Using multidimensional scaling with Duchon splines for reliable finite area smoothing

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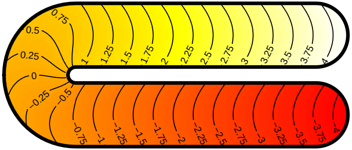
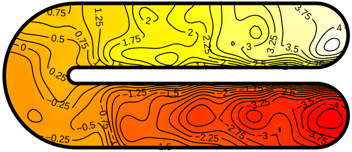
Spatial smoothing

- Have (x, y) locations and some response, z.
- Want a smooth map or to explain spatial auto-correlation.
- Thanks to `mgcv`, `inla`, `sp`, etc spatial smoothing now easy.
- *But* still some problems – e.g. *leakage*.





Smoothing using splines

- Take some set of basis functions, estimate coefficients, penalize based on integrated derivatives (roughness).

$$||f(\mathbf{x}, \mathbf{y}) - \mathbf{z}||^2 + \lambda J_{m,d}$$

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

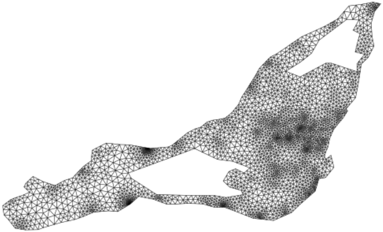
- Here f is a thin plate regression spline:

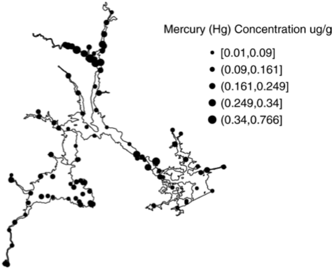
$$f(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} \delta_i \eta_{md}(r) + \sum_{j=1}^{M} \alpha_j \phi_j(\mathbf{x}, \mathbf{y})$$

- Integrate into bigger models (GAMs/GAMMs/etc).

Solutions to leakage

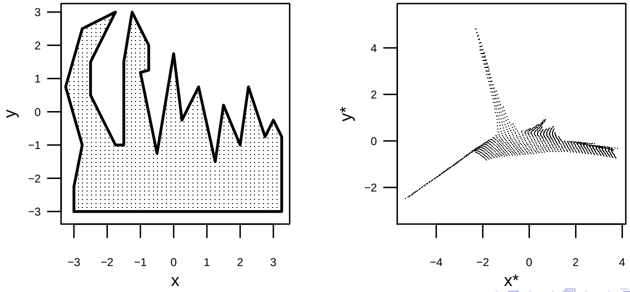
- Boundary conditions - soap film smoothing (Wood *et al.*, 2008), FELSPLINE (Ramsay, 2002).
- Within-area distance metrics - GLTPS (Wang and Ranalli, 2007).
- Domain transformation - what I'm going to talk about.



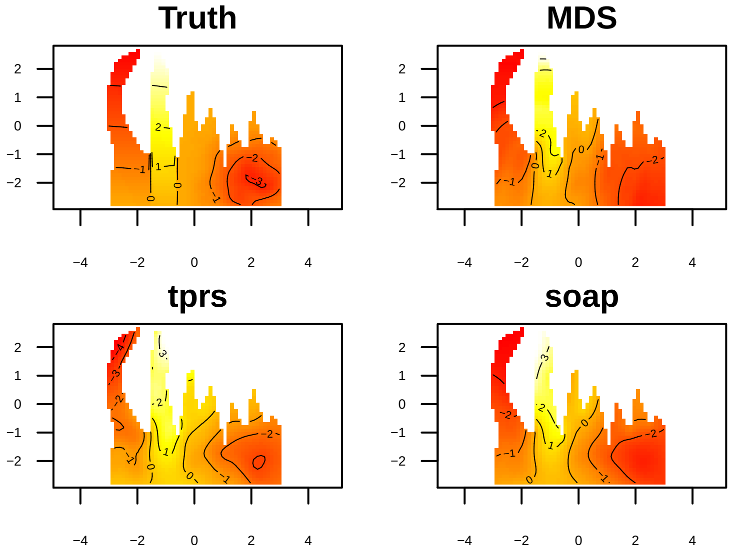


Multidimensional scaling + within-area distances = domain transform

- MDS: Take ($n \times n$) symmetric distance matrix, project into ($< n$) dimensions.
- Using Euclidean distances $\Rightarrow$ same point set (up to scale/rotate).
- Use *within-area* distances reflect distances travelled by objects in domain.



