Module 4: Coping with Multiple Predictors

Multidimensional Splines Recap

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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)

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

  $n \propto \left(\frac{c}{\delta}\right)^{\frac{d}{4}}$

- Why? Using data in local nbhd
  - In high dim, few points in any nbhd

  everything is far away in high dim

- Consider example with *n* uniformly distributed points in $[-1,1]^d$
  - d=1: In $[-0.1,0.1]$, $\approx \frac{n}{10}$ obs. in interval
  - d=10 In $[-0.1,0.1]^d$,

  roughly $n\left(\frac{0.2}{2}\right)^{10} = \frac{n}{10{,}000{,}000{,}000}$

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Figure from Yoshua Bengio's website

Natural Thin Plate Splines

$x_i \in \mathbb{R}^d$

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

d=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: ***natural thin plate spline*** with knots at the x_{ij}
- For general λ, solution is a linear basis expansion of the form

  The image

  $\beta_0 + \beta^T x + \sum_{j=1}^{n} b_j h_j(x)$

  with

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  RBF

- Interpretation: We take an elastic flat plate that interpolates points (x_i, y_i) and penalize its "bending energy"

Tensor Product Splines

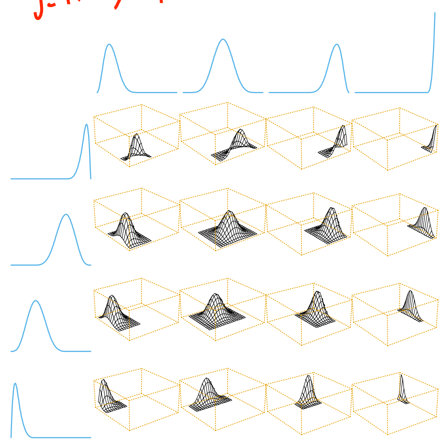
- We use this tensor product basis univariate basis

$d=2$ example $\rightarrow$ $g_{jk}(x) = h_{1j}(x_1)h_{2k}(x_2)$ $j=1,\dots,M_1$ $k=1,\dots,M_2$

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 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:

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

- Is this model identifiable? No, can change α and shift f_j's to compensate $\rightarrow$ exactly same $g(\mu)$.

Fix: Constrain $\sum_{i=1}^{n} f_j(x_{ij}) = 0$

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

many, many choices here (see all of module 2) or GPs...

Backfitting Algorithm

Algorithm 9.1 *The Backfitting Algorithm for Additive Models.*

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

init f_j

take avg., then fix

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

partial res.

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

smoother chosen for x_j

fit using partial res.

numerical reasons

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

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

From Hastie, Tibshirani, Friedman book

Other GAM formulations

- Semiparametric models:

$$g(\mu) = X^T\beta + \alpha + f(z)$$

model linearly

model nonparam.

- ANOVA decompositions:

combination of standard GAMs + (low-dim) multivar models

$$f(x) = \alpha + \sum_j f_j(x_j) + \sum_{j<k} f_{jk}(x_j, x_k) + \ldots$$

main effects

capture interactions

Choice of:
- Maximum order of interaction
- Which terms to include – maybe not all main effects + interactions
- What representation

–reg. splines + tensor product for interactions or thin plate ...

- 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

$$f(x) = f_1(x_1) + \dots + f_d(x_d)$$

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

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

Module 4: Coping with Multiple Predictors

Multidimensional Kernel Methods

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Nadaraya-Watson Estimator

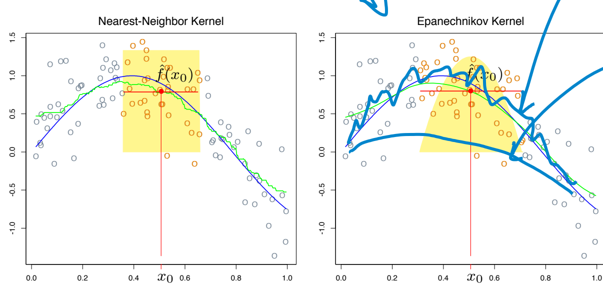
$$\hat{f}(x_0) = \frac{\sum_{i=1}^{n} K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^{n} K_\lambda(x_0, x_i)}$$

