Basis expansions, kernels and support vector machines

Hastie, Tibshirani, Friedman Ch 5, 6, 12

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Basis Expansion

HTF Ch5

Move beyond linearity

- Linear regression, logistic regression, LDA
  - Classification by linear hyperplanes
  - Easy to fit and to interpret

- $f(Y|\mathbf{X})$ is typically non-linear and non-additive
  - augment X with transformations of $\mathbf{X}$
  - use as input in linear models
  - Denote mth transformation $h_m(\mathbf{X}) : \mathbb{R}^p \to \mathbb{R}^p$
  - Model $f(\mathbf{X}) = \sum_{m=1}^{M} \beta_m h_m(\mathbf{X})$
  - $f(\mathbf{X})$ is linear in $h_m(\mathbf{X})$
  - This is a *linear basis expansion* in $\mathbf{X}$

Linear basis expansion

- Linear model
  - $h_m(\mathbf{X}) = X_m$
- Polynomial terms (Taylor expansion)
  - $h_m(\mathbf{X}) = X_m^2$ or $h_m(\mathbf{X}) = X_i X_j^2$
  - # variables $\uparrow$ exponentially in p
  - tweak one region $\uparrow$ flap another
- Functions of a vector
  - $h_m(\mathbf{X}) = log(X_j)$, $h_m(\mathbf{X}) = \sqrt{X_j}$, $h_m(\mathbf{X}) = ||\mathbf{X}||$
- Indicators $h_m(\mathbf{X}) = I(L_m \leq X_k < U_m)$
  - Break the range of X_k into regions
  - Piecewise constant model in each region
- Piece-wise polynomials and splines
  - Dictionary $\mathcal{D}$ of basis functions
  - Method for controlling model complexity: *restriction, selection, regularization*
  - Restriction: $f(\mathbf{X}) = \sum_{j=1}^{p} f_j(X_j) = \sum_{j=1}^{p} \sum_{m=1}^{M_j} \beta_{jm} h_{jm}(X_j)$

Piecewise fits

- Assume $\mathbf{X}$ is one-dimensional (i.e., X)
  - Divide domain(X) into contiguous intervals
  - $f(X)$: a separate polynomial in each interval

- Example: piecewise constant
  - $h_1(X) = I(X < \xi_1),\ h_2(X) = I(\xi_i \leq X \leq \xi_2),$
    $h_3 = I(\xi_2 \leq X)$
  - $f(X) = \sum_{m=1}^{3} \beta_m h_m(X)$
  - $\widehat{\beta}_m = \bar{Y}_m$, the mean of mth region

- Example: piecewise linear
  - Need extra basis $h_{m+3} = h_m(X) \cdot X,\ m = 1, \ldots, 3$

- Example: restricted piecewise linear
  - $f(\xi_1^-) = f(\xi_1^+) \ \rightarrow\ \beta_1 + \xi_1\beta_4 = \beta_2 + \xi_1\beta_5$
  - 3 intervals: 4 free parameters out of 6
  - Alternatively: $h_1(X) = 1,\ h_2(X) = X,$
    $h_3(X) = (X - \xi_1)_+,\ h_4(X) = (X - \xi_2)_+$

