Module 4: Coping with Multiple Predictors

Multidimensional Splines (Continued…)

STAT/BIOSTAT 527, University of Washington
Emily Fox
May 8th, 2014

Curse of Dimensionality

- To maintain a fixed level of accuracy for a given nonparametric estimator, the sample size must increase exponentially in *d*
- Set MSE = δ

$$n \propto \left(\frac{c}{\delta}\right)^{d/4}, \quad c > 0$$

- Why? Using data in local nbhd
  - In high dim, few points in any nbhd
- Consider example with *n* uniformly distributed points in $[-1,1]^d$
  - d=1: in $[-0.1, 0.1] \sim n \times \left(\frac{1}{10}\right)$
  - d=10 in $[-0.1, 0.1]^{10} \sim n \times \left(\frac{1}{10}\right)^{10} = \frac{n}{10^{10}}$ obs in interval

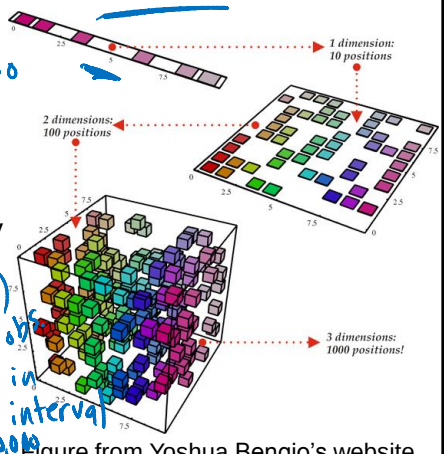


Figure from Yoshua Bengio's website

Natural Thin Plate Splines

$$\min_f \sum_{i=1}^{n} \{y_i - f(x_i)\}^2 + \lambda J(f)$$

$x_i \in \mathbb{R}^2$ "bending energy"

$$J(f) = \int\int_{\mathbb{R}^2} \left[\left(\frac{\partial^2 f(x)}{\partial x_1^2} \right)^2 + 2 \left(\frac{\partial^2 f(x)}{\partial x_1 x_2} \right)^2 + \left(\frac{\partial^2 f(x)}{\partial x_2^2} \right)^2 \right] dx_1 dx_2$$

- Solution: Unique minimizer is the ***natural thin plate spline*** with knots at the x_{ij}
- Proof: See Green and Silverman (1994) and Duchon (1977)

- Similar properties and intuition as in 1d:
  - As λ→0, Sol'n approaches an interpolator
  - As λ→∞, LS plane (no 2nd derivative)

Tensor Product Splines

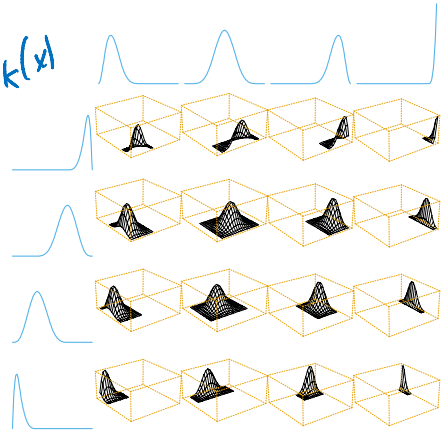
- We use this tensor product basis

  $g_{jk}(x) = h_{1j}(x_1) h_{2k}(x_2)$

  to model $f(x)$

$$f(x) = \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \theta_{jk} g_{jk}(x)$$

- This formulation extends (in theory) to any dimension d
- Note that as the dimension of the basis grows exponentially with the input dimension d



From Hastie, Tibshirani, Friedman book

Generalized Additive Models

- Both for computational reasons and added interpretability, models that assume an additive structure are very popular
- Assuming a GLM framework:

$$g(\mu(x)) = \alpha + f_1(x_1) + \ldots + f_d(x_d)$$

LM: $y = \alpha + f_1(x_1) + f_2(x_2) + \ldots + f_d(x_d)$

- Is this model identifiable?

