Moving Beyond Linearity

1. Polynomial regression
2. Step functions
3. Regression splines
4. Smoothing spline
5. Local regression
6. Generalized additive Models

About this chapter

- Linear model is the most fundamental statistical model.
- Its limitation is the mean response must be a linear function of inputs/covariates.
- This relation in practice often does not hold.
- Nonlinear models are needed.

The nonlinear models.

- Polynomial regression.
- Step functions
- Regression splines
- Smoothing splines
- Local regression
- Generalized additive models.
- Trees, SVM, neural nets, ...

- Data: $(\mathbf{x}_i, y_i), i = 1, ..., n$.
- The general model
$$y_i = f(\mathbf{x}_i) + \epsilon_i.$$
- We assumed f is linear before.
- Linearity assumption is almost always an approximation, and sometimes a poor one.
- What kind of functions of $f(\cdot)$ we should assume?

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- What kind of functions of $f(\cdot)$ we should assume?
- Cannot search for arbitrary function $f(\cdot)$.
- Limit the search space.
- by Polynomial functions, or step functions, or certain basis functions,...

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- All linear regression results apply.
- Problem: how to determine the appropriate degree d.
- it is unusual to use d greater than 3 or 4.

The generalized linear model

- Generalized linear model:

$$E(Y|X) = g(X^T\beta)$$

  where g is a given *link function*.
- Examples:
  1. linear regression: $g(x) = x$
  2. logistic regression: $g(x) = 1/(1+e^{-x})$, the sigmoid function. $Y = 1$ or 0.
  3. Probit model: $g(x) = \Phi(x)$, the cdf of $N(0,1)$. $Y = 1$ or 0.
  4. Poisson model: $g(x) = e^x$. Y is count data.
  5. ...
- They can be extended to generalized non-linear model in the same fashion.

Logistic model with polynomial regression

- For binary response y_i, coded the binary events as 1 and 0.

$$p(y_i = 1|x_i) = \frac{\exp(\beta_0 + \beta_1 x_i + ... + \beta_d x_i^d)}{1 + \exp(\beta_0 + \beta_1 x_i + ... + \beta_d x_i^d)}.$$

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- This is essentially just logistic model with d inputs.
- All results on logistic model apply here.

Basis functions

- Let $b_1(x), ..., b_p(x)$ be a set of *basis functions.*
- We limit the search space of $f(\cdot)$ to the space that is linearly spanned by these basis functions:

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- Again a multiple linear regression model.
- The polynomial functions are special cases of basis functions approach.

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- Create the cutpoints

$$-\infty = c_0 < c_1 < ... < c_p < c_{p+1} = \infty$$

- The entire real line is cut into $p + 1$ intervals.
- Set $c_k(x) = I(c_k \leq x < c_{k+1})$, for $k = 0, ..., p$.
- Any x must be in exactly one of the $p + 1$ intervals.

$$c_0(x) + \cdots + c_p(x) = 1, \ \forall \ x.$$

Regression model based on step functions

- Use linear combination of $c_k(x)$ to approximate functions.

$$f(x) = \beta_0 + \beta_1 c_1(x) + \cdots + \beta_p c_p(x).$$

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- Again a multiple linear regression model.
- Same extension works for generalized linear model

$$f(x) = g(\beta_0 + \beta_1 c_1(x) + \cdots + \beta_p c_p(x)).$$

Piecewise polynomial functions

1. Cut the entire real line (or the range of values of covariates) into sub-intervals same as step function approach.
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$$p_k(x) = \begin{cases} \text{a polynomial}, & x \in [c_k, c_{k+1}), \\ 0, & \text{others.} \end{cases}$$

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$$p_k(x) = \begin{cases} \text{a polynomial}, & x \in [c_k, c_{k+1}), \\ 0, & \text{others.} \end{cases}$$

- These cutpoints are called *knots*.
- Step function approach is a special case of piecewise polynomial of degree 0.