Piecewise fit

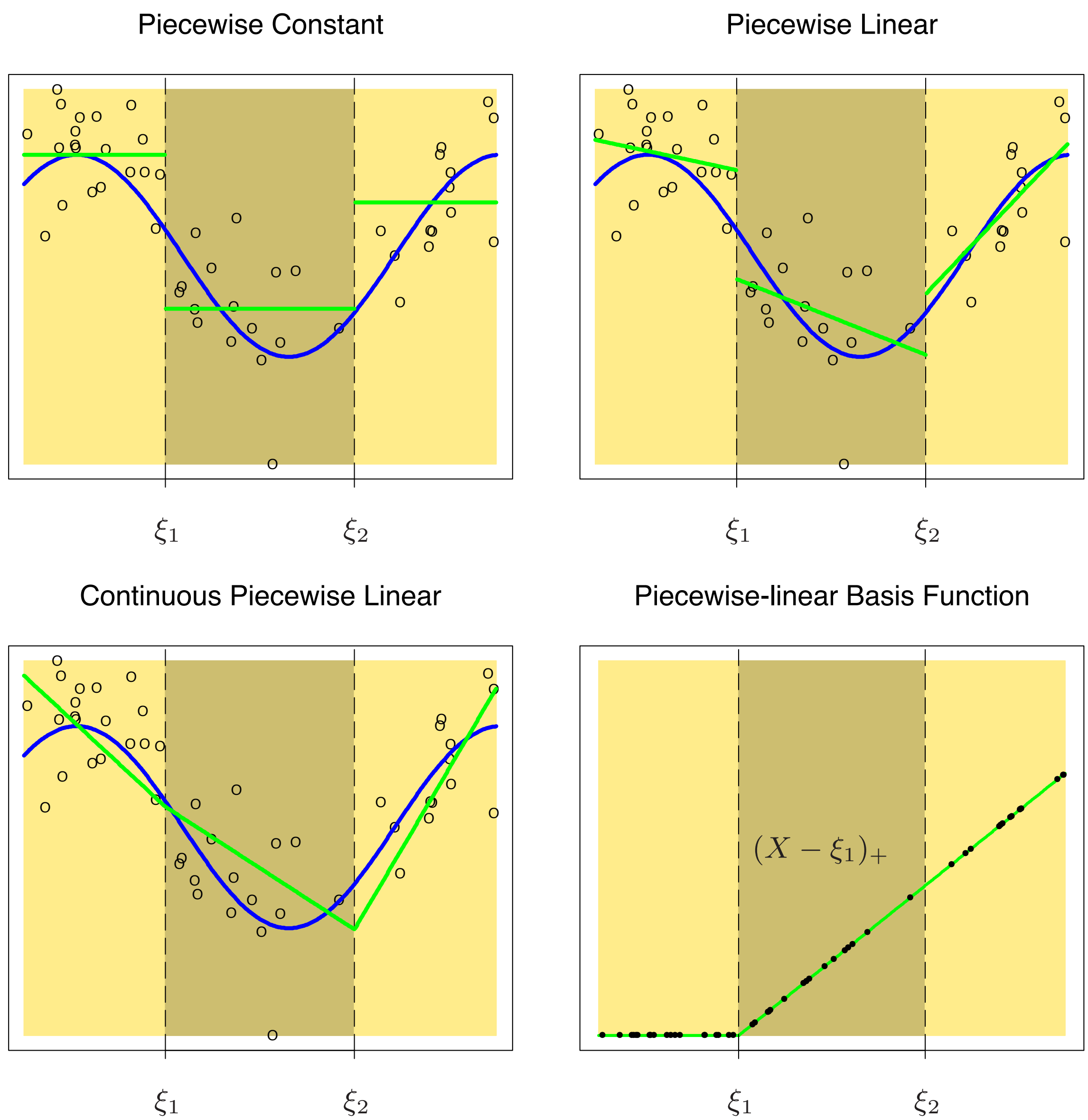


Fig. 5.1. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

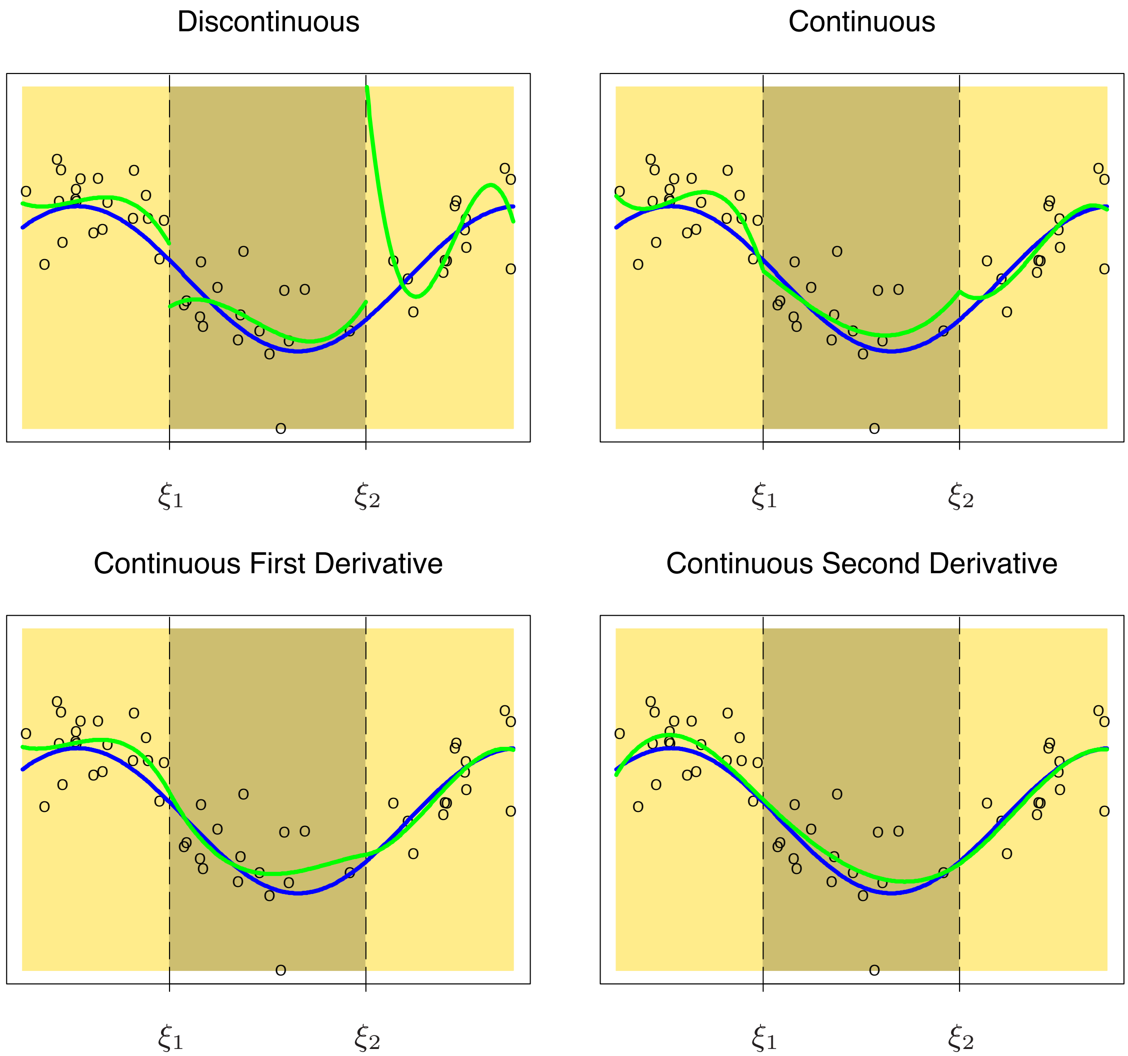
Splines

- Smoother functions
  - Increase the order of polynomials
  - Cubic splines: continuous to second derivative
  - $h_1(X) = 1, h_s(X) = X, h_3(X) = X^2, h_4(X) = X^3$
    $h_5(X) = (X - \xi_1)_+^3,\ h_6(X) = (X - \xi_2)_+^3$

- Example on the next page
  - 6 basis functions
  - 6-dimensional linear space of functions
  - (3 regions) $\times$ (4 parameters per region)
    - (2 knots) $\times$ (3 constrains per knot) $= 6$

- Order-M spline with knots ξ_j, $j = 1, \ldots, K$
  - Piecewise polynomial up to order M
  - Has continuous derivatives up to order $M - 2$.
  - Piecewise constant fit is order-1 spline.
    Piecewise continuous fit is order-2 spline.
    Cubic spline is order-4 spline.
  - Basis set: $h_j(X) = X^{j-1},\ j = 1, \ldots, M$ and
    $h_{M+l}(X) = (X - \xi_l)_+^{M-1},\ l = 1, \ldots, K$

Piecewise cubic polynomials



Cubic spline is the lowest-order spline for which the knot-discontinuity is not visible to human eye

Fig. 5.2. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Natural cubic splines

- Need for extra stability
  - Polynomials and splines have erratic behavior near the boundaries
  - Variance explodes
  - Extrapolation is problematic

- Natural cubic splines: extra constraints
  - Linear functions beyond boundary knots
  - K knots $=$ K basis functions
  - Basis for cubic splines $\rightarrow$ impose constraints
  - Start from basis set, impose boundary constraint, derive reduced basis:

$$N_1(X) = 1,\ N_2(X) = X,$$
$$N_{k+2}(X) = d_k(X) - d_{K-1}(X)$$
$$\text{where } d_k(X) = \left\{(X-\xi_k)_+^3 - (X-\xi_K)_+^3\right\} / \{\xi_K - \xi_k\}$$