No, can shift α and shift f_j's to compensate → exactly same $g(\mu)$

Fix: constrain $\sum_{i=1}^{n} f_j(x_{ij}) = 0$ → $\hat{\alpha} = \bar{y}$ to match change

- Can model $f_j(x_j)$ using any smoother

many choices! (spline, kernel methods, etc.) (modulez)

GAM Example

GLM: $g(\mu) = X^T\beta$

- Consider using a penalized regression spline of order p_j with L_j knots for each covariate x_j

or y

$$g(\mu) = \beta_0 + \sum_{j=1}^{d} \left[\sum_{k=1}^{p_j} \beta_{jk} x_j^k + \sum_{l=1}^{L_j} b_{jl} (x_j - \xi_{jl})_+ \right] = f_j(x_j)$$

- Penalization is applied to the spline coefficients b_j

$$\sum_{j=1}^{d} \lambda_j \sum_{\ell=1}^{L_j} b_{j\ell}^2$$

Comments:

- The GAM is very interpretable
  - $f_i(x_i)$ is not influenced by the other $f_j(x_j)$
  - Can plot f_j to straightforwardly see the relationship between x_i and y
- Will see that this also leads to computational efficiencies

Backfitting

- To begin, assume a standard (non-GLM) regression setting
- For concreteness, consider
- Result is an ***additive cubic spline model*** with knots at the unique values of x_{ij}
  - For X full column rank, can show that solution is unique. Otherwise, linear part of $f_j(x_j)$ is not uniquely determined
- Here, clearly $\hat{\alpha} =$
- How do we think about fitting the other parameters??

Backfitting

- ***Backfitting*** is an iterative fitting procedure
- Since $f(x)$ is additive, if we condition on the fit of all other components $f_j(x_j)$, $j \neq i$, then we know how to fit $f_i(x_i)$
- Iterate the estimation procedure until convergence

Backfitting Algorithm

Algorithm 9.1 *The Backfitting Algorithm for Additive Models.*

1. Initialize: $\hat{\alpha} = \frac{1}{N}\sum_1^N y_i$, $\hat{f}_j \equiv 0, \forall i, j$.

2. Cycle: $j = 1, 2, \ldots, p, \ldots, 1, 2, \ldots, p, \ldots,$

$$\hat{f}_j \leftarrow \mathcal{S}_j\left[\{y_i - \hat{\alpha} - \sum_{k \neq j} \hat{f}_k(x_{ik})\}_1^N\right],$$

$$\hat{f}_j \leftarrow \hat{f}_j - \frac{1}{N}\sum_{i=1}^N \hat{f}_j(x_{ij}).$$

until the functions $\hat{f}_j$ change less than a prespecified threshold.

From Hastie, Tibshirani, Friedman book

Review of GLMs

- Mean parameters are a linear combination of inputs, passed through a possibly nonlinear function

- Assume a distribution in the exponential family

Focus on canonical form

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

natural param; log-partition fcn; dispersion; const. wrt θ

  - Using theory of exponential families,

$$\mu(x) = E[Y \mid x] = b'(\theta(x))$$

$$\text{var}(Y \mid x) = \sigma^2 b''(\theta(x)) \triangleq \sigma^2 V_x$$

Review of GLMs

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Mean parameters are a linear combination of inputs, passed through a possibly nonlinear function
- A parametric GLM assumes

$$g(\mu(x)) = \beta^T x$$

"link fcn"

  - With a canonical link function,

$$\theta(x) = g(\mu(x))$$

  - The link function is assumed to be invertible

$\mu(x) = g^{-1}(\theta(x))$

Examples

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Linear regression

$\theta_i := \theta(x_i)$, $b(\theta)$

$$\log p(y_i \mid x_i, \beta, \sigma^2) = \frac{y_i \tilde{\mu}_i - \frac{\tilde{\mu}_i^2}{2}}{\sigma^2} - \frac{1}{2}\left(\frac{y_i^2}{\sigma^2} + \log(2\pi\sigma^2)\right)$$

$c(y_i, \sigma^2)$

$\theta_i = \tilde{\mu}_i = \beta^T x_i$

$b(\theta) = \frac{\theta^2}{2}$

$\mu(x) = b'(\theta(x)) = \theta(x) = \tilde{\mu}(x)$

$b''(\theta) = 1 \Rightarrow \text{var}(y_i) = \sigma^2 b''(\theta) = \sigma^2$

$\theta = g(\mu(x))$

$= \tilde{\mu}(x) = \mu(x)$

$\Rightarrow g(\cdot) = I(\cdot)$

$g(t) = t$ Identity link fcn

Examples

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Binomial regression

$$\log p(y_i \mid x_i, \beta, \sigma^2) = y_i \underbrace{\log\left(\frac{\pi_i}{1-\pi_i}\right)}_{\theta_i} + \underbrace{m \log(1-\pi_i)}_{-b(\theta)} + \underbrace{\log\binom{m}{y_i}}_{c}$$

