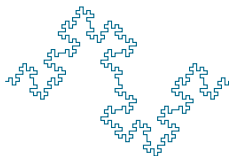


Bivariate Penalized Splines for Geo-Spatial Models

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MOTIVATION

BIVARIATE SPLINES

TRIANGULATIONS

BIVARIATE PENALIZED SPLINE ESTIMATORS

PARTIALLY LINEAR BIVARIATE SPLINE

IMAGE OF LENA SÖDERBERG



Damaged image with 50% of missing data observations

IMAGE OF LENA SÖDERBERG



Image recovered using thin-plate splines

IMAGE OF LENA SÖDERBERG



Face of Lena Söderberg with 8401 pixels.

IMAGE OF LENA SÖDERBERG



Lena Söderberg from November 1972 issue of Playboy

SPATIAL DATA AND MODELING

- ▶ **Spatial** is relating to the position, area, shape, and size of things.
- ▶ **Spatial** describes how objects fit together in space.
- ▶ **Data** are facts and statistics collected together for inference and analysis.
- ▶ **Spatial Data** are data/information about the location and shape of, and relationships among, geographic features, usually stored as coordinates and topology.

SPATIAL MODEL

- ▶ **A common goal in spatial modeling:** predicting the value of a target variable Y over a two-dimensional domain.
- ▶ Let $\{\mathbf{X}_i = (X_{1i}, X_{2i})\}_{i=1}^n$ be a set of n points range over a bounded domain $\Omega \subseteq \mathbb{R}^2$ of an arbitrary shape.
- ▶ Let Y_i be the value of Y observed at point \mathbf{X}_i .
- ▶ Given n observations $\{(\mathbf{X}_i, Y_i)\}_{i=1}^n = \{(X_{1i}, X_{2i}, Y_i)\}_{i=1}^n$, we assume

$$Y_i = m(\mathbf{X}_i) + \sigma(\mathbf{X}_i) \epsilon_i, \quad i = 1, \dots, n$$

- ▶ ϵ_i 's are random errors and independent of \mathbf{X}_i ;
- ▶ m is an unknown smooth function.
- ▶ **Goal:** to estimate a function of m based on the n observations.

1-D SMOOTHING SPLINES

- ▶ The **smoothing spline** estimate of m is defined as a solution to the optimization problem:

$$\sum_{i=1}^n [Y_i - m(X_i)]^2 + \lambda \int [m''(t)]^2 dt$$

with λ as a fixed constant (**roughness penalty parameter**).

- ▶ The 1st term ensures the closeness of the estimate to the data;
- ▶ The 2nd term penalizes the curvature of the function;
- ▶ **Small λ** \Rightarrow an interpolating estimate;
- ▶ **Large λ** $\Rightarrow m''(x) \rightarrow 0 \Rightarrow$ the least squares fit.

BIVARIATE SMOOTHING

Suppose we have two input variables X_1 and X_2 .

- ▶ **Thin-plate spline smoother:** Wood (2003)
 - ▶ By penalizing the curvature of the spline surface, **thin-plate spline** is defined as a solution to the optimization problem

$$\sum_{i=1}^n (Y_i - m(X_{1i}, X_{2i}))^2 + \lambda \int \sum_{i+j=2} \binom{2}{i} (D_{x_1}^i D_{x_2}^j f)^2 dx_1 dx_2.$$

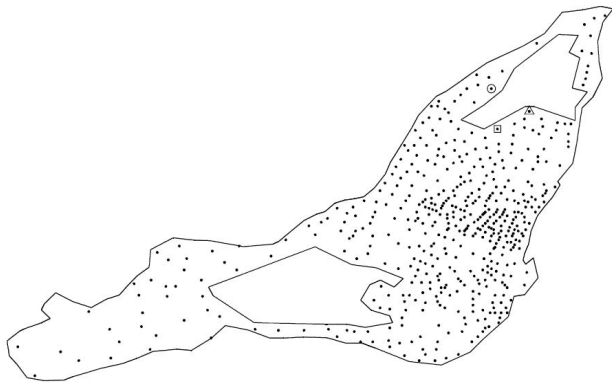
- ▶ **Tensor product spline smoother:**

$$m(x_1, x_2) = \sum_{j,k} \beta_{jk} B_j(x_1) B_k(x_2).$$

- ▶ Useful when the data are observed on a **regular grid in a rectangular domain**;
- ▶ Undesirable when data are located in domains with **complex boundaries and holes**.

