

# Two new approaches to smoothing over complex regions

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# Outline

## Smoothing over complex regions

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Solutions

## Domain morphing with the Schwarz-Christoffel transform

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## Multidimensional Scaling

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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

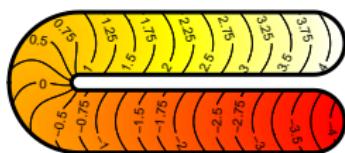
- ▶ Objective function takes the form:

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

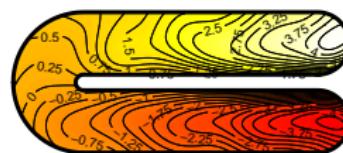
- ▶  $f$  is the function you want to estimate, made up of some combination of basis functions.
- ▶  $P$  is some squared derivative penalty operator, usually  $P = (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})^2$ .
- ▶ This can be generalized to an additive model or GAM.

# 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

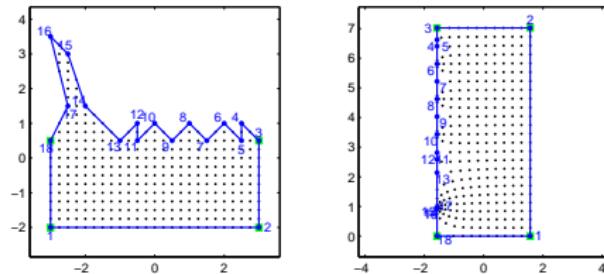
- ▶ FELSPLINE (Ramsay, (2002).)
- ▶ Domain morphing (Eilers, (2006).)
- ▶ Within-area distance (Wang and Ranalli, (2007).)
- ▶ Soap film smoothers (Wood *et al*, (2008).)

# 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.



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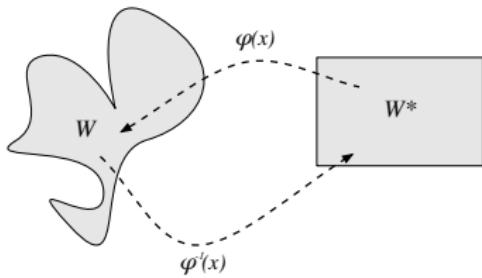
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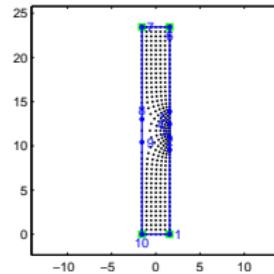
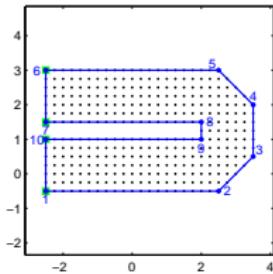
# The Schwarz-Christoffel transform

- ▶ 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.

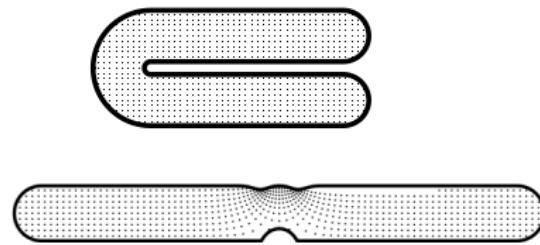


## The mapping

- ▶ Use a bounding box around the horseshoe.

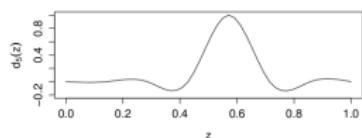
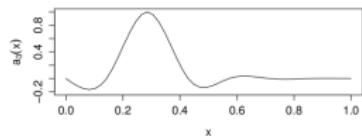


- ▶ Morphing the horseshoe shape still gives a slightly odd domain however, we are still doing better than before.

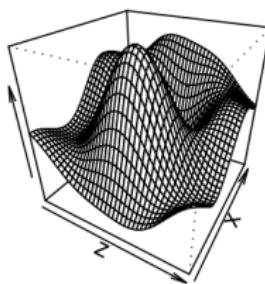
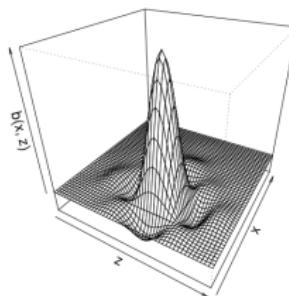


# Results

- ▶ 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 prediction points.