$\sigma^2 = 1$

$\theta(x) = \log \frac{\pi(x)}{1-\pi(x)}$

$b(\theta(x)) = m \log(1 + e^{\theta(x)})$

$\mu(x) = b'(\theta(x)) = \frac{m}{1+e^{\theta(x)}} e^{\theta(x)} = m\,\pi(x)$ ✓

$\mathrm{var}(y) = b''(\theta(x)) = m\,\pi(x)(1-\pi(x))$

$\theta(x) = g(\mu(x))$

$= \log \frac{\frac{\mu(x)}{m}}{1 - \frac{\mu(x)}{m}}$ ✓

$= \log \frac{\mu(x)}{m - \mu(x)}$

$g(t) = \log \frac{t}{m-t}$

ML Estimation

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

$\theta_i = \beta^T x_i$

- Maximize the log-likelihood

$$\log p(y_1, \ldots, y_n \mid \beta) = \sum_{i=1}^{n} \frac{y_i \theta_i - b(\theta_i)}{\sigma^2} + \text{const}$$

$$\frac{d\ell_i}{d\beta_j} = \frac{d\ell_i}{d\theta_i}\frac{d\theta_i}{d\beta_j} = \sum_{i=1}^{n} \frac{y_i - b'(\theta_i)}{\sigma^2} \frac{d\theta_i}{d\beta_j} x_{ij} = 0$$

- No closed-form solution, so use iterative methods
  - 2nd order methods like IRLS require Hessian

$$H = -\frac{1}{\sigma^2} X^T S X \qquad S = \mathrm{diag}\left(\frac{d\mu_1}{d\theta_1}, \ldots, \frac{d\mu_n}{d\theta_n}\right)$$

ML Estimation

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- IRLS Newton updates: iteratively reweighted LS

$$\beta_{t+1} = (X^T S_t X)^{-1} X^T S_t z_t$$

$$z_t = \theta_t + S_t^{-1}(y - \mu_t)$$

$$\theta_t = X\beta_t \qquad \mu_t = g^{-1}(X\beta_t)$$

Nonparametrics + GLMs

$$p(y \mid x) = \exp\left[\frac{y\theta(x) - b(\theta(x))}{\sigma^2} + c(y, \sigma^2)\right]$$

- Consider a more general form

$$g(\mu(x)) = f(x) \qquad \theta(x) = g(\mu(x))$$

prev. $= \beta^T x$

- Can consider many forms for *f*(x) that we have studied in this course, e.g.
  - Smoothing splines
  - Penalized regression splines
  - Local regression (kernel methods)
  - …

GAMs and Logistic Regression

- A generalized additive logistic regression model has the form

- The functions $f_1, \ldots, f_d$ can be estimated using a backfitting algorithm, too
- First, recall IRLS algorithm for *parametric* logistic regression

$$z = X\beta^{\text{old}} + W^{-1}(y - p)$$

$$\beta^{\text{new}} \leftarrow \arg\min_{\beta} (z - X\beta)^T W (z - X\beta)$$

GAMs and Logistic Regression

Algorithm 9.2 *Local Scoring Algorithm for the Additive Logistic Regression Model.*

1. Compute starting values: $\hat{\alpha} = \log[\bar{y}/(1-\bar{y})]$, where $\bar{y} = \text{ave}(y_i)$, the sample proportion of ones, and set $\hat{f}_j \equiv 0\ \forall j$.

2. Define $\hat{\eta}_i = \hat{\alpha} + \sum_j \hat{f}_j(x_{ij})$ and $\hat{p}_i = 1/[1+\exp(-\hat{\eta}_i)]$.
   Iterate:

   (a) Construct the working target variable

   $$z_i = \hat{\eta}_i + \frac{(y_i - \hat{p}_i)}{\hat{p}_i(1-\hat{p}_i)}.$$

   (b) Construct weights $w_i = \hat{p}_i(1-\hat{p}_i)$

   (c) Fit an additive model to the targets z_i with weights w_i, using a weighted backfitting algorithm. This gives new estimates $\hat{\alpha}, \hat{f}_j,\ \forall j$