  - Second and third derivatives are 0 for $X \geq \xi_K$

Pointwise variance curve

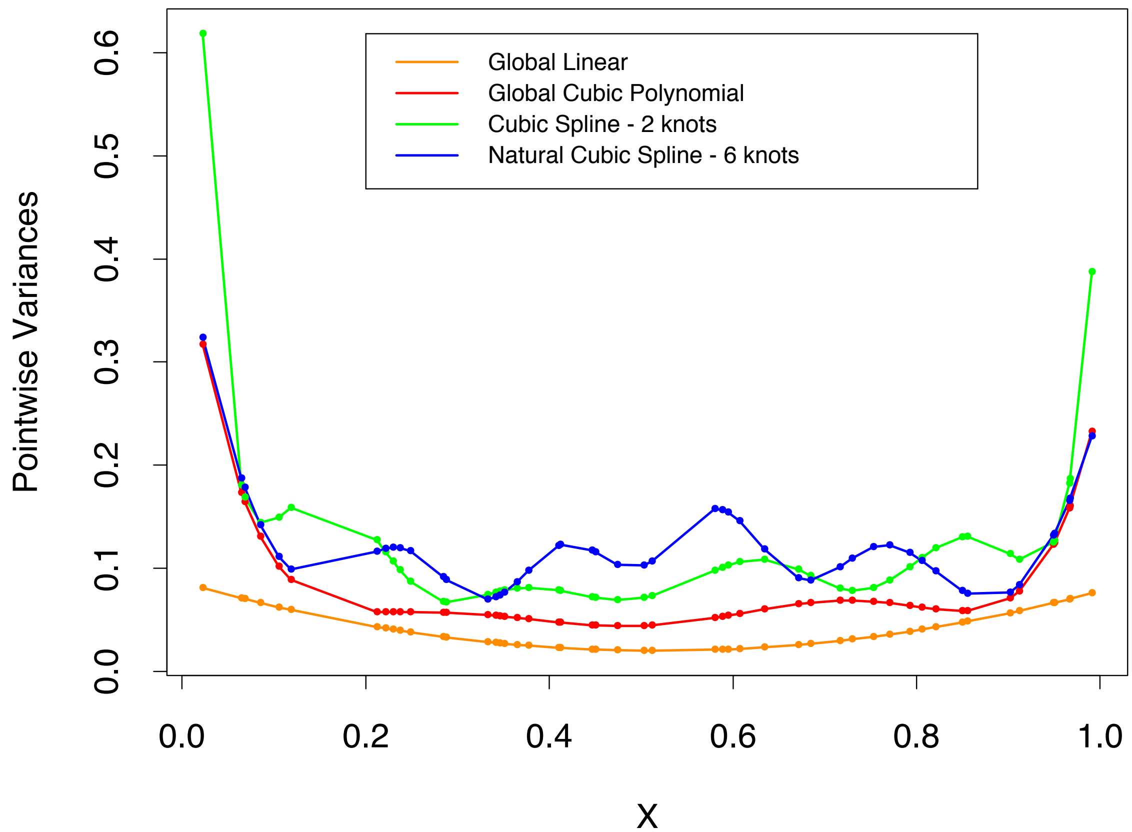


Fig. 5.3. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Example: South African Heart Disease

- Logistic regression

$$\frac{\Pr\{\texttt{chd} = 1|X\}}{1 - \Pr\{\texttt{chd} = 1|X\}} = \theta_0 + h_1(X_1)'\theta_1 + \ldots + h_p(X_p)'\theta_p$$

  - θ_j are vectors of coefficients multiplying the vector of natural spline basis functions h_j
  - Use 4 natural spline basis functions for each term in the model
  - Knots chosen at uniform quantiles of X_j:
    3 internal knots +
    2 boundary knots at the extremes of X_j
  - Binary predictor has a single coefficient
  - More compactly: combine p vectors of basis functions + constant term in a big vector $h(X)$, and model $h(X)'\theta$
  - Backward stepwise selection + AIC to drop terms
  - Plot prediction $\pm 2 \cdot SE$