- $f(x) = \beta_0 p_0(x) + \cdots \beta_d p_d(x)$.
- The model is

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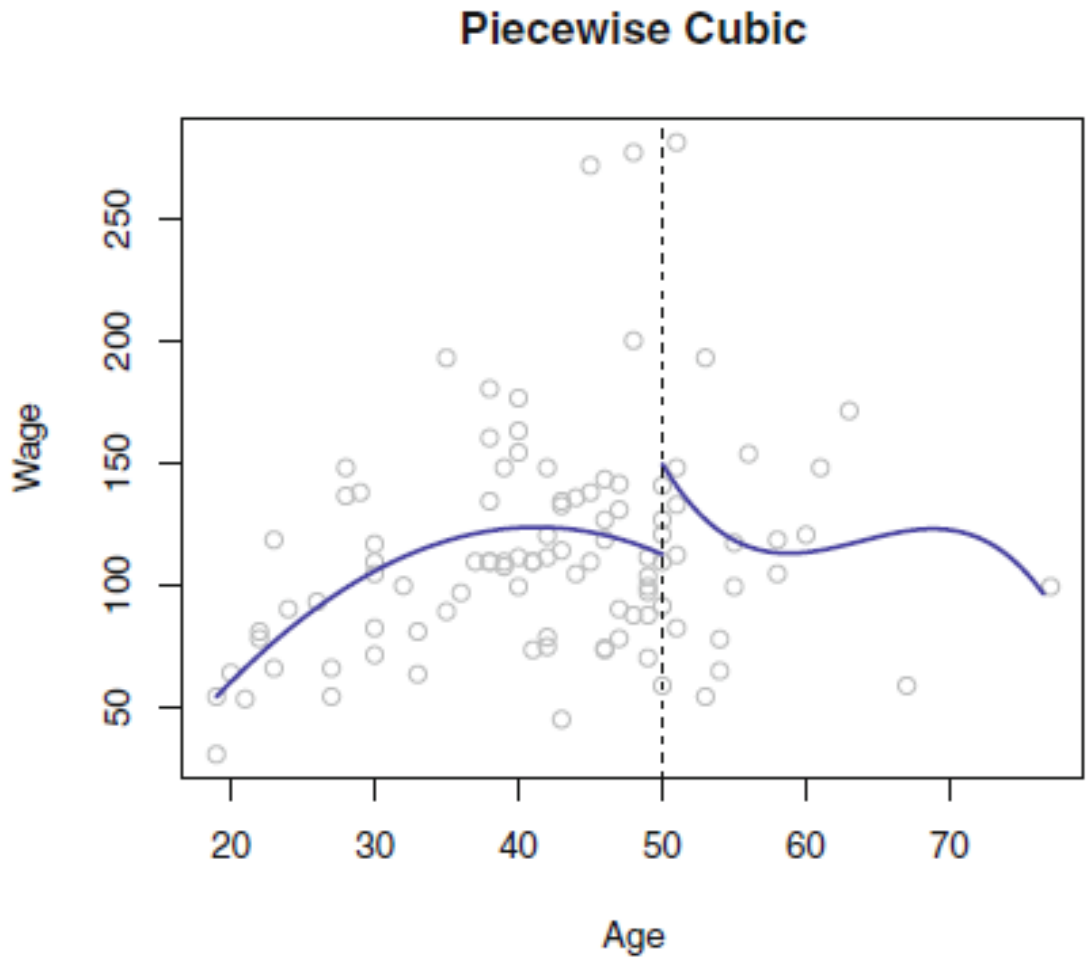
- Still a multiple linear regression model.
- Difficulty in creating the number and locations of cutpoints
- Drawback: non-smooth, not even continuous.



- Advantage:
  - capture local variation;
  - the degree of polynomial is generally low.
- disadvantage:
  - dis-continuity at knots.

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- ...

The effect of constraints

- Each constraint can be expressed as on linear equation.
- It reduces one degree of freedom.
- And reduces the complexity of the model.

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- Cubic spline: piecewise cubic polynomials but are continuous and have continous 1st and 2nd derivatives at knots.
- The degree of freedom of a cubic spline with K knots is:

$$4 \times (K+1) - 3K = K + 4.$$

Totally $K+1$ cubic functions, each has 4 free parameters, but each of the K knot has 3 constraints on continuity, continuity of 1st and 2nd derivatives.