SMOOTHING OVER DIFFICULT REGIONS

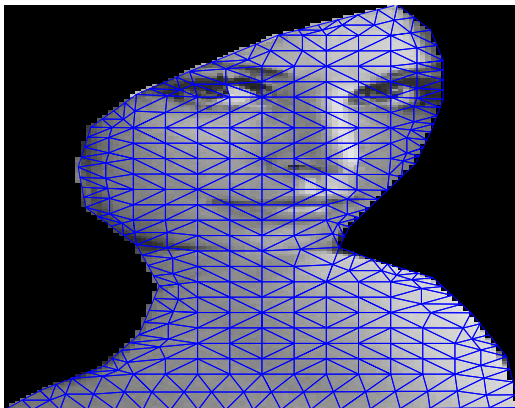
Ramsay (2002, JRSSB): estimate the per capita income for the Island of Montreal, Canada.



Island of Montreal with 493 data points defined by the centroids of census enumeration areas. Source: Ramsay (2002, JRSSB)

BIVARIATE SPLINES OVER TRIANGULATION

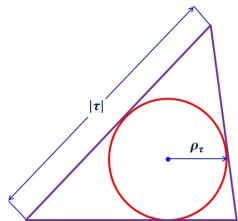
- ▶ We consider **bivariate splines on triangulations** to handle the irregular domains.



Triangulation of the image of Lena Söderberg

TRIANGLE: SIZE AND SHAPE

- ▶ Let τ be a **triangle**, i.e., a convex hull of three points not located in one line.
- ▶ Given any triangle τ ,
 - ▶ Let $|\tau|$ be the length of its longest edge;
 - ▶ Let ρ_τ be the radius of the largest disk inscribed in τ ;
 - ▶ Define the ratio $\beta_\tau = |\tau|/\rho_\tau$ the **shape parameter** of τ ;
 - ▶ For an equilateral triangle, $\beta_\tau = 2\sqrt{3}$;
 - ▶ Any other triangle has a larger shape of parameter;
 - ▶ When β_τ is small, the triangles are relatively uniform (all angles of triangles in the triangulation τ are relatively the same).

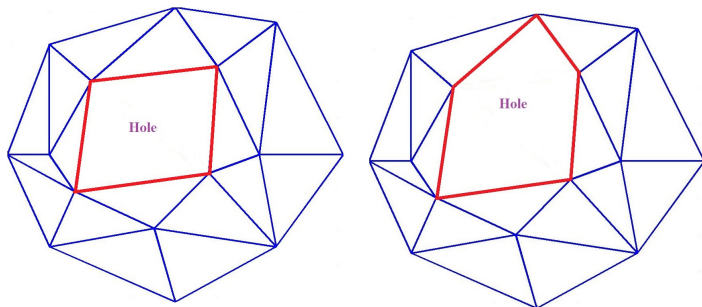


TRIANGULATIONS

A collection $\Delta = \{\tau_1, \dots, \tau_N\}$ of triangles is called a **triangulation** of $\Omega = \cup_{i=1}^N \tau_i$ if a pair of triangles in Δ intersect, then their intersection is either a common vertex or a common edge.

TRIANGULATIONS

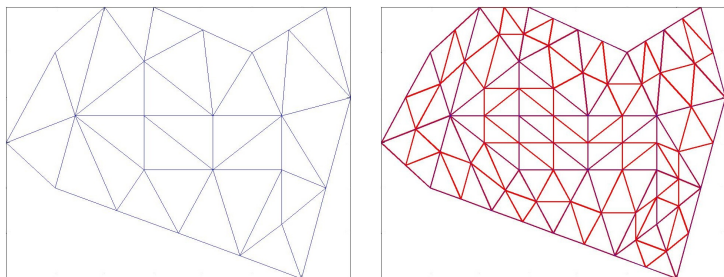
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Two triangulation examples.

UNIFORM REFINEMENT OF A TRIANGULATION

Let Δ be a given triangulation. A **uniform refinement** of Δ can be obtained by splitting each triangle $\tau \in \Delta$ into four subtriangles by connecting the midpoints of the edges of τ .