- 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



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Local Linear Regression

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

- Reinterpretation:

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

$\to \hat{f} = \bar{Y}$

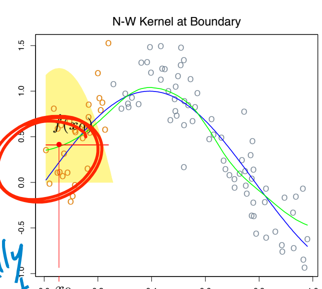
$K\left(\frac{|x_i - x|}{\lambda}\right)$

const.

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

restrict to locally constant

$\to \hat{f}(x) = \frac{\sum w_i(x) y_i}{\sum w_i(x)}$



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

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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:

$$\min_{\beta_{x_0}} \sum_i K_\lambda(x_0, x_i)\big(y_i - \overbrace{\beta_{0x_0} - \beta_{1x_0}(x_i - x_0)}^{\text{local linear model}}\big)^2$$

- 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

Corrects bias up to 1st order

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Local Polynomial Regression

- Consider local polynomial of degree ~~d~~ p centered about x_0

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

- 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: $\hat{f}(x_0) = \hat{\beta}_{0x_0}$
- Bias only has components of degree *d+1* and higher

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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 $x \in \mathbb{R}^d$

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

multivar local polynomial

  - Need *d*-dimensional kernel

$$K_\lambda(x_0, \cdot) : \mathbb{R}^d \to \mathbb{R}$$ kernel weights

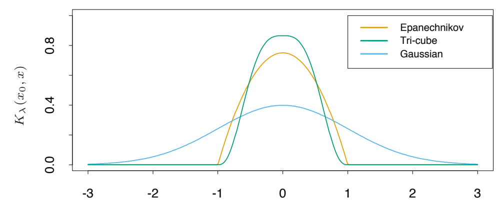
  - Nadaraya-Watson kernel smoother fits locally constant model
  - Local linear regression fits local hyperplane via weighted LS
  - …

- Challenges:
  - Defining kernel
  - Curse of dimensionality

Example Univariate Kernels $x \in \mathbb{R}$

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

ind. on -1, 1



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Multivariate Kernels

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

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

just compute distance in $\mathbb{R}^d$ and apply kernel as before

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

SE $K_\lambda(x_0, x) = e^{\frac{-\|x_0 - x\|^2}{2\lambda}}$

Multivariate Kernels

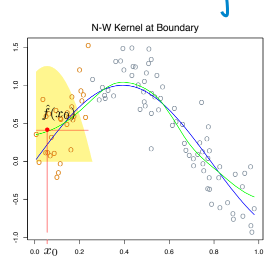
- Many choices, even more than in 1d
- Examples:
  - Product kernels

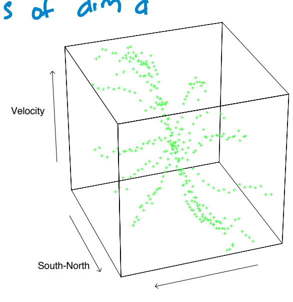
$$K_{\lambda_1,\lambda_2}(x_0, x) = K_1\left(\frac{x_{01}-x_1}{\lambda_1}\right) K_2\left(\frac{x_{02}-x_2}{\lambda_2}\right)$$

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

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 regardless of dim d





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Local Linear Regression

- Assume a RBF kernel $K_\lambda(x_0, x_i) = K\left(\frac{\|x_0 - x_i\|}{\lambda}\right) \stackrel{\Delta}{=} w_i(x_0)$
- For each target location x_0, goal is to minimize

$$\min_{\beta_{x_0}} \sum_{i=1}^{n} K_\lambda(x_0, x_i)\Big(y_i - \underbrace{\beta_{0x_0} - \sum_{j=1}^{d} \beta_{jx_0}(x_{ij} - x_{0j})}_{\text{local linear model}}\Big)^2$$