Spline basis representation

- Suppose the K knots $\xi_1 < ... < \xi_K$ are determined.
- We may find $1, b_1(x), ..., b_{K+3}$ to form the space of cubic splines with knots at $\xi_1, ..., \xi_K$.

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- How to find these basis functions $b_k(x)$?
- **Require**: each must be a polynomial of order 3 and must be continuous, continous at 1st and 2nd derivates at all knots.

Spline basis representation

- x , x^2 and x^3 satisfy the requirement.
- Let

$$h(x,\xi) = (x-\xi)_+^3 = \begin{cases} (x-\xi)^3 & \text{if } x > \xi \\ 0 & \text{otherwise} \end{cases}$$

- $h(x,\xi_k)$ also satisfy the requirement.
- The basis functions of cubic splines can be

$$1, x, x^2, x^3, h(x,\xi_1), ..., h(x,\xi_K)$$

- Totally $K+4$ dimension with $K+3$ features.

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- The behavior of the cubic spline at boundary can be quite unstable.
- *Natural cubic spline* is cubic spline but require the function to be *linear* on $(-\infty, \xi_1]$ and $[\xi_K, \infty)$.

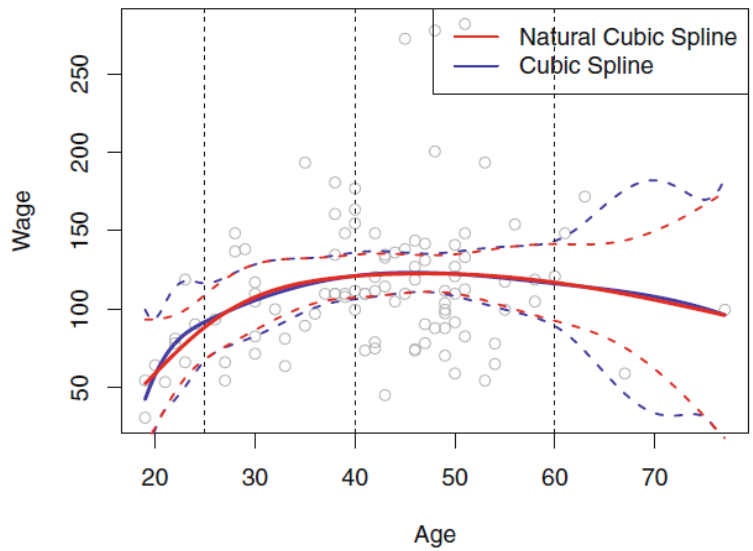

Figure: 7.4. A cubic spline and a natural cubic spline, with three knots, fit to a subset of the Wage data. Natural spline has narrower confidence intervals near boundary

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- Example: natural cubic splines has $4 = K - 1$ degree of freedom corresponds to $K = 5$ knots and $K - 2 = 3$ interior knots.

Choice of number and locations of knots

- Usually choose equally spaced knots within the range of values of inputs.
- If we know a function is highly varying somewhere, place more knots there, so that the spline function is also highly varying in the area.
- Try several choices of the number of knots, and use validation/cross-validation approach to determine the best.
- Many statistics software provide automatic choice of number and location of knots.

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- Polynomial function has poor boundary behavior.
- Natural spline is much better.

Smoothing spline

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- specifying a set of knots,
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- The most common constraint is f'', the second derivative do not vary much.

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- This is equivalent to with λ being the tuning parameter

$$\sum_{i=1}^{n}(y_i - f(x_i))^2 + \lambda \int f''(x)^2 dx \qquad (7.11).$$

- The function f minimizing the above is called *smoothing spline.*
- The function that minimize that loss+roughness penalty is *skrunken* version of a natural cubic spline with knots $x_1, ..., x_n$.

The tuning parameter

λ controls the amount of roughness penalty.

- $\lambda = 0$: no penalty, exactly interpolate the training observations, degree of freedom $= n$; maybe overfit.

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- What the degree of freedom when $\lambda > 0$ and is finite?
- We call it *effective degree of freedom*, denoted as df_λ.