A triangulation and its uniform refinement

TRIANGULATIONS IN PRACTICE

- ▶ **Maxmin-angle triangulation:** we seek to maximize the smallest angle in a triangulation.
- ▶ There is no triangle that contains no data points.
- ▶ Find a polygon Ω containing all the design points of the data and triangulate Ω by hand or computer to have a triangulation Δ_0 .
- ▶ **Uniformly refine** Δ_0 several times to have a desired triangulation.
- ▶ The **Delaunay** algorithm is a good way to triangulate the convex hull of an arbitrary dataset; see MATLAB program “delaunay.m”.

DEFINITION OF SPLINE FUNCTIONS

- ▶ Let $\tau = \langle (x_1, y_1), (x_2, y_2), (x_3, y_3) \rangle$. For any point $v = (x, y) \in \mathbb{R}^2$, let b_1, b_2, b_3 be the solution of

$$x = b_1x_1 + b_2x_2 + b_3x_3,$$

$$y = b_1y_1 + b_2y_2 + b_3y_3,$$

$$1 = b_1 + b_2 + b_3,$$

where coefficients (b_1, b_2, b_3) are called the **barycentric coordinates** of point v with respect to the triangle τ .

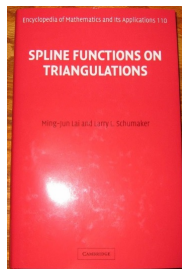
- ▶ Fix a degree $d > 0$. For $i + j + k = d$, let

$$B_{ijk}^d(x, y) = \frac{d!}{i!j!k!} b_1^i b_2^j b_3^k \text{ (Bernstein-Bézier polynomials).}$$

- ▶ Let $s|_\tau = \sum_{i+j+k=d} c_{ijk}^\tau B_{ijk}^d(x, y)$, $\tau \in \Delta$.

SPLINE FUNCTIONS ON TRIANGULATIONS

- ▶ **Lai and Schumaker (2007):** all basics about multivariate splines
 - ▶ Evaluation
 - ▶ Differentiation
 - ▶ Integration
 - ▶ Refinement schemes of a triangulation
- ▶ **Lai and Schumaker (2007):** advanced properties
 - ▶ Dimension of various spline spaces
 - ▶ Construction of various locally supported basis functions
 - ▶ Approximation properties of various spline spaces



Lai and Schumaker
(2007, Cambridge Univ. Press)

BIVARIATE PENALIZED SPLINE ESTIMATOR

- ▶ Given $\lambda > 0$ and $\{\mathbf{X}_i, Y_i\}_{i=1}^n$, consider the minimization:

$$\min_s \sum_{i=1}^n \{Y_i - s(\mathbf{X}_i)\}^2 + \lambda \mathcal{E}_v(s), \quad (1)$$

where

$$\mathcal{E}_v(f) = \sum_{\tau \in \Delta} \int_{\tau} \sum_{i+j=2} \binom{2}{i} (D_{x_1}^i D_{x_2}^j f)^2 dx_1 dx_2$$

is the energy functional.

- ▶ Let \hat{m}_λ be the minimizer of (1) and we call it the **bivariate penalized spline estimator over triangulation (BPSOT estimator)** of m corresponding to λ .

PENALTY PARAMETER SELECTION

- ▶ Partition the original data randomly into K subsamples with: one subsample \Rightarrow test set, $K - 1$ subsamples \Rightarrow training set.
- ▶ Define the K -fold cross-validation score as

$$CV_\lambda = \sum_{i=1}^n \left\{ Y_i - \hat{m}_\lambda^{-k[i]}(\mathbf{X}_i) \right\}^2$$

- ▶ $k[i]$: the subsample containing the i th observation.
- ▶ $\hat{m}_\lambda^{-k[i]}$: the estimate of the mean with the measurements of the $k[i]$ th part of the data points removed.
- ▶ Select $\lambda = \arg \min CV_\lambda$.