- Equivalently,

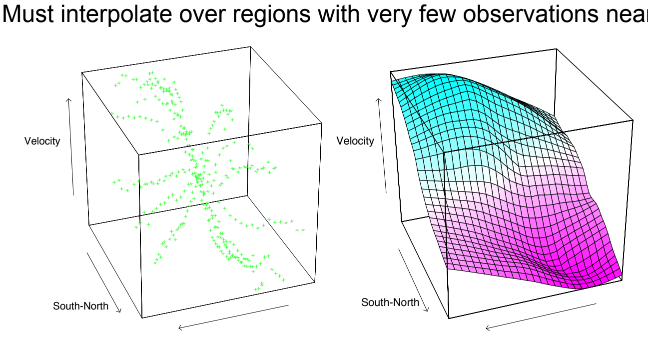
$$\min_{\beta_{x_0}} (y - X_{x_0}\beta_{x_0})^T W_{x_0} (y - X_{x_0}\beta_{x_0})$$

$$X_{x_0} = \begin{bmatrix} 1 & x_{11}-x_{01} & \cdots & x_{1d}-x_{0d} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1}-x_{01} & \cdots & x_{nd}-x_{0d} \end{bmatrix} \qquad W_{x_0} = \mathrm{diag}(w_1(x_0), \ldots, w_n(x_0))$$

- 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: $\hat{f}(x_0) = \hat{\beta}_{0x_0}$

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



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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

2nd order Taylor expansion

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

- Suggests the use of a local polynomial: interaction terms

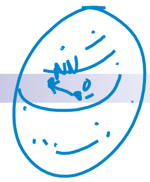
$$P_{x_0}(x;\beta_{x_0}) = \beta_{0x_0} + (x_1 - x_{01})\beta_{1x_0} + (x_2 - x_{02})\beta_{2x_0}$$
$$+ (x_1 - x_{01})^2\beta_{3x_0} + \ldots \text{ (all other terms above)}$$

- 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

Most pts are closer to boundary of sample than to any other data pt

- 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 $V(R) \propto R^d$
- The volume fraction is therefore:

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

as d grows, even for small ϵ

- 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

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

- Places equal weight on all dimensions of *x*
  - Typically, standardize data so all dimensions have unit variance
- More generally, can consider structured kernels

modifies distance metric

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

A: d×d matrix

e.g., SE $e^{-(x_0 - x)^T \Sigma^{-1} (x_0 - x)}$

- Choices for A
  - Diagonal → increase, decrease, or omit influence of x_j via A_{jj}
  - Low rank → useful in presence of corr. pred.
  - General

$A = U^T \overset{k \times d}{U}$ $k \ll d$ $\quad \overset{k\times 1}{z} = \overset{k\times d}{U} \overset{d\times 1}{x} \Rightarrow x^T A x = z^T z$

Projection Pursuit Regression

- To help deal with high-dimensional nonparam. regression, consider

additive model, but in terms of derived features $V_m = w_m^T x$ rather than x itself

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

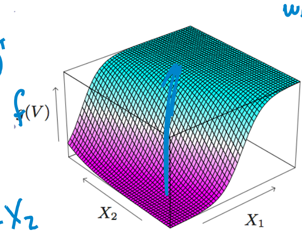
Projection of X into subspace

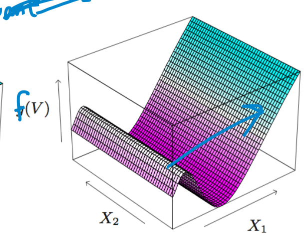
d×1 unit vector

"ridge fcn" in $\mathbb{R}^d$ only varies in direction w_m

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

$w = \frac{1}{\sqrt{2}}(1,1)^T$ so only varying in $X_1 + X_2$





$w = (1,0)$ only varying in X_1 dir

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

"universal approximator"