Fit: $\hat{f}_j(X_j) = h_j(X_j)' \hat{\theta}_j$

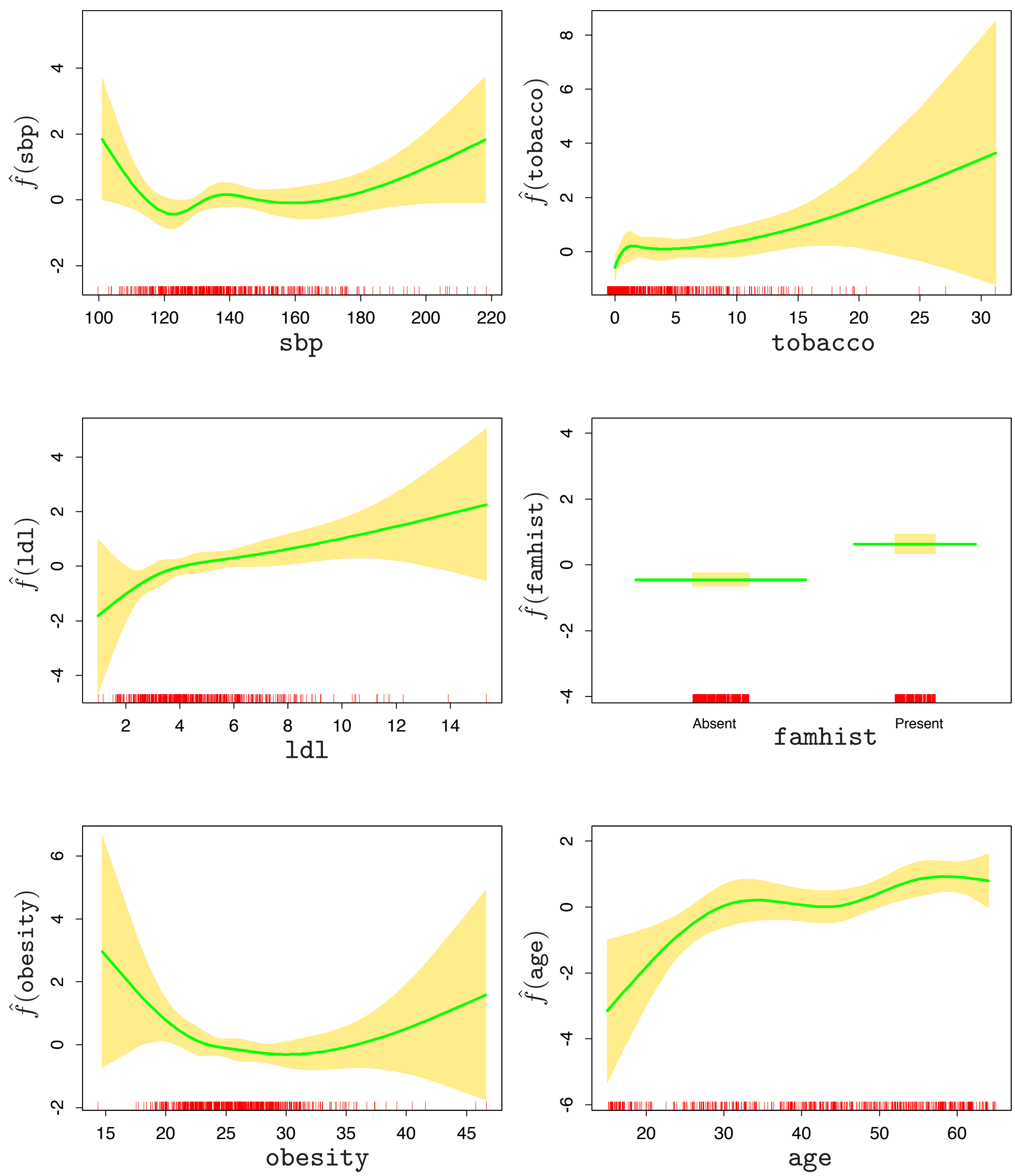
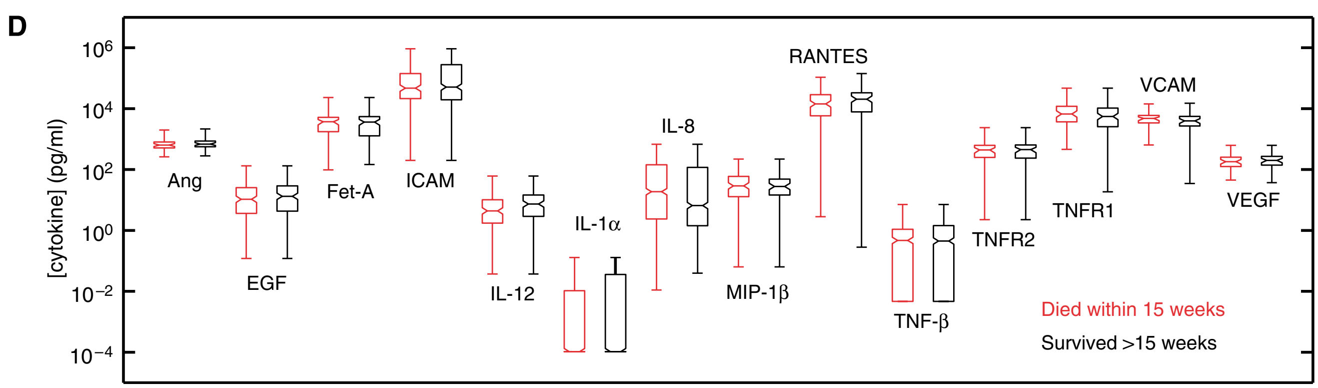


Fig. 5.4. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Example: disease classification

Knickerbocker *et al.* "An integrated approach to prognosis using protein microarrays and nonparametric methods". *Molecular Systems Biology*, 2007

- Goal: predict mortality in patients w/kidney dialysis
  - 468 patients, 208 died within 15 weeks of diagnoses
  - 14 proteins ("messenger" molecule that allows cells to communicate and alter function)
  - 11 clinical characteristics (age, race, bmi...)
  - Proteins were uninformative in isolation