IMAGE OF LENA SÖDERBERG: TRIANGULATIONS

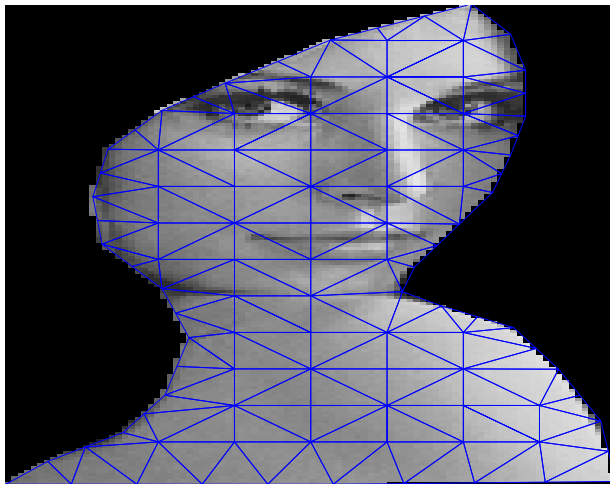
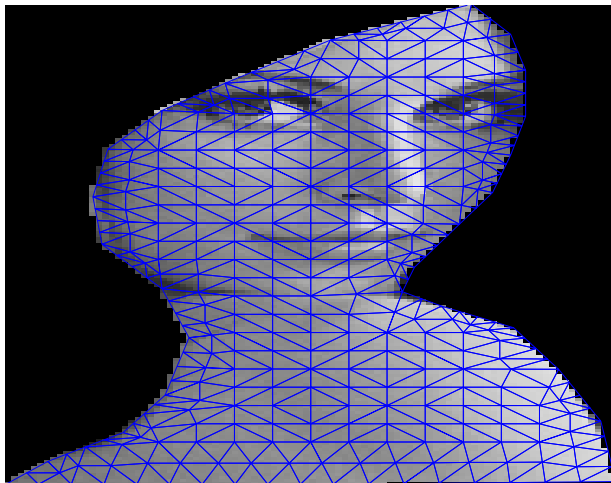
Triangulation Δ_0

IMAGE OF LENA SÖDERBERG: TRIANGULATIONS



Triangulation Δ_1

IMAGE OF LENA SÖDERBERG: TRIANGULATIONS

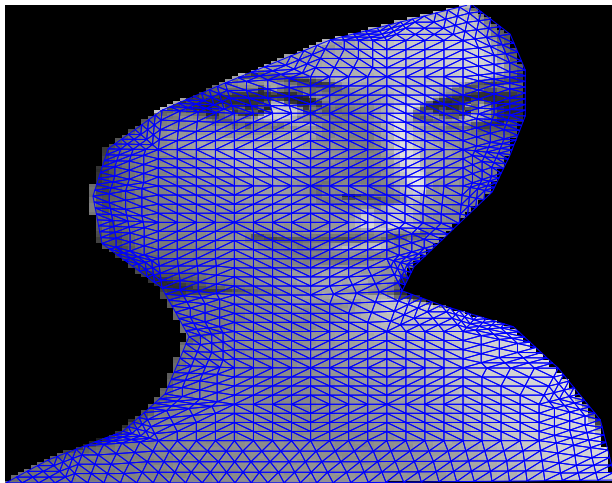
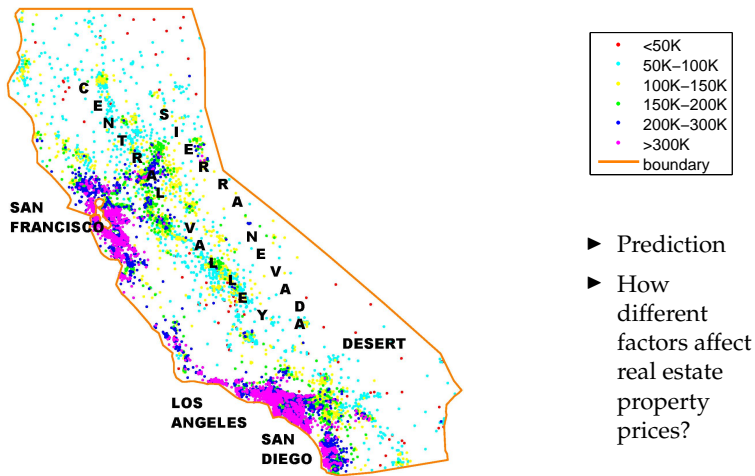
Triangulation Δ_2

IMAGE OF LENA SÖDERBERG: TRIANGULATIONS



Recovered image using bivariate splines over triangulation Δ_1

MOTIVATION: CALIFORNIA HOUSE VALUE DATA



- ▶ Prediction
- ▶ How different factors affect real estate property prices?