- Interpretation can be hard
- M=1 "single index model" in econometrics → interpretable
- **Goal:** Seek to minimize over $\{ f_m, w_m \}$

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

how? First, choose smoother $S(\cdot)$ for f_m

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

before standardizing data :)

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~~ max.

residuals if we add w to model

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

prev. residuals

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

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

Structure = eliminate some of the higher order terms

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 $S_j(\cdot)$

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Varying Coefficient Models

- Special case of a structured model
- Divide the set of *d* covariates into two sets

$$((X_1, \ldots, X_q), (Z_1, \ldots, Z_{d-q})) \quad q<d$$

- Consider a ***conditionally linear*** model

$$f(x) = \alpha(z) + \beta_1(z)x_1 + \ldots + \beta_q(z)x_q$$

linear given z, but coeff. vary w/ z.

- Due to its local nature, it's natural to fit such a model using locally weighted LS

$$\min_{\alpha(z_0), \beta(z_0)} \sum_{i=1}^n K_\lambda(z_0, z_i)(y_i - \alpha(z_0) - x_{1i}\beta_1(z_0) - \cdots - x_{qi}\beta_q(z_0))^2$$

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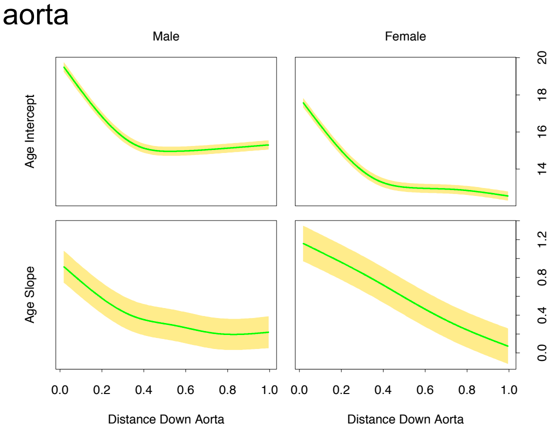
Varying Coefficient Models

- Example = Human aorta data
- Response = diameter of aorta
- Covariates
  - Linear in "age"
  - Coefficients vary in "gender" and "depth"
- Separate model for M/F
- Results:
  - Aorta thickens with age
  - Relationship is less clear for larger depth



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Varying Coefficient Models

- Alternatively, one can use splines instead of local regression as a smoother for the varying coefficient functions $\beta_j(z)$

↑ what we want to model nonparam.

- Consider penalized linear splines with *L* knots
  - For univariate *x* and *z*, for simplicity, we have

$$E[y \mid x, z] = \underbrace{\alpha_0^{(0)} + \alpha_1^{(0)} z + \sum_{\ell=1}^{L} b_\ell^{(0)} (z - \xi_\ell)_+}_{\beta_0(z)}$$

$$+ \underbrace{\left(\alpha_0^{(1)} + \alpha_1^{(1)} z + \sum_{\ell=1}^{L} b_\ell^{(1)} (z - \xi_\ell)_+ \right)}_{\beta_1(z)} x$$

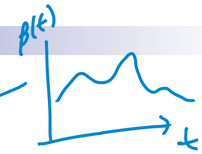
↑ linear in x given z

Example: Time-Varying Coeff

- Let z correspond to time t, a simple case being:

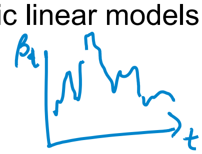
$$y_t = \alpha + \beta(t) X_t + \epsilon_t$$

no time variation, but could have that



- This model directly relates to (Bayesian) dynamic linear models

$$y_t = \alpha + z_t \beta_t + \epsilon_t \quad \epsilon_t \sim N(0, \sigma_\epsilon^2)$$
$$\beta_t = \beta_{t-1} + \nu_t \quad v_t \sim N(0, \sigma_\nu^2)$$



varying coef. model w/ smoothing via a 1st order Markov model

See West and Harrison 1997

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