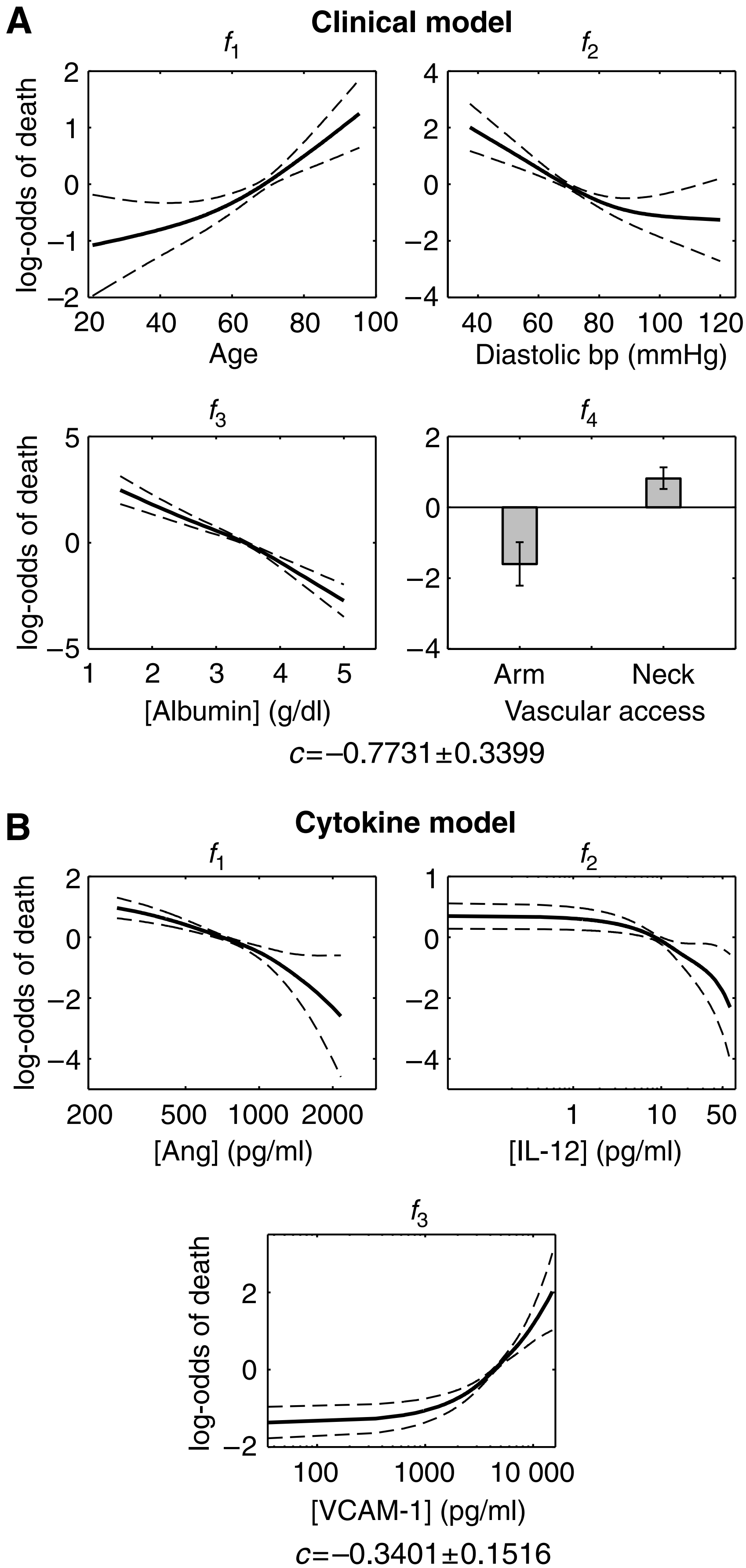
Approach

- Separate predictive model for clinical and molecular measurements
  - Logistic regression (Y = death within 15 weeks)

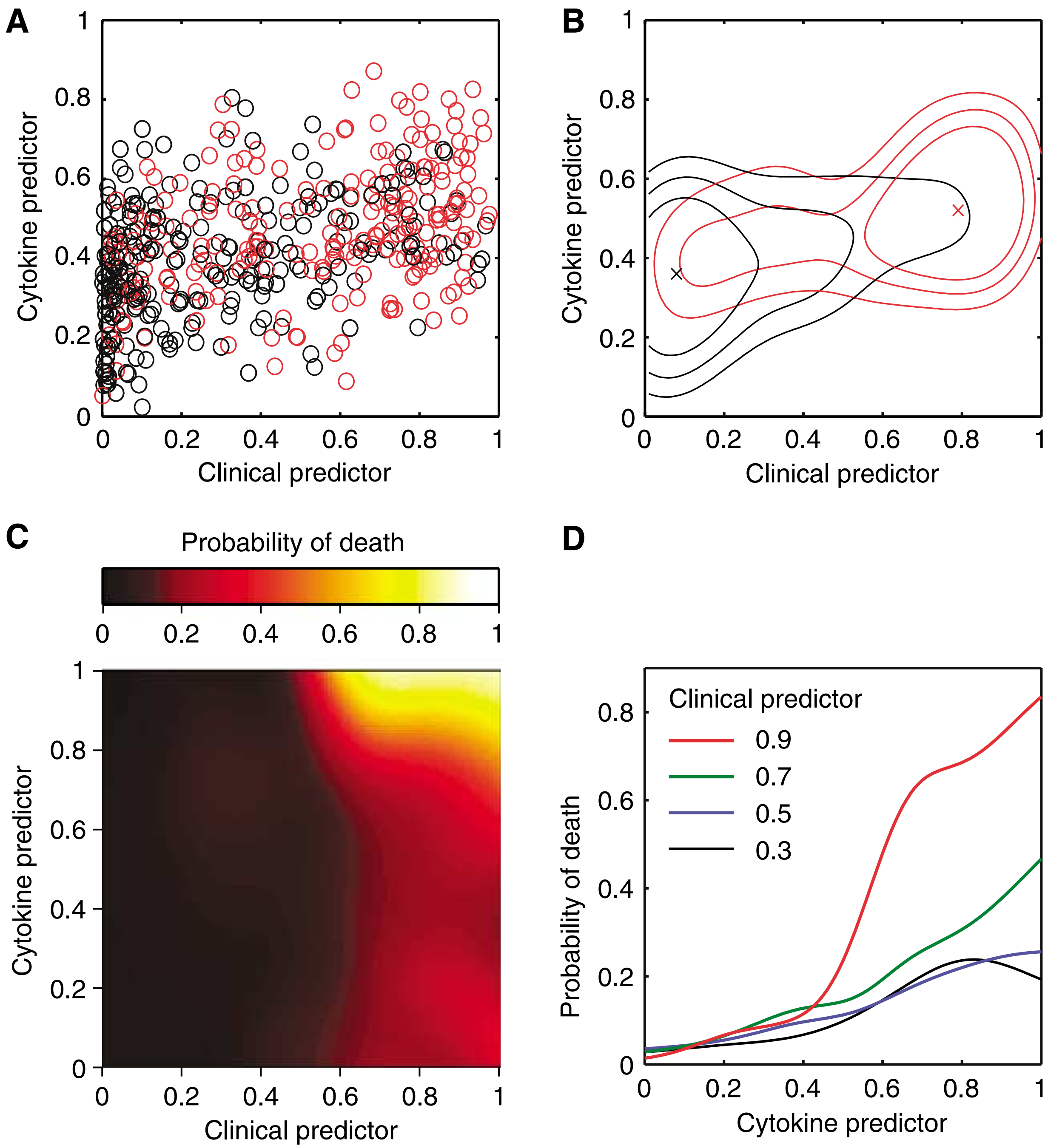
$$\text{log-odds of death} = \log(P_{\text{sample}}(\text{death})/P_{\text{sample}}(\text{survival})) = c + \sum_{p=1}^{M} b_p x_p$$

  - Additive model to reduce feature space
  - Exhaustive search for best M-variable model
  - Non-parametric version of the best model: splines

$$\log - \text{odds of death} = \log(P_{\text{sample}}(\text{death})/P_{\text{sample}}(\text{survival})) = c + \sum_{p=1}^{M} f_p(x_p)$$