Effective degree of freedom

- The df_λ is a measure of the flexibility of the smoothing spline
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Effective degree of freedom

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  - the higher it is, the more flexible.
  - the lower-bias but higher-variance.
- Minimizing (7.11), let the fitted values be

$$\hat{\mathbf{y}} = \mathbf{S}_\lambda \mathbf{y} \tag{7.12}$$

  where $\hat{\mathbf{y}} = (y_1, ..., y_n)^T$ is an n-vector.
- Then, the effective degree of freedom is

$$df_\lambda = \text{trace}(\mathbf{S}_\lambda).$$

Choice of λ

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- For leave-one-out cross-validation (LOOCV), it can be shown

$$\mathrm{RSS}_{\mathrm{cv}}(\lambda) = \sum_{i=1}^{n}(y_i - \hat{f}_\lambda^{(-i)}(x_i))^2 = \sum_{i=1}^{n}\left[\frac{y_i - \hat{f}_\lambda(x_i)}{1 - s_{\lambda,ii}}\right]^2$$

  where $s_{\lambda,ii}$ is the i-th diagonal element of $\mathbf{S}_\lambda$.
- $\hat{f}_\lambda^{(-i)}(x_i)$ – fitted value for this smoothing spline evaluated at x_i, where the fit uses all of the training observations except for the ith observation (x_i, y_i).
- $\hat{f}_\lambda(x_i)$ – the smoothing spline function fit to all of the training observations and evaluated at x_i.

Fast computation of cross-validation I

- The leave-one-out cross-validation statistic is given by

$$CV = \frac{1}{N}\sum_{i=1}^{N} e_{[i]}^2,$$

where $e_{[i]} = y_i - \hat{y}_{[i]}$, the observations are given by $y_1, \ldots, y_N$, and $\hat{y}_{[i]}$ is the predicted value obtained when the model is estimated with the ith case deleted.

- Suppose we have a linear regression model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{e}$. The $\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$ and $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ is the hat matrix. It has this name because it is used to compute $\hat{\mathbf{Y}} = \mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{HY}$. If the diagonal values of $\mathbf{H}$ are denoted by $h_1, \ldots, h_N$, then the leave-one-oout cross-validation statistic can be computed using

$$CV = \frac{1}{N}\sum_{i=1}^{N} [e_i/(1-h_i)]^2,$$

where $e_i = y_i - \hat{y}_i$ is predicted value obtained when the model is estimated with all data included.

Fast computation of cross-validation II

Proof

- Let $\mathbf{X}_{[i]}$ and $\mathbf{Y}_{[i]}$ be similar to $\mathbf{X}$ and $\mathbf{Y}$ but with the ith row deleted in each case. Let $\mathbf{x}_i^T$ be the ith row of $\mathbf{X}$ and let

$$\hat{\boldsymbol{\beta}}_{[i]} = (\mathbf{X}_{[i]}^T\mathbf{X}_{[i]})^{-1}\mathbf{X}_{[i]}^T\mathbf{Y}_{[i]}$$

  be the estimate of $\boldsymbol{\beta}$ without the ith case. Then $e_{[i]} = y_i - \mathbf{x}_i^T\hat{\boldsymbol{\beta}}_{[i]}$.
- Now $\mathbf{X}_{[i]}^T\mathbf{X}_{[i]} = (\mathbf{X}^T\mathbf{X} - \mathbf{x}_i\mathbf{x}_i^T)$ and $\mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i = h_i$. So by the Sherman-Morrison-Woodbury formula,

$$(\mathbf{X}_{[i]}^T\mathbf{X}_{[i]})^{-1} = (\mathbf{X}^T\mathbf{X})^{-1} + \frac{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i\mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}}{1-h_i}.$$