Tensor product



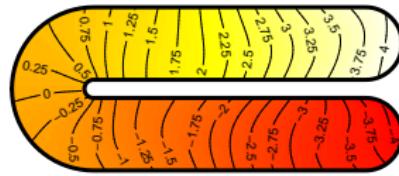
Thin plate

# Horseshoe plots

Truth



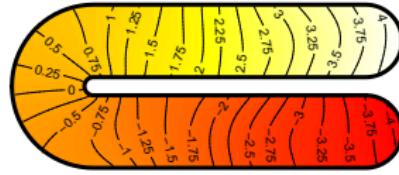
SC+PS



SC+TPRS

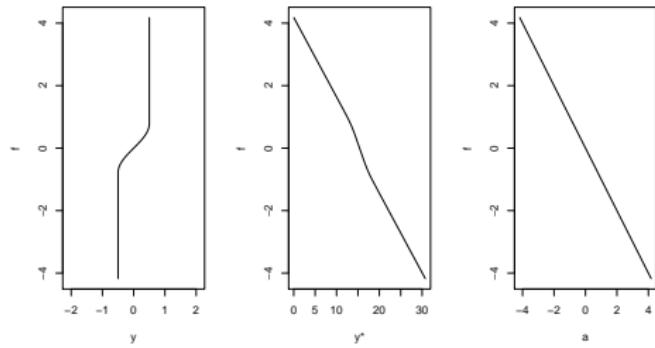
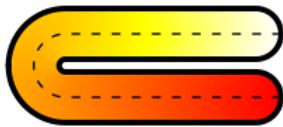


Soap film



# Why does it do well?

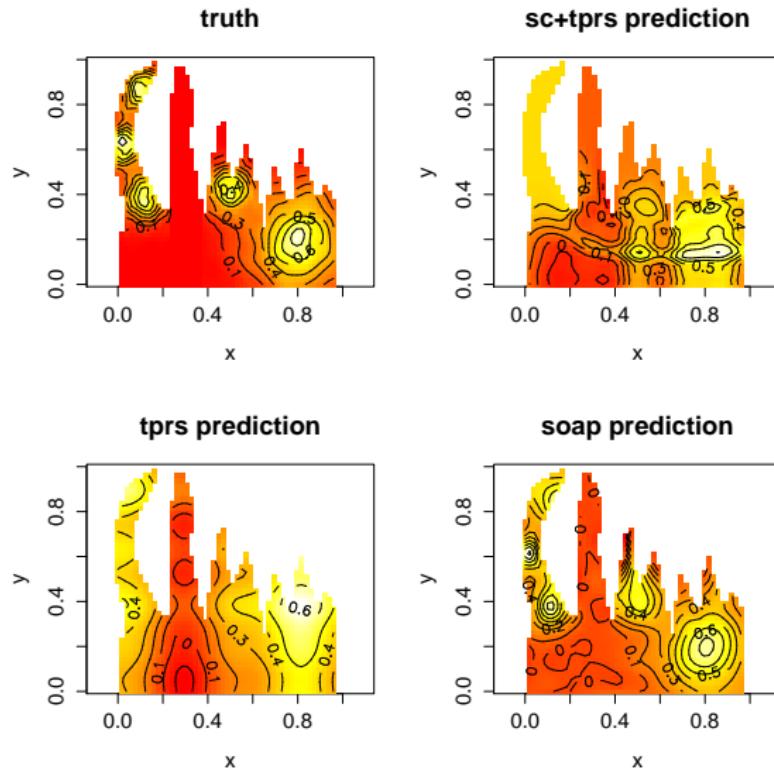
- ▶ Looking at line plots, we can see the difference in gradient.
- ▶ SC method seems to approximate the gradient better.



# Problems

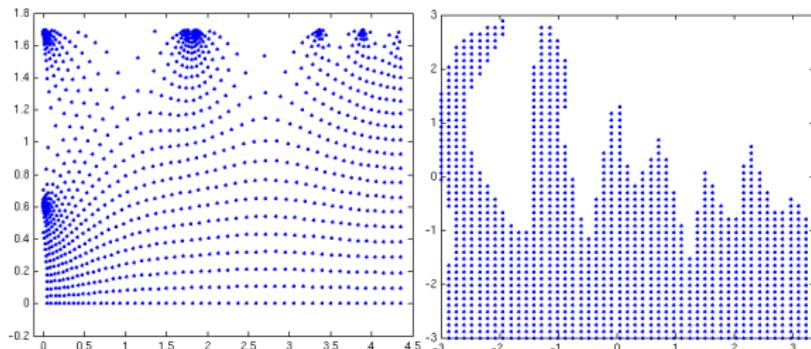
- ▶ Small:
  - ▶ Implementation is Matlab+R. (YUCK!)
- ▶ **BIG:**
  - ▶ Weird artifacts.
  - ▶ Morphing of domain appears to cause features to be smoothed over.
  - ▶ Arbitrary selection of vertices.