A
Clinical model
f_1
log-odds of death
2
1
0
−1
−2
20
40
60
80
100
Age
f_2
4
2
0
−2
−4
40
60
80
100
120
Diastolic bp (mmHg)
f_3
log-odds of death
5
0
−5
1
2
3
4
5
[Albumin] (g/dl)
f_4
2
0
−2
−4
Arm
Neck
Vascular access
c=−0.7731±0.3399
B
Cytokine model
f_1
log-odds of death
2
0
−2
−4
200
500
1000
2000
[Ang] (pg/ml)
f_2
1
0
−2
−4
1
10
50
[IL-12] (pg/ml)
f_3
log-odds of death
2
0
−2
100
1000
10 000
[VCAM-1] (pg/ml)
c=−0.3401±0.1516

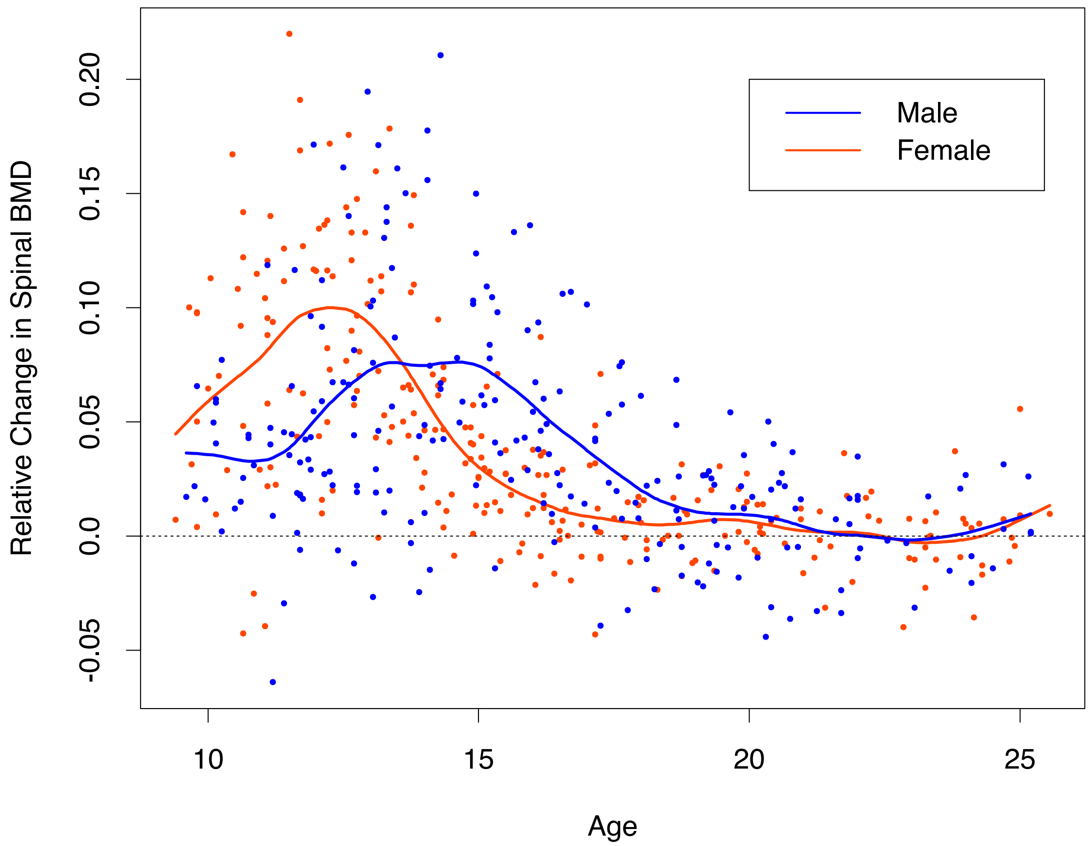
Combined prediction



Controlling model complexity (fixed knots)

- Restriction
  - Limit the class of functions
    $$f(\mathbf{X}) = \sum_{j=1}^{p} f_j(X_j) = \sum_{j=1}^{p} \sum_{m=1}^{M_j} \beta_{jm} h_{jm}(X_j)$$
  - Model complexity $\sim$ number of basis functions
- Selection
  - AIC, BIC, significance testing
  - Adaptively include basis functions that contribute to prediction (include CART, boosting...)
- Regularization
  - Include the entire dictionary of basis functions, but restrict the coefficients
    $$\text{RSS}(f, \lambda) = \sum_{i=1}^{N} \{y_i - f(x_i)\}^2 + \lambda \int \left\{f''(t)\right\}^3 dt$$
  - λ is a smoothing parameter ($\lambda = 0$: any function; $\lambda = \infty$: linear fit)
  - Maximized with a natural cubic spline
  - Equivalent to generalized ridge regression

Example



Rel. change in bone mineral density $\sim$ age, $\lambda = 0.00022$

$$\begin{aligned} \text{EPE}(\hat{f}_\lambda) &= E\left(Y - \hat{f}_\lambda\right)^2 \\ &= \text{Var}(Y) + E\left[\text{Bias}^2(\hat{f}_\lambda) + \text{Var}(\hat{f}_\lambda)\right] \\ &= \sigma^2 + \text{MSE}(\hat{f}_\lambda) \end{aligned}$$

Choose λ by cross-validation

Fig. 5.6. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Kernel Methods

HTF Ch6

One-dimensional kernel smoothers

- Different model at each point x_0
  - Only use observations close to target x_0
  - Weigh the neighbors x_1 with a kernel $K_\lambda(x_0, x_i)$

  - Weight based on distance from x_0
  - λ is a parameter
  - The resulting function is smooth

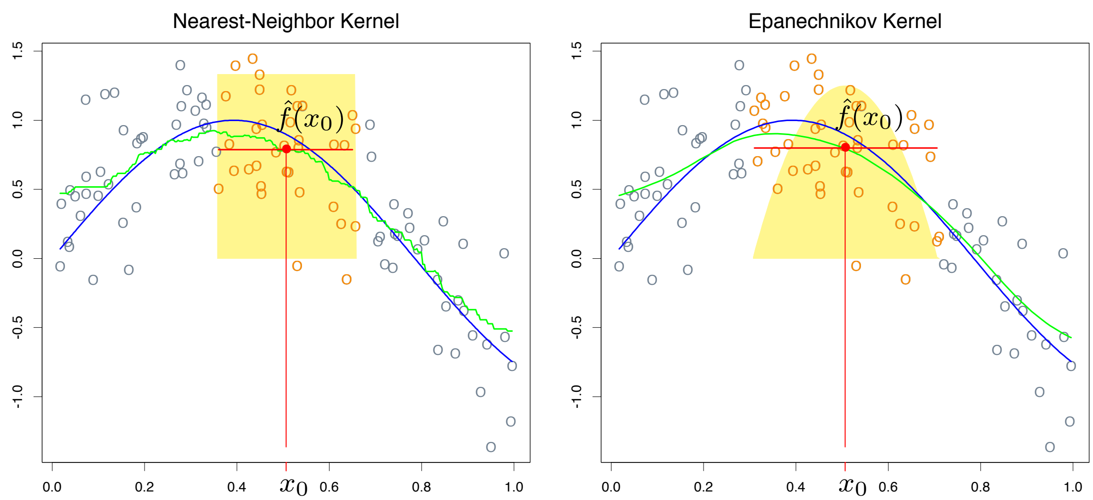
- K nearest neighbors
  - $\hat{f}(x_0) = \text{Ave}(y_i | x_i \in N_k(x_0))$ (discontinuous in x)