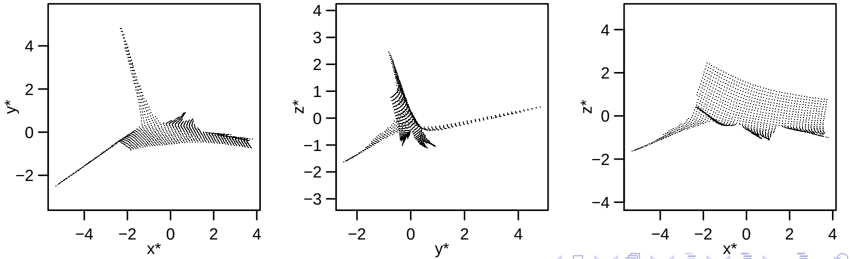
MDS+TPRS smooths



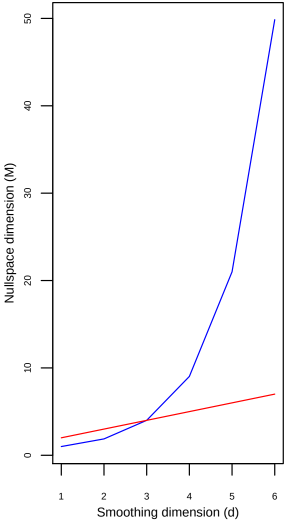
Projections in higher dimensions

- Ordering and crowding issues.
- Using `rgl`, 3-D projections look like manifolds.
- Unreliable smoothing with thin plate in high dimensions.
- Nullspace++ (in size and function complexity)

$$f(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^{n} \delta_i \eta_{md}(r) + \sum_{j=1}^{M} \alpha_j \phi_j(\mathbf{x}, \mathbf{y})$$



Nullspace explosion



Duchon splines (I)

- Usual thin plate penalty:

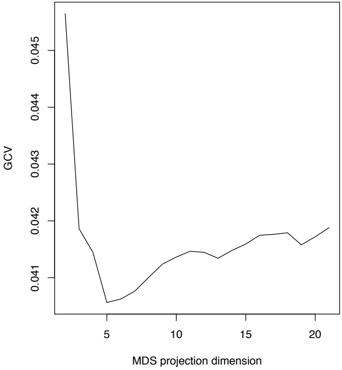
$$J_{m,d} = \int \cdots \int_{\mathbb{R}^d} \sum_{\nu_1+\cdots+\nu_d=m} \frac{m!}{\nu_1! \ldots \nu_d!} \left(\frac{\partial^m f(x_1, \ldots, x_d)}{\partial x_1^{\nu_1} \ldots \partial x_d^{\nu_d}} \right)^2 \mathrm{d}x_1 \ldots \mathrm{d}x_d$$

- Take Fourier transform and weight on frequencies.
- Fudge nullspace (radial basis makes up for global polys).
- Penalize the "smoother" parts of the radial functions less.
- Becomes:

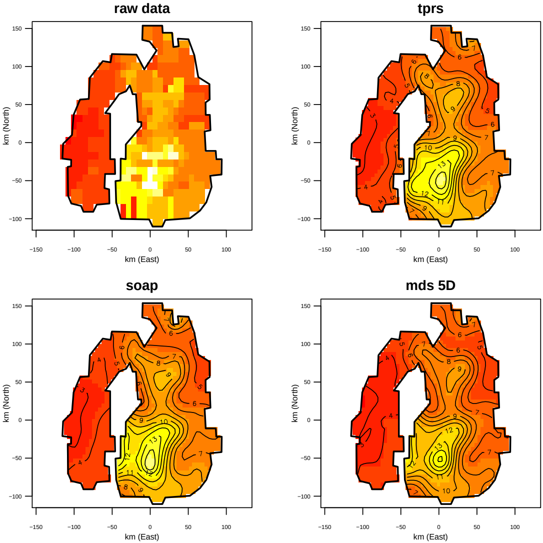
$$\breve{J}_{m,d} = \int \cdots \int_{\mathbb{R}^d} |\boldsymbol{\tau}|^{2s} \sum_{\nu_1+\cdots+\nu_d=m} \frac{m!}{\nu_1! \ldots \nu_d!} \left(\mathfrak{F} \frac{\partial^m f}{\partial x_1^{\nu_1} \ldots \partial x_d^{\nu_d}} (\boldsymbol{\tau}) \right)^2 \mathrm{d}\boldsymbol{\tau}$$

Duchon splines (II)

- Smooth in very high dimensions without huge nullspaces.
- Projection dimension selection by GCV score.



Cholorphyll levels in the Aral sea



Generalized distance smoothing

- Distance matrix could be any set of disparities:
  - MP voting records.
  - Distance between patient's gene expressions.
  - Socio-economic indicators.
- Most variation $\neq$ best predictors.
- Column-wise variance non-constant.
- Issue may be in the metric used.

msg - Multidimensional Scaling for Gams

- Implemented in R as an extra basis in mgcv.
- If you know how to use mgcv, you know how to use msg.

```
b<-gam(z~s(x,y,bs="msg",
xt=list(bnd=boundary,mds.dim=4)),data=data)
```

- GCV dimension selection coming *soon*.

Conclusion

- `msg` performs at least as well as soap film in simulation.
- Duchon splines very useful for high dimensional smoothing.
- Can do smoothing of general distance matrices.
- *But* no killer examples (yet!).
- Do you have any interesting (distance) data?
- Package `msg` available at `http://github.com/dill/msg`.

Calculating within-area distances