3. Continue step 2. until the change in the functions falls below a prespecified threshold.

From Hastie, Tibshirani, Friedman book

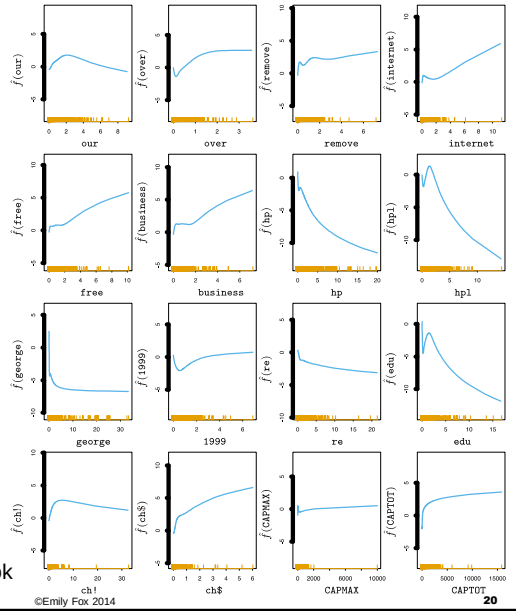
GAM Logistic Example

- Example: *predicting spam*
- Data from UCI repository
- Response variable: *email* or *spam*
- 57 predictors:
  - 48 quantitative – percentage of words in email that match a give word such as “business”, “address”, “internet”,…
  - 6 quantitative – percentage of characters in the email that match a given character (; , [! $ #)
  - The average length of uninterrupted capital letters: CAPAVE
  - The length of the longest uninterrupted sequence of capital letters: CAPMAX
  - The sum of the length of uninterrupted sequences of capital letters: CAPTOT

GAM Logistic Example

- Test set of 1536 emails
- Training set: n=3065
- Use a GAM with a cubic smoothing spline
  - Each with 4 dof
- Estimated functions for significant predictors
  - Note large discontinuity near 0 for many
- Test error of 6.6%

From Hastie, Tibshirani, Friedman book



Other GAM formulations

- Semiparametric models:

$$g(\mu) =$$

- ANOVA decompositions:

$$f(x) =$$

Choice of:

- Maximum order of interaction
- Which terms to include
- What representation

- Tradeoff between full model and decomposed model

Connection with Thin Plate Splines

- Recall formulation that lead to natural thin plate splines:

$$\min_f \sum_{i=1}^{n} \{y_i - f(x_i)\}^2 + \lambda J(f)$$

$$J(f) = \int\int_{\mathbb{R}^2} \left[\left(\frac{\partial^2 f(x)}{\partial x_1^2} \right)^2 + 2 \left(\frac{\partial^2 f(x)}{\partial x_1 x_2} \right)^2 + \left(\frac{\partial^2 f(x)}{\partial x_2^2} \right)^2 \right] dx_1 dx_2$$

- There exists a $J(f)$ such that the solution has the form

- However, it is more natural to just assume this form and apply

$$J(f) = J(f_1 + f_2 + \cdots + f_d) = \sum_{j=1}^{d} \int f_j''(t_j)^2 dt_j$$

What you need to know

- Nothing is conceptually hard about multivariate *x*
- In practice, nonparametric methods struggle from curse of dimensionality
- Options considered:
  - Thin plate splines
  - Tensor product splines
  - Generalized additive models
  - Combinations (to model some interaction terms)

Readings

- Wakefield – 12.1-12.3
- Hastie, Tibshirani, Friedman – 5.7, 9.1
- Wasserman – 4.5, 5.12

Multidimensional Kernel Methods

STAT/BIOSTAT 527, University of Washington
Emily Fox
May 8th, 2014

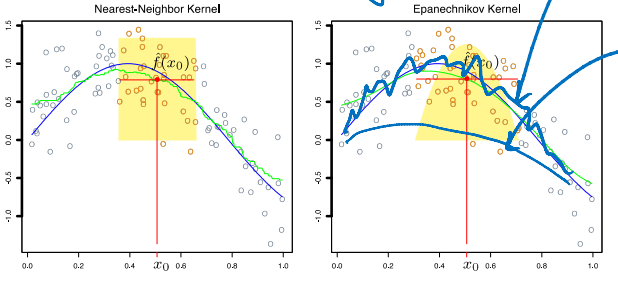
Nadaraya-Watson Estimator

$$\hat{f}(x_0) = \frac{\sum_{i=1}^n K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^n K_\lambda(x_0, x_i)}$$

- Example:
  - Boxcar kernel → local avgs
  - Epanechnikov
  - Gaussian typical
- Often, choice of kernel matters much less than choice of λ

small λ, low bias, high var

large λ high bias, low var



From Hastie, Tibshirani, Friedman book

Local Linear Regression

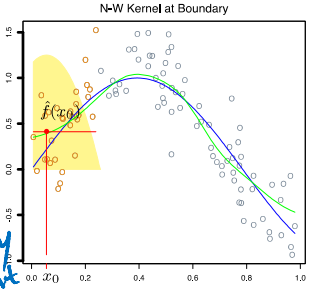
- Locally weighted averages can be badly biased at the boundaries because of asymmetries in the kernel
- Reinterpretation:

$$\hat{f} = \arg\min_a \sum (y_i - a)^2 \;\rightarrow\; \hat{f} = \bar{Y}$$

$$K\left(\frac{|x_i - x|}{\lambda}\right)$$

$$\hat{f}(x) = \arg\min_a \sum w_i(x)(y_i - a)^2 \;\rightarrow\; \hat{f}(x) = \frac{\sum w_i(x) y_i}{\sum w_i(x)}$$

restrict to locally constant



From Hastie, Tibshirani, Friedman book

- Equivalent to the Nadaraya-Watson estimator
- Locally constant estimator obtained from weighted least squares

