Two new approaches to smoothing over complex regions

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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.

Smoothing with penalties

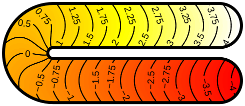
- Objective function takes the form:

$$\sum_{i=1}^{n}(z_i - f(x_i, y_i; \theta))^2 + \lambda \int_\Omega Pf(x, y; \theta) d\Omega$$

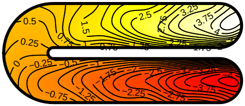
- f is the function you want to estimate, made up of some combination of basis functions.
- P is some squared derivative penalty operator, usually $P = (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})^2$.
- This can be generalized to an additive model or GAM.

Smoothing over complex domains

- Smoothing of complex domains makes this a lot more difficult.
- Problem of leakage.
- Euclidean distance doesn't always make sense.
- Models need to incorporate information about the intrinsic structure of the domain.



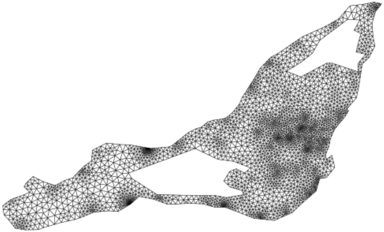
(modified) Ramsay test function

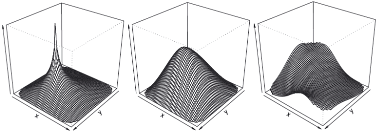


Thin plate spline fit

Possible solutions to leakage problems

- FELSPLINE (Ramsay, (2002).)
- Domain morphing (Eilers, (2006).)
- Within-area distance (Wang and Ranalli, (2007).)
- Soap film smoothers (Wood *et al*, (2008).)



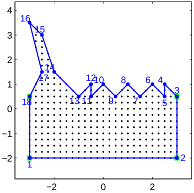
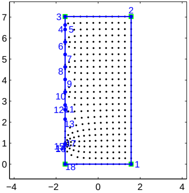


Why morph the domain?

- Takes into account within-area distance.
- Gives a known domain that is easier to smooth over.
- Potentially less computationally intensive.

However:

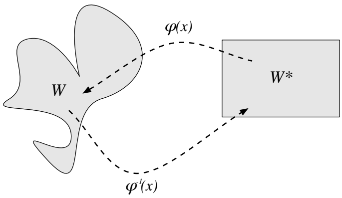
- Don't maintain isotropy - distribution of points odd.
- Not clear what this does to the smoothness penalty.

Outline

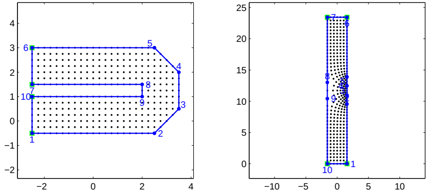
The Schwarz-Christoffel transform

- Take a polygon in some domain W and morph it to a new domain W^*.
- Do this by starting at the new domain and working back to the polygon.
- Can draw a polygonal bounding box around some arbitrary shape.



Schwarz-Christoffel algorithm

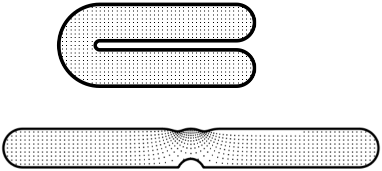
- Start with a rectangle.
- Add vertices.
- Iteratively deform by changing angles.
- Continue until the new shape is identical to the polygon.
- We then have a function for the mapping, $\varphi(x, y)$.
- $\varphi(x, y)$ is a conformal mapping.



The mapping

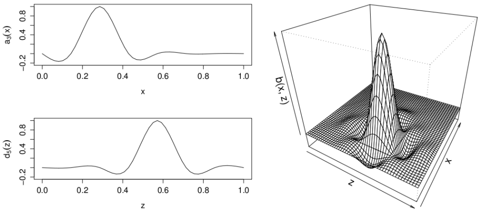
- Use a bounding box around the horseshoe.

- Morphing the horseshoe shape still gives a slightly odd domain however, we are still doing better than before.

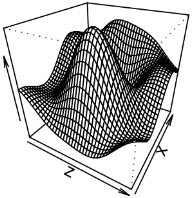


Results

- Fit using both thin plate regression splines and P-splines with a comparison to the soap film (current best.)
- MSE used to compare over a grid of predicition points.