# A more realistic domain



# A more realistic domain - what's happening?

- ▶ Weird “crowding” effect.
- ▶ Different with each vertex choice. All bad.



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# Multidimensional scaling and within-area distances

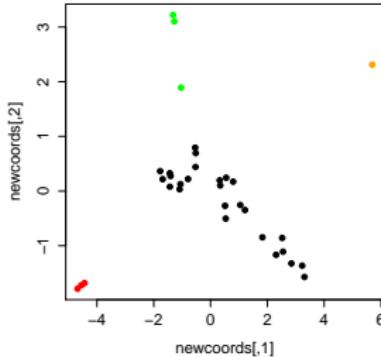
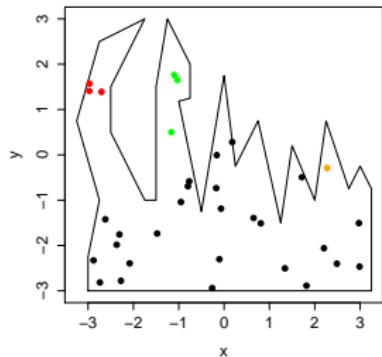
- ▶ Idea: use MDS to arrange points in the domain according to their “within-domain distance.”

## Scheme:

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

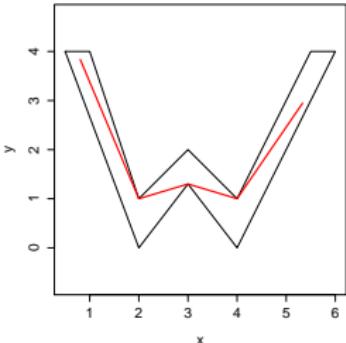
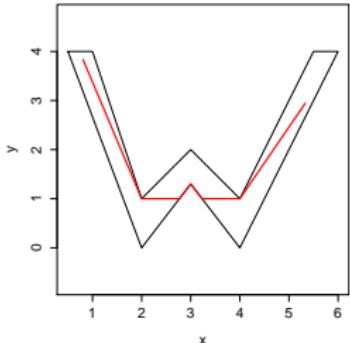
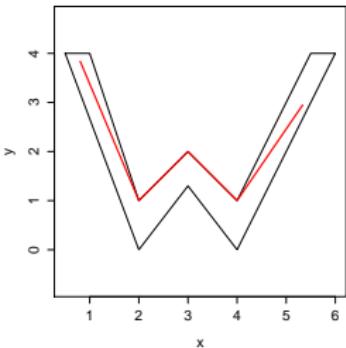
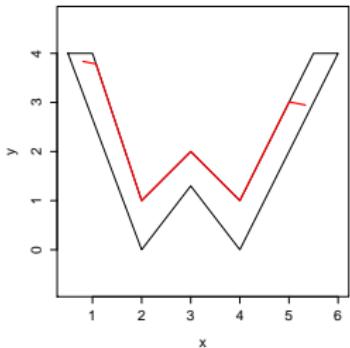
# Multidimensional scaling refresher

- ▶ 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`.



