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Outline

- Penalized least squares
- Implied priors.
- Something completely different





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Penalized least squares

An abstraction of Grace's model and estimate is *Observe:*

$$y_i = f(x_i) + e_i$$

f is smooth and $\{e_i\}$ iid normal

A spline:

$$\hat{f}(x) = \sum_{j=1}^{n} c_j K(x, x_j)$$

where \boldsymbol{c} minimizes

$$||\boldsymbol{y} - K\boldsymbol{c}||^2 + \lambda \boldsymbol{c}^T K \boldsymbol{c}$$

The RKHS: $K_{i,j} = K(x_i, x_j)$ and K is a reproducing kernel (or a covariance function). What problem are we solving?

If f is Gaussian process with mean zero and with covariance K

- then \hat{f} is the "Kriged" curve.
- then \hat{f} is the conditional expectation of f given \boldsymbol{y} .
- then \hat{f} is the posterior mean/mode with a Gaussian process prior on f



Instead of

$$||\boldsymbol{y} - K\boldsymbol{c}||^2 + \lambda \boldsymbol{c}^T K \boldsymbol{c}$$

 \boldsymbol{c} minimizes

$$||oldsymbol{y} - Koldsymbol{c}||^2 + \lambda \sum_{j=1}^n |c_j|$$

This forces some components to be identically zero the number being controlled by λ .

What problem are we solving? What about the L_1 penalty?

$$||\boldsymbol{y} - K\boldsymbol{c}||^2 + \lambda \sum_{j=1}^n |c_j|$$

-log likelihood log prior (minus some constants)

The prior is $\{c_i\}$ are iid double exponential RVs. i.e.

$$f(c) = \lambda/2e^{-|c|/\lambda}$$

minimizing this is the same as maximizing the posterior.

Instead of

$$||\boldsymbol{y} - K\boldsymbol{c}||^2 + \lambda \boldsymbol{c}^T K \boldsymbol{c}$$

 $Kriging/spatial\ statistics\ version$

$$||\boldsymbol{y} - K^{1/2}\boldsymbol{\beta}||^2 + \lambda ||\boldsymbol{\beta}||^2$$

 $(\boldsymbol{\beta} = K^{-1/2}\boldsymbol{c})$

Version of hard thresholding with wavelets

$$||oldsymbol{y}-K^{1/2}oldsymbol{eta}||^2+\lambda\sum\limits_{j=1}^n|eta_j|$$

If $K^{1/2}$ has columns that are an orthogonal wavelet basis.

What are the priors for f like?

 ${\cal K}$ generalized covariance related to cubic smoothing spline

$$f(x) = \sum_{j} a_{j} \psi_{j}(x)$$

Four (2×2) interesting cases

- Cubic smoothing spline prior a_j iid normal, $\psi_j = K^{1/2}(., x_j)$
- Wavelet type prior a_j iid double exponential and ψ_j same.
- \approx Grace's model. $a_j = c_j$ iid double exponential but $\psi_j = K(., x_j)$
- Gaussian analog $a_j = c_j$ iid normal and $\psi_j = K(., x_j)$

... and also a mixture $\pi \delta_0, (1-\pi)N(0,\sigma^2)$

Sample paths for cubic smoothing spline prior



Adding sample paths with double exponential coefficients

(and using same set of generating uniforms RVs)



dashed = double exponential

Realizations from prior related to Grace's talk

Cubic spline prior

Basis pursuit prior



Comparison to Gaussian process



dashed = double exponential

Comparison to mixture $(\pi = .8)$



A project at NCAR

From a numerical simulation of turbulence find individual vortices and expand them in a parsimonious basis.

The whole image: $\zeta(\boldsymbol{x}) = \sum_{k=1}^{K} v_k(\boldsymbol{x}) + e(\boldsymbol{x})$ The k^{th} vortex: $v_k = \sum_{i=1}^{3J+1} c_{k,i} \psi_j(\boldsymbol{x} - \mu_k)$





Basis pursuit raises issues about what priors are good for functional structure.

Distinguish variable selection from function estimation.