + \left(\frac{\partial^2 f(x,y)}{\partial y^2}\right)^2\right)\mathrm{d}x\mathrm{d}y.$$

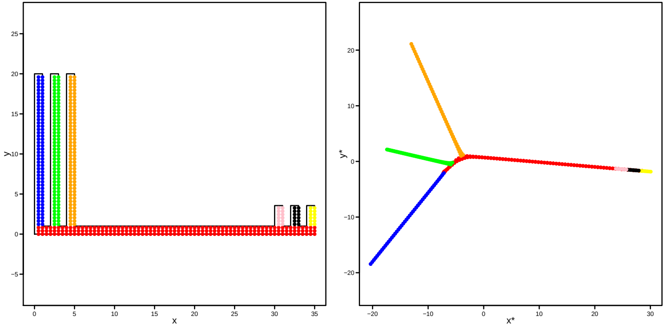
- Some improvements in MSE terms, doesn't get rid of all artefacts.

Calculating $\mathcal{L}^*(x, y)$



Ordering

- So, where are the artefacts coming from?
- Taking projections of n-dimensional space.
- Points can lose ordering.



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Final comments

- Clearly, not that useful in practise.
- Smoothing on manifolds?
- Better idea of what is required to make domain transformation work in general.

Criteria for domain transformation techniques:

- No crowding.
- Maintain order.
- Smooth mapping.
- Fast mapping.

The key: transform "just enough" but no more.

References

- S.N. Wood, M.V. Bravington, and S.L. Hedley. *Soap film smoothing. JRSSB, 2008*
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- T.A. Driscoll and L.N. Trefethen. *Schwarz-Christoffel Mapping. Cambridge, 2002*
- T. Ramsay. *Spline smoothing over difficult regions. JRSSB, 2002*
- P.H.C. Eilers. *P-spline smoothing on difficult domains. University of Munich seminar, 2006*
- J.C. Gower. *Adding a point to vector diagrams in multivariate analysis. Biometrika, 1968.*

Slides available at `http://people.bath.ac.uk/dlm27`

Appendix - Ordering problems in 4-D