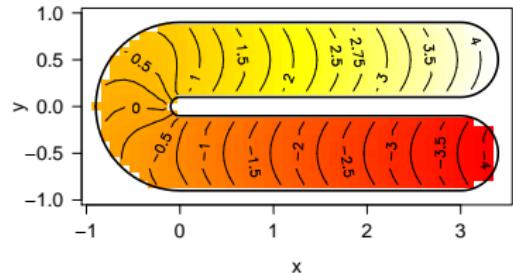
# Finding within-area distances

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

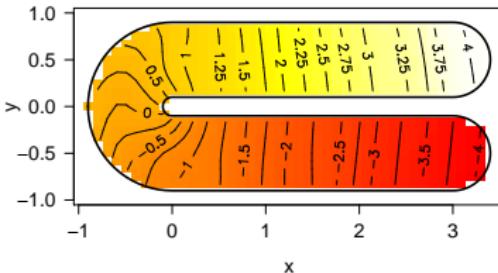


# Ramsay simulations (low noise)

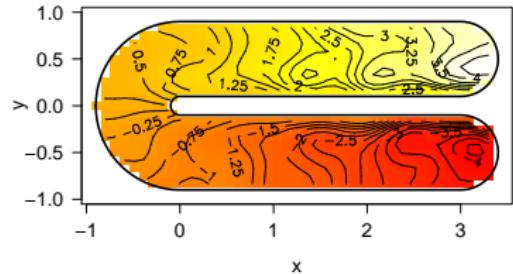
truth



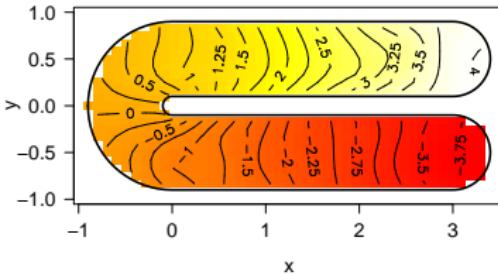
MDS



tprs

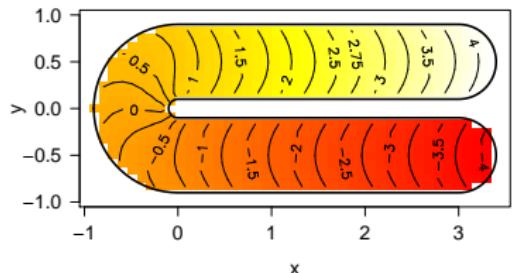


soap

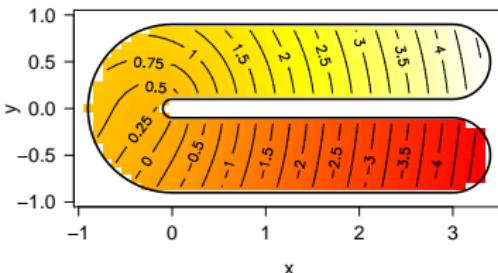


# Ramsay simulations (high noise)

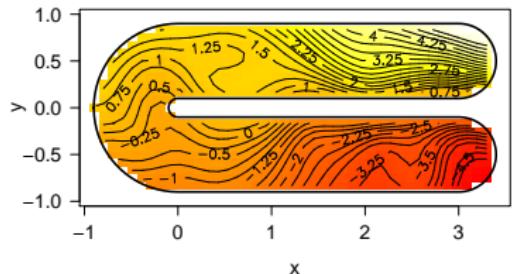
truth



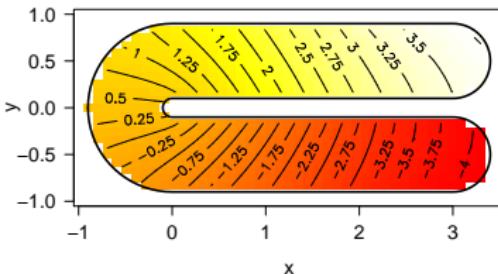
MDS



tprs

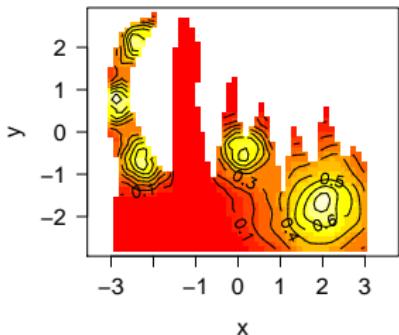


soap

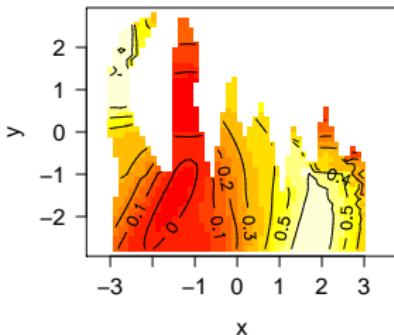


# A different domain

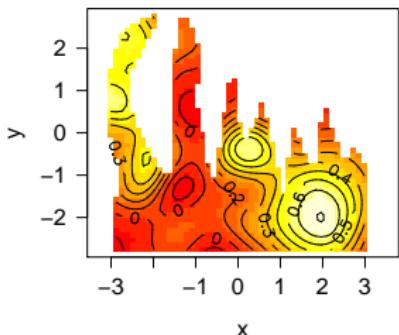
truth



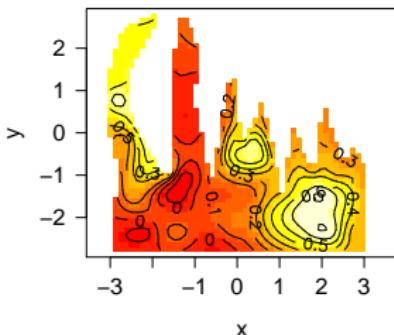
mds



tprs



soap



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- ▶ 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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Slides available at <http://people.bath.ac.uk/dlm27>