Local Linear Regression

- Consider locally weighted linear regression instead
- Local linear model around fixed target x_0 :

$$\beta_{0x_0} + \beta_{1x_0}(x - x_0)$$

- Minimize:

$$\min_{\beta_{x_0}} \sum_i K_\lambda(x_0, x_i)\left(y_i - \beta_{0x_0} - \beta_{1x_0}(x_i - x_0)\right)^2$$

- Return: $\hat{f}(x_0) = \hat{\beta}_{0x_0}$ ← fit at x_0

Note: not equivalent to fitting a local constant!

- Fit a new local polynomial for *every* target x_0

Local Polynomial Regression

- Consider local polynomial of degree *d* centered about x_0

$$P_{x_0}(x;\beta_{x_0}) = \beta_{0x_0} + \beta_{1x_0}(x-x_0) + \frac{\beta_{2x_0}}{2!}(x-x_0)^2 + \cdots + \frac{\beta_{dx_0}}{d!}(x-x_0)^d$$

- Minimize: $\min_{\beta_{x_0}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)(y_i - P_{x_0}(x;\beta_{x_0}))^2$
- Equivalently:

$$\min_{\beta_{x_0}} (y - X_{x_0}\beta_{x_0})^T W_{x_0} (y - X_{x_0}\beta)$$

$$X_{x_0} = \begin{bmatrix} 1 & x_1 - x_0 & \cdots & \frac{(x_1-x_0)^d}{d!} \\ \vdots & & & \\ 1 & x_n - x_0 & \cdots & \frac{(x_n-x_0)^d}{d!} \end{bmatrix}$$

- Return: $\hat{f}(x_0) = \hat{\beta}_0 x_0$
- Bias only has components of degree *d+1* and higher

Local Polynomial Regression

- Rules of thumb:
  - Local linear fit helps at boundaries with minimum increase in variance
  - Local quadratic fit doesn't help at boundaries and increases variance
  - Local quadratic fit helps most for capturing curvature in the interior
  - Asymptotic analysis → local polynomials of odd degree dominate those of even degree (MSE dominated by boundary effects)
  - Recommended default choice: **local linear regression**

Local Polynomial Regression

- Kernel smoothing and local regression extend straightforwardly to the multivariate *x* scenario

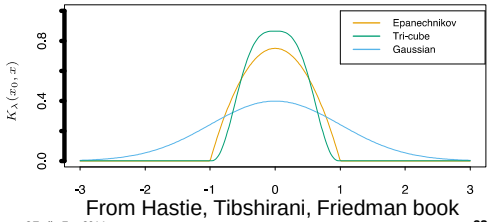
$$\min_{\beta_{x_0}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)(y_i - P_{x_0}(x; \beta_{x_0}))^2$$

  - Need *d*-dimensional kernel
  - Nadaraya-Watson kernel smoother fits locally constant model
  - Local linear regression fits local hyperplane via weighted LS
  - …

- Challenges:
  - Defining kernel
  - Curse of dimensionality

Example Univariate Kernels

- *Gaussian* $K(x) = \frac{1}{2\pi} e^{-\frac{x}{2}}$
- *Epanechnikov* $K(x) = \frac{3}{4}(1-x)^2 I(x)$ ← ind. on -1, 1
- *Tricube* $K(x) = \frac{70}{81}(1-|x|^3)^3 I(x)$
- *Boxcar* $K(x) = \frac{1}{2} I(x)$



From Hastie, Tibshirani, Friedman book

Multivariate Kernels

- Many choices, even more than in 1d
- Examples:
  - Radial basis kernels

$$K_\lambda(x_0, x) =$$

E.g., radial Epanechnikov, tricube, squared exponential (Gaussian)

Multivariate Kernels

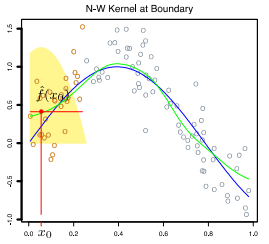
- Many choices, even more than in 1d
- Examples:
  - Product kernels

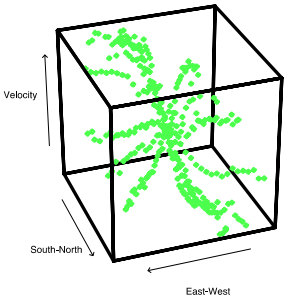
$$K_{\lambda_1,\lambda_2}(x_0, x) =$$

- Choices:
  - Form
  - Kernel(s)
  - Bandwidth(s)