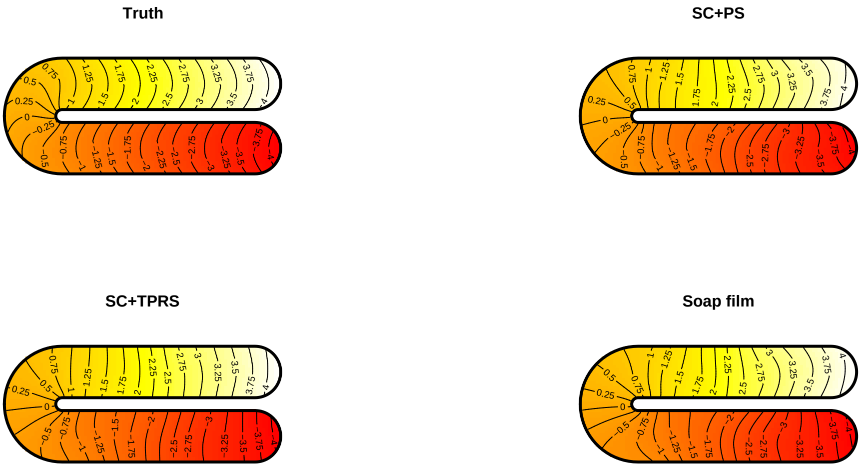


Tensor product



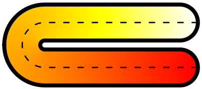
Thin plate

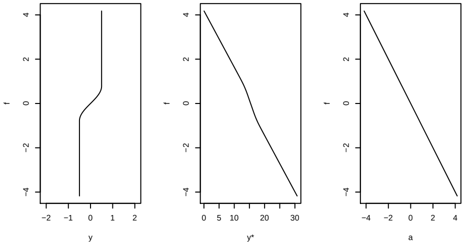
Horseshoe plots



Why does it do well?

- Looking at line plots, we can see the difference in gradient.
- SC method seems to approximate the gradient better.

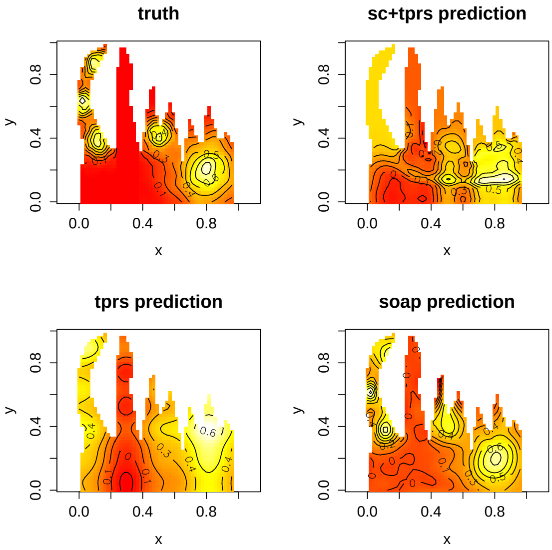




Problems

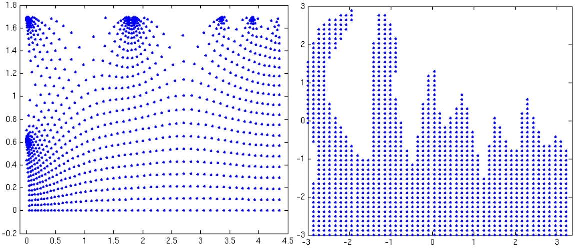
- Small:
  - Implementation is Matlab+R. (YUCK!)
- **BIG**:
  - Weird artifacts.
  - Morphing of domain appears to cause features to be smoothed over.
  - Arbitrary selection of vertices.

A more realistic domain



A more realistic domain - what's happening?

- Weird "crowding" effect.
- Different with each vertex choice. All bad.



Outline

Multidimensional scaling and within-area distances

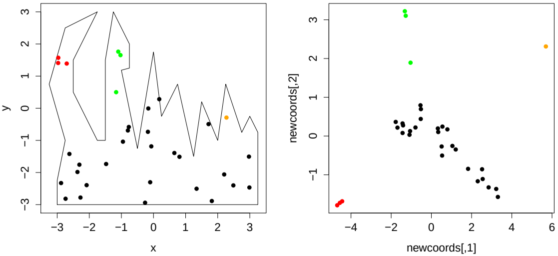
- Idea: use MDS to to arrange points in the domain according to their “within-domain distance.”