20,532 blocks defined by centroids of census enumeration areas (1990 Census).

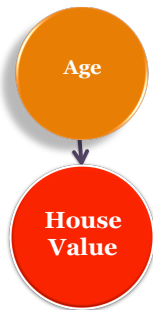
CALIFORNIA HOUSE VALUE DATA

- ▶ **Data:** all the block groups in California from the 1990 Census
- ▶ **Target:** House value



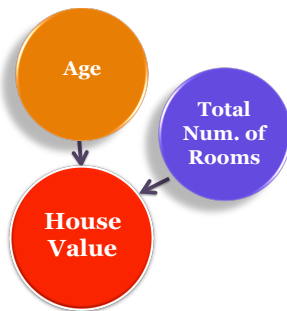
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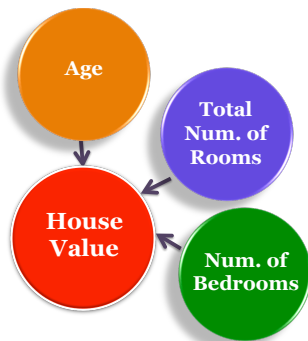
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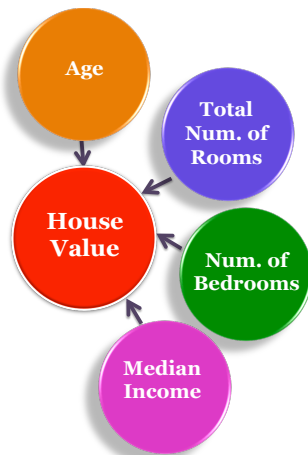
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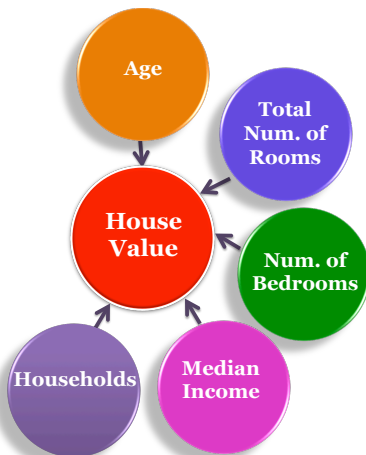
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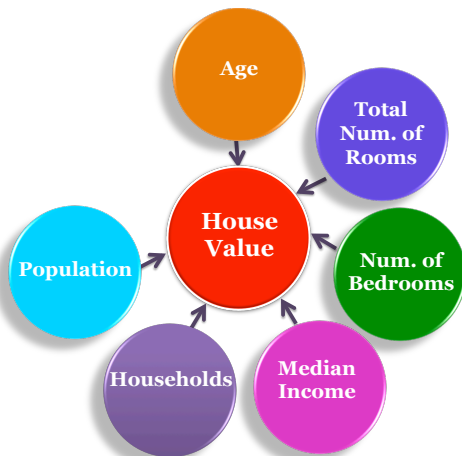
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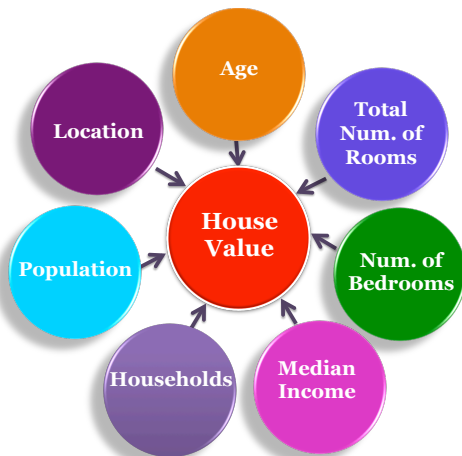
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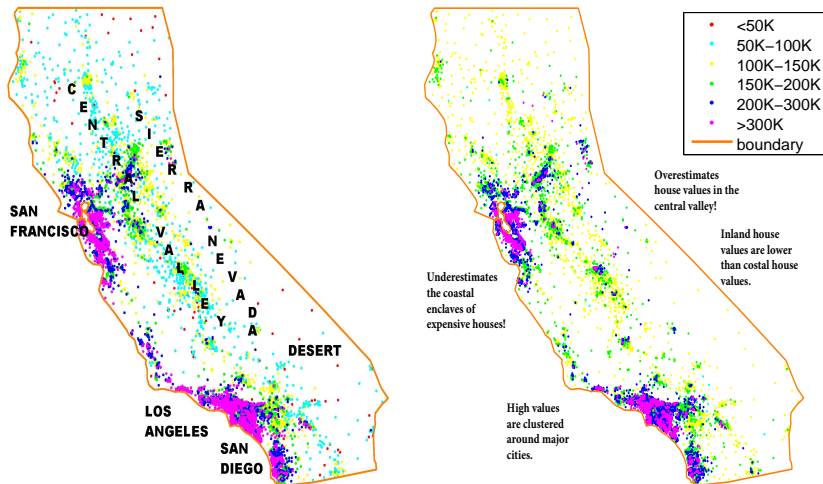
6-FACTOR GLM