- Nadaraya-Watson kernel-weighted averaga
  - $\hat{f}(x_0) = \frac{\sum_{i=1}^N K_\lambda(x_0, x_i) y_i}{\sum_{i=1}^N K_\lambda(x_0, x_i)}$, where
    $K_\lambda(x_0, x) = D\left(\frac{|x - x_0|}{\lambda}\right)$ and

$$D(t) = \begin{cases} \frac{3}{4}(1 - t^2) & if \quad |t| \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

  - Points near the boundary have weight ~ 0
    $\rightarrow$ smoothing

Example



- 100 pairs (x_i, y_i)
- Green: Left: 30-NN running mean.
  Right: Kernel-weighted average, $\lambda = 0.2$
- Orange: observations contributing to the fit

Fig. 6.1. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Adaptive width

- Define $h_\lambda(x_0)$ a width function that determines the neighborhood of x_0

- Define $K_\lambda = D\left(\frac{|x-x_0|}{h_\lambda(x_0)}\right)$

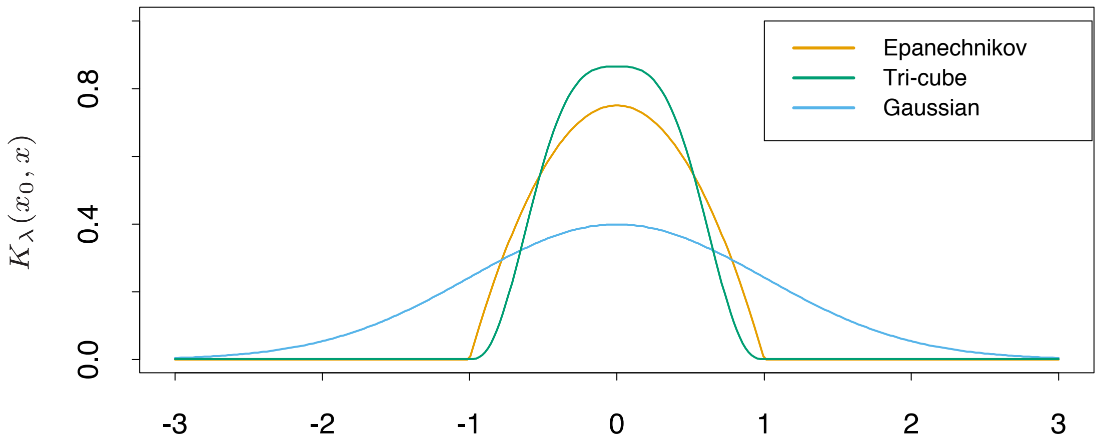
- Concerns:

  - Determine λ. Larger $\lambda \rightarrow$ lower variance but higher bias

  - $h_\lambda(x)$ constant $\rightarrow$ variance inversely proportional to density of points

  - Nearest neighbor $\rightarrow$ bias inversely proportional to density of points

Kernel examples



- Epanechnikov quadratic kernel $K_\lambda(x_0, x) = D\left(\frac{|x-x_0|}{\lambda}\right)$

$$D(t) = \begin{cases} \frac{3}{4}(1 - t^2) & if \quad |t| \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

- Tri-cube function

$$D(t) = \begin{cases} (1 - t^3)^3 & if \quad |t| \leq 1 \\ 0 & \text{otherwise} \end{cases}$$

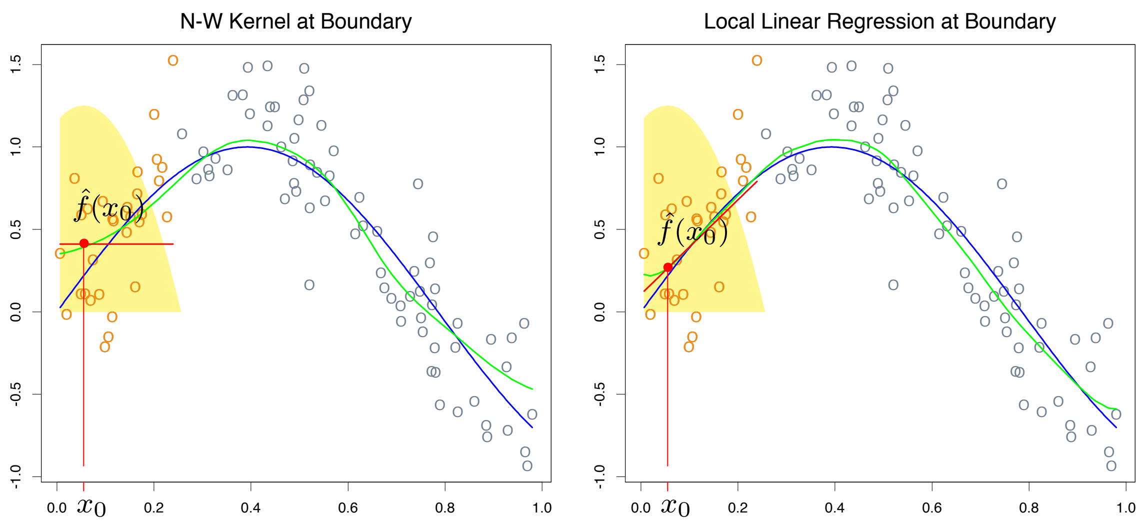
Fig. 6.2. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Local linear regression