Motivating Local Linear Regression

- Nadaraya-Watson smoothing can be applied to multivariate *x*
- However, boundary issues are even worse in higher dimensions
  - Messy to correct for boundary even in 2d (esp. for irregular boundaries)
  - Fraction of points close to the boundary increases with dimension
- Local polynomial regression corrects boundary errors up to desired order





From Hastie, Tibshirani, Friedman book

Local Linear Regression

- Assume a RBF kernel
- For each target location x_0, goal is to minimize

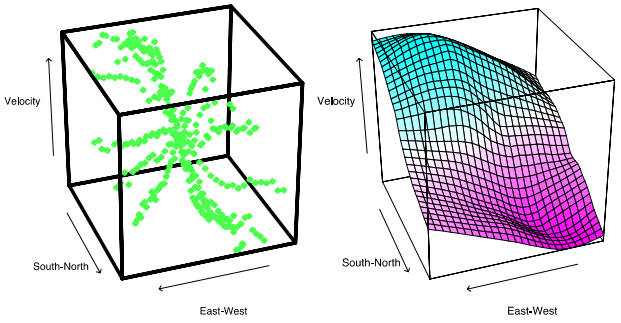
$$\min_{\beta_{x_0}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)\left(y_i - \beta_{0x_0} - \sum_{j=1}^{d} \beta_{jx_0}(x_{ij} - x_{0j})\right)^2$$

- Equivalently,

- Solution: $\hat{\beta}_{x_0} = (X_{x_0}^T W_{x_0} X_{x_0})^{-1} X_{x_0}^T W_{x_0} y$
- Return:

Local Linear Example

- Astronomical study
  - Response = velocity measurements on a galaxy
  - Predictors = two positions
- Note the unusual star-shaped design → very irregular boundary
  - Must interpolate over regions with very few observations near boundary



From Hastie, Tibshirani, Friedman book

Motivating Local Polynomial

- One way to think about motivating local polynomials is as follow
- Consider 2d example for simplicity
- For a suitably smooth function $f(x) = f(x_1,x_2)$, we can approximate it for values $x=[x_1,x_2]$ in a nbhd of $x_0=[x_{01},x_{02}]$ as

$$f(x) \approx f(x_0) + (x_1 - x_{01})\frac{\partial f}{\partial x_{01}} + (x_2 - x_{02})\frac{\partial f}{\partial x_{02}}$$
$$+ (x_1 - x_{01})^2 \frac{1}{2}\frac{\partial^2 f}{\partial x_{01}^2} + (x_1 - x_{01})(x_2 - x_{02})\frac{1}{2}\frac{\partial^2 f}{\partial x_{01}\partial x_{02}} + (x_2 - x_{02})^2 \frac{1}{2}\frac{\partial^2 f}{\partial x_{02}^2}$$

- Suggests the use of a local polynomial:

- Then, $\min_{\beta_{x_0}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)(y_i - P_{x_0}(x;\beta_{x_0}))^2$

Scaling to High Dimensions

- Local regression becomes less useful in dimensions greater than 2 or 3
  - Impossible to maintain localness (low bias) and large sample size (low variance) without the total sample size increasing exponentially in *d*
- Again, curse of dimensionality
  - Sparsity of data
  - Points concentrate at boundaries
- Visualization of the fitted function is also hard in high dimensions, and visualization is often a key goal in smoothing

Boundary Effects

- Everything is far away in high dimensions
- Consider *n* data points uniformly distributed in a *d*-dimensional unit ball
- Example task: Consider nearest neighbor estimate at origin
- Median distance to closest data point is $\left(1 - \frac{1}{2}^{1/n}\right)^d$
  - For *n*=500 and *d*=10, distance ≈ 0.52
  - Closest point is likely more than ½ way to the boundary
- Prediction is harder near the edges of the sample boundary

Boundary Effects II

- Another way to think of this effect is in terms of volume
- We want to compute the fraction of volume that lies between radius R = 1 − ε and R = 1
- The volume of a sphere is proportional to
- The volume fraction is therefore:

$$\frac{V_d(1) - V_d(1-\epsilon)}{V_d(1)} = 1 - (1-\epsilon)^d$$

- Most of the volume of a sphere is concentrated in a thin shell near the surface

Structured Local Regression

- As we have seen before, when faced with data scarcity relative to model complexity, assume structure
- Structured kernels
  - Place more or less importance on certain dimensions (or combinations thereof) by modifying the kernel
- Structured regression functions
  - Just as with splines, decompose the target regression function
  - E.g., ANOVA decompositions and fit low-dim terms with local regression