- ▶ 6-factor GLM of house value as a linear combination of:
 - House Age (Age)
 - Total # of Rooms (TR)
 - # of Bedrooms (BR)
 - Median Income (Income)
 - Population (Pop)
 - Household (Hhd)

Model 1: 6-Factor GLM (Pace and Barry, 1997)

$$\begin{aligned}\log(\text{Value}) = & \beta_0 + \beta_1 \text{Income} + \beta_2 \log(\text{Age}) \\ & + \beta_3 \log(\text{TR}/\text{Pop}) + \beta_4 \log(\text{BR}/\text{Pop}) \\ & + \beta_5 \log(\text{Pop}/\text{Hhd}) + \beta_6 \log(\text{Hhd})\end{aligned}$$

6-FACTOR GLM ESTIMATES



A. California house value data

B. GLM fit with 6 factors

LOCATION, LOCATION, LOCATION!

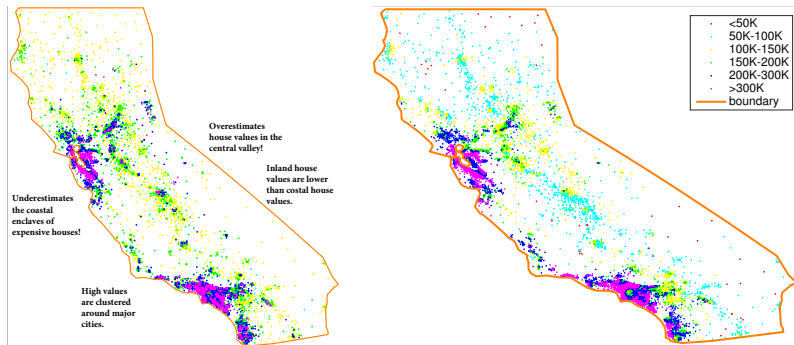
- ▶ **“Location matters”!**
- ▶ **We need to adjust for the location effect:**
 - House Age (Age)
 - Total # of Rooms (TR)
 - # of Bedrooms (BR)
 - Median Income (Income)
 - Population (Pop)
 - Household (Hhd)
 - **Latitude**
 - **Longitude**

Model 2: A Flexible Semiparametric Model

$$\begin{aligned} \log(\text{Value}) = & \beta_0 + \beta_1 \text{Income} + \beta_2 \log(\text{Age}) \\ & + \beta_3 \log(\text{TR}/\text{Pop}) + \beta_4 \log(\text{BR}/\text{Pop}) \\ & + \beta_5 \log(\text{Pop}/\text{Hhd}) + \beta_6 \log(\text{Hhd}) \\ & + g(\text{Latitude}, \text{Longitude}), \end{aligned}$$

where $g(\cdot, \cdot)$ is a smooth bivariate function to be estimated.

ESTIMATED HOUSE VALUES



(a) GLM fit with 6 factors

(b) Bivariate penalized splines

Prediction errors of the logarithm of house values.

LINEAR	KRIG	TPS	SOAP	BPST
0.146	0.083	0.081	0.079	0.052

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