- Smoothly varying locally weighted average
  - Problem: asymmetry of the kernel on the boundary of the domain $\rightarrow$ bias
  - Solution: fit straight lines rather than constants
  - Also helps if values of x are unequally spaced

- Separate weighted least squares problem
  - At each target point x_0:
    $$\min_{\alpha(x_0),\beta(x_0)} \sum_{i=1}^{N} K_\lambda(x_0, x_i)\,[y_i - \alpha(x_0) - \beta(x_0)x_i]^2$$
  - Define $b(x)' = (1, x)$
    $\mathbf{B}$ the $X \times 2$ regression matrix with ith row $b(x)'$
    $\mathbf{W}(x_0)$ the $N \times N$ diagonal matrix diag$(K_\lambda(x_0, x_i))$.
    Then $\hat{f}(x_0) = b(x_0)'\,(\mathbf{B}'\mathbf{W}(x_0)\mathbf{B})^{-1}\,\mathbf{B}'\mathbf{W}(x_0)\mathbf{y}$
  - Estimate at a single point
    $\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0$

Example



- Left: locally weighted average:
  bias near the boundaries of X

- True function is linear, but most observations in the neighborhood exceed the target point.

- Right: locally weighted linear regression removes the bias to first order

Fig. 6.3. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Extensions / comments

- Local polynomial regression
  - Minimize
    $$\min_{\alpha(x_0),\beta_j(x_0),j=1,\ldots,d} \sum_{i=1}^{N} K_\lambda(x_0,x_i)\left[y_i-\alpha(x_0)-\sum_{j=1}^{d}\beta_j(x_0)x_i^j\right]^2$$
  - Solution $\hat{f}(x_0)=\hat{\alpha}(x_0)+\sum_{j=1}^{d}\hat{\beta}_j(x_0)x_0^j$
  - Avoid "trimming the hills and filling the valleys"

- Bias-variance tradeoff
  - Small window $\rightarrow$ low bias, high variance

- Default hoice of λ
  - Epanechnikov or tri-cube: radius of support region
  - Gaussian: standard deviation
  - Better option: cross-validation

Example

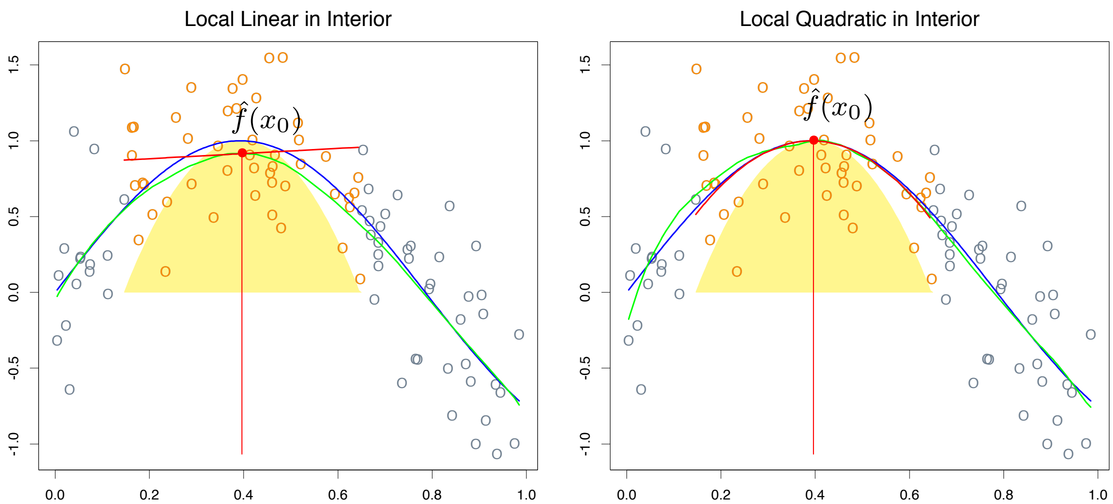
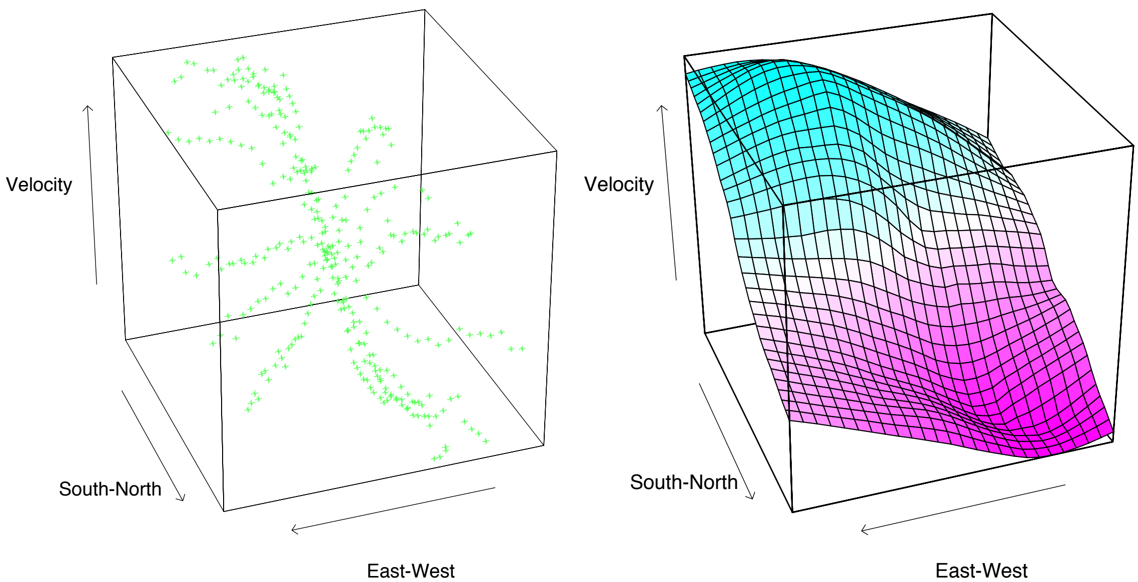


Fig. 6.5. Hastie, Tibshirani, Friedman
The Elements of Statistical Learning 2008

Local regression in $\mathbb{R}^p$



$$\min_{\beta(x_0)} \sum_{i=1}^{N} K_\lambda(x_0, x_i)\left(y_i - \beta(x_i)'\beta(x_0)\right)^2$$

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

Fig. 6.8. Hastie, Tibshirani, Friedman
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