Structured Kernels

- In many scenarios, RBF or *spherical* kernels are considered
- Places equal weight on all dimensions of *x*
  - Typically, standardize data so all dimensions have unit variance
- More generally, can consider structured kernels

$$K_{\lambda,A}(x_0, x) = K\left(\frac{(x - x_0)^T A(x - x_0)}{\lambda}\right)$$

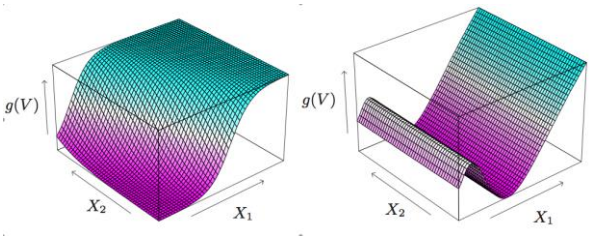
- Choices for A
  - Diagonal →
  - Low rank →
  - General

Projection Pursuit Regression

- To help deal with high-dimensional regression, consider

$$f(x_1, \ldots, x_d) = \alpha + \sum_{m=1}^{M} f_m(w_m^T x)$$

  - $||w_m|| = 1$ for $m=1,\ldots, M$
- Seek w_m so the model fits well



PPR Comments

$$f(x_1, \ldots, x_d) = \alpha + \sum_{m=1}^{M} f_m(w_m^T x)$$

- If *M* is arbitrarily large, and for appropriate choice of f_m, PPR can approximate any continuous function in R^d arbitrarily well
- Interpretation can be hard
- *M*=1 "single index model" in econometrics → interpretable
- **Goal:** Seek to minimize over { f_m, w_m }

$$\sum_{i=1}^{n} \left(y_i - \sum_{m=1}^{M} f_m(w_m^T x_i) \right)^2$$

PPR Fitting Algorithm

- Direction vectors w_m chosen in a forward-stagewise procedure to minimize the fraction of unexplained variance
- Start by standardizing data to 0 mean and scale each covariate to have the same variance

1. Set $\hat{\alpha} = \text{avg}(y_i)$
2. Initialize $\hat{\epsilon}_i = y_i, i = 1, \ldots, n \quad \text{and} \quad m = 0$
3. Find the direction (unit vector) *w** that minimizes

$$I(w) = 1 - \frac{\sum_{i=1}^{n} (\hat{\epsilon}_i - S(w^T x_i))^2}{\sum_{i=1}^{n} \hat{\epsilon}_i^2}$$

4. Set $\hat{f}_m(w^{*T} x_i) = S(w^{*T} x_i)$
5. Set *m* = *m* + 1 and update the residuals:

$$\hat{\epsilon}_i \leftarrow \hat{\epsilon}_i - \hat{f}_m(w^{*T} x_i)$$

If *m*=M, stop.

PPR Fitting Algorithm Comments

$$f(x_1, \ldots, x_d) = \alpha + \sum_{m=1}^{M} f_m(w_m^T x)$$

- Algorithm considered is a greedy forward-wise procedure
- After each step, the f_m's from the previous steps can be readjusted using backfitting
- Can lead to fewer terms, but unclear if it improves predictions
- Typically the w_m's are not readjusted
- Choice of M can be based on a threshold in improvement of fit or using CV

Structured Regression Functions

- Often, instead of structuring the kernel, it makes sense and is simpler to structure the regression function itself
- Just as with splines, we can consider ANOVA decompositions

$$f(x_1, x_2, \ldots, x_p) = \alpha + \sum_j f_j(x_j) + \sum_{k<\ell} f_{k\ell}(x_k, x_\ell) + \ldots$$

or, more simply, standard GAMs

$$f(x_1, x_2, \ldots, x_p) = \alpha + \sum_j f_j(x_j)$$

- Can use ***1d (or low-dim) local regression*** as the smoother for each term and fit using backfitting algorithm

Kernel Density Estimation

- Kernel methods are often used for density estimation (actually, classical origin)
- Assume random sample $X_1, \ldots, X_n \overset{iid}{\sim} P$
- Choice #1: empirical estimate? $\hat{P} = \frac{1}{n}\sum \delta_{X_i}$

- Choice #2: as before, maybe we should use an estimator

$$\hat{p}(x_0) = \frac{\#x_i \in \text{Nbhd}(x_0)}{n\lambda}$$

λ ← width of nbhd

- Choice #3: again, consider kernel weightings instead

$$\hat{p}(x_0) = \frac{1}{n\lambda}\sum K_\lambda(x_0, x_i)$$ Parzen est.