Scheme:

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

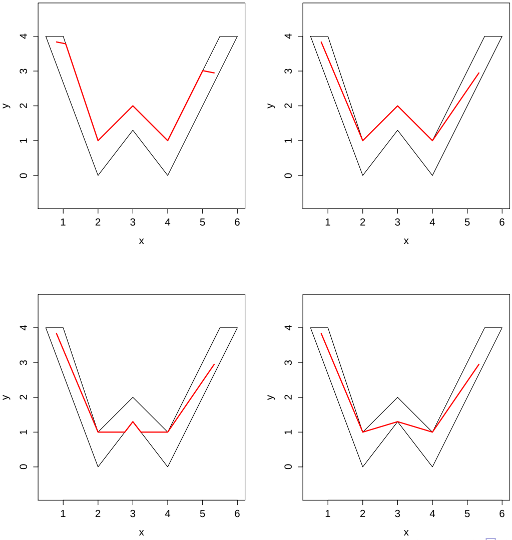
Multidimensional scaling refresher

- Double centre matrix of between point distances, D, (subtract row and column means) then find DD^T.
- Finds a configuration of points such that Euclidean distance between points in new arrangement is approximately the same as distance in the domain.
- Already implemented in R by `cmdscale`.

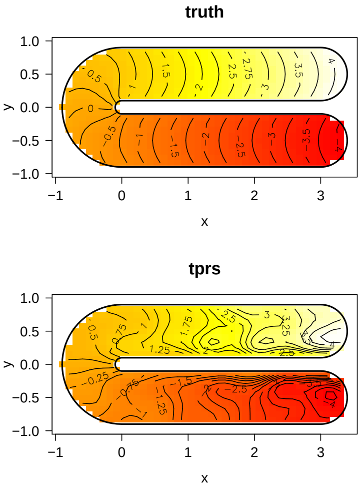


Finding within-area distances

- Use a new algorithm to find the within area distances.



Ramsay simulations (low noise)



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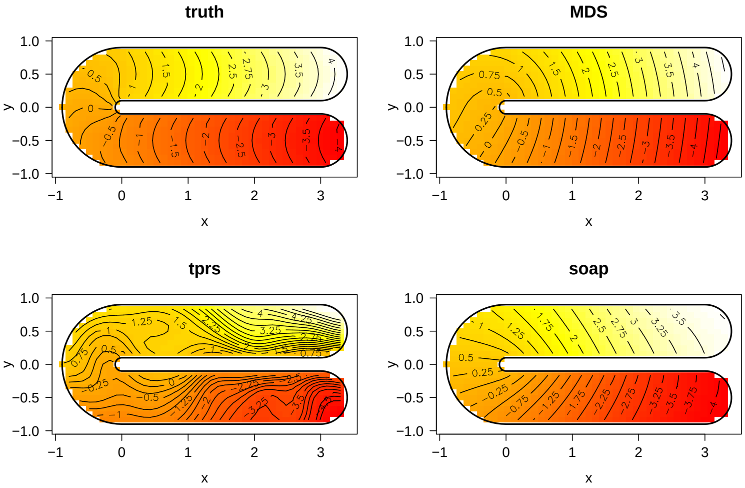
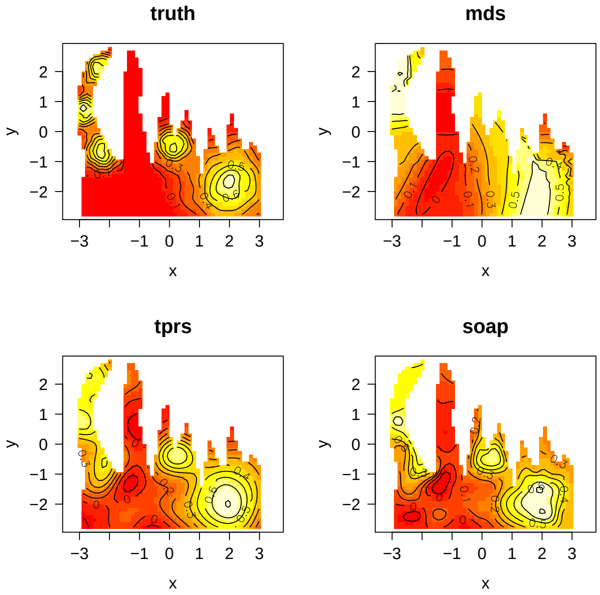


A different domain



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Conclusions

- Seems that the S-C transform does not have much utility.
- MDS shows more promise, easier to transfer to higher dimensions.
- MDS does not impose strict boundary conditions so leakage still possible.
- After initial “transform” calculation, both methods only use the same computational time as a thin plate regression spline. (Soap is expensive.)

Further work

- Real data!
- Implement insertion of new points using method of Gower (1968).
- Current within-area distance algorithm is pure R, very slow. Need to re-write in C/Fortran.
- Pushing the data into more dimensions might be useful to separate points.

References

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- C. Chatfield and A.J. Colins. *Introduction to multivariate analysis. CRC, 1980*
- J.C. Gower. *Adding a point to vector diagrams in multivariate analysis. Biometrika, 1968.*

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