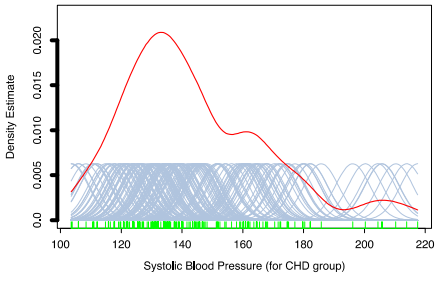
Kernel Density Estimation

- Popular choice = Gaussian kernel → ***Gaussian KDE***

$$\hat{p} = \frac{1}{n}\sum_{i=1}^{n} \phi_\lambda(x - x_i)$$ ϕ_λ

$$= (\hat{p} * \phi_\lambda)(x)$$

↑ empirical dist.



From Hastie, Tibshirani, Friedman book

Multivariate KDE

- In 1d $$\hat{p}(x_0) = \frac{1}{n\lambda} \sum_{i=1}^{n} K_\lambda(x_0, x_i)$$
- In R^d, assuming a product kernel,

$$\hat{p}(x_0) = \frac{1}{n\lambda_1 \cdots \lambda_d} \sum_{i=1}^{n} \left\{ \prod_{j=1}^{d} K_{\lambda_j}(x_{0j}, x_{ij}) \right\}$$

- Typical choice = Gaussian RBF

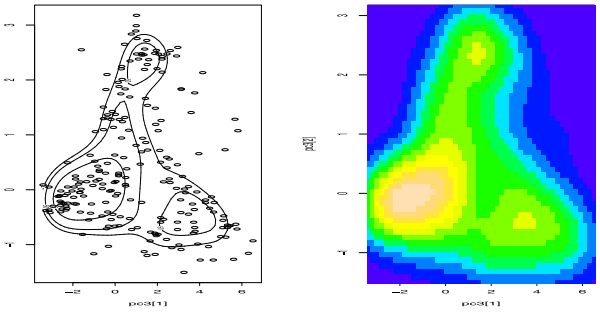
Multivariate KDE

$$\hat{p}(x_0) = \frac{1}{n\lambda_1 \cdots \lambda_d} \sum_{i=1}^{n} \left\{ \prod_{j=1}^{d} K_{\lambda_j}(x_{0j}, x_{ij}) \right\}$$

- Risk grows as $O(n^{-4/(4+d)})$
- Example: To ensure relative MSE < 0.1 at 0 when the density is a multivariate norm and optimal bandwidth is chosen
- Always report confidence bands, which get wide with *d*

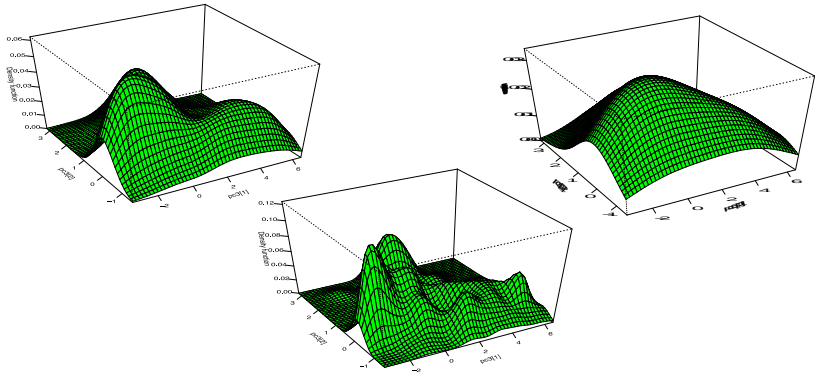
Multivariate KDE Example

- Data on 6 characteristics of aircraft (Bowman and Azzalini 1998)
- Examine first 2 principle components of the data
- Perform KDE with independent kernels



Multivariate KDE Example

- Data on 6 characteristics of aircraft (Bowman and Azzalini 1998)
- Examine first 2 principle components of the data
- Perform KDE with independent kernels



What you need to know

- As with splines:
  - Nothing is conceptually hard about multivariate *x*
  - In practice, nonparametric methods struggle from curse of dimensionality
- For multivariate kernel methods, need multivar kernel
  - Radial basis kernels
  - Product kernels
  - Structured kernels, including learning like projection pursuit
- Methods:
  - Local polynomial regression
  - Local polynomial regression in structured regression like GAMs
  - KDE

Readings

- Wakefield – 12.4-12.6
- Hastie, Tibshirani, Friedman – 6.3-6.4, 11.2
- Wasserman – 5.12, 6.5