Fast computation of cross-validation III

Proof

- Also note that $\mathbf{X}_{[i]}^T \mathbf{Y}_{[i]} = \mathbf{X}^T\mathbf{Y} - \mathbf{x}y_i$. Therefore

$$\begin{aligned}\hat{\boldsymbol{\beta}}_{[i]} &= \left[(\mathbf{X}^T\mathbf{X})^{-1} + \frac{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i\mathbf{x}_i^T(\mathbf{X}^T\mathbf{X})^{-1}}{1-h_i}\right](\mathbf{X}^T\mathbf{Y} - \mathbf{x}_i y_i) \\ &= \hat{\boldsymbol{\beta}} - \left[\frac{(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i}{1-h_i}\right][y_i(1-h_i) - \mathbf{x}_i^T\hat{\boldsymbol{\beta}} + h_i y_i] \\ &= \hat{\boldsymbol{\beta}} - (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i e_i/(1-h_i)\end{aligned}$$

- Thus

$$\begin{aligned}e_{[i]} &= y_i - \mathbf{x}_i^T\hat{\boldsymbol{\beta}}_{[i]} \\ &= y_i - \mathbf{x}_i^T\left[\hat{\boldsymbol{\beta}} - (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}_i e_i/(1-h_i)\right] \\ &= e_i + h_i e_i/(1-h_i) = e_i/(1-h_i)\end{aligned}$$

Local regression

- Rather than considering fitting a function f to the data, we just focus on a target point, say x_0, and try to estimate $f(x_0) = \beta_0$.
- Consider a weight function, often called kernel function, $k(t)$.
  - $k(t)$ is nonnegative symmetric,
  - becomes small when $|t|$ is large.

Typical choice of kernels

- Uniform kernel: $k(t) = 1/2 I(|t| \leq 1)$.
- Triangle kernel: $k(t) = (1 - |t|) I(|t| \leq 1)$.
- Gaussian kernel: $k(t) = e^{-t^2/2}/\sqrt{2\pi}$
- Epanecknikov kernel: $k(t) = 3/4(1 - t^2)_+$
- Logistic kernel: $k(t) = 1/(e^t + e^{-t} + 2)$.
- Sigmoid kernel: $k(t) = 2/(\pi(e^t + e^{-t}))$.

Local view

- use the kernel function to create *weights* on each observation so that those with x_i closer to x_0 gets more weights:

$$K_{i0} = \frac{1}{h} k(\frac{x_i - x_0}{h})$$

- These weights create the "Localness" surrounding x_0. h is the bandwidth that is usually small.
- we can consider minimization

$$\sum_{i=1}^{n} K_{i0}(y_i - \beta_0 - \beta_1(x_i - x_0))^2$$

  Then, $\hat{\beta}_0$ is the estimator of $f(x_0)$.
- This estimator is local linear estimator, since locally around x_0, we used linear function to approximate $f(x)$.
- One can certainly consider local polynomial estimation, by considering local polynomial approximation.

Remark.

- Local linear estimate is also a linear function of $\mathbf{y}$, and there has expression of the form of (7.12).
- The degree of freedom controled by the bandwidth.
- Small bandwidth results in small bias but high variance (and high effective degree of freedom).
- Can be difficult to implement with high dimension data, by the curse of dimensionality.

Generalized additive Models (GAMs)

- With p inputs, the general model should be

$$y_i = f(x_{i1}, ..., x_{ip}) + \epsilon_i.$$

- Difficult to model multivariate nonlinear function.
- Restrict search space to

$$\{f(x_1, ..., x_p) : f_1(x_1) + f_2(x_2) + ...f_p(x_p)\}$$

- The multivariate function is simple sum of nonlinear function of each varible.
- This leads to the generalized additive model (GAM).

The GAMs

- The model:

$$y_i = f_1(x_{i1}) + f_2(x_{i2}) ... + f_p(x_{ip}) + \epsilon_i$$

- The statistical estimation of f_1, ..., f_p can be solved by taking advantage of
- 1. the methodologies for nonlinear model for single input case.
- 2. a backfit algorithm.

The backfitting algorithm

- Initialize the estimator of f_1, ..., f_p, denoted as $\hat{f}_1, ..., \hat{f}_p$.
- Given estimates $\hat{f}_1, .., \hat{f}_{k-1}$, $\hat{f}_{k+1}$, ..., $\hat{f}_p$, compute

$$\tilde{y}_i = y_i - \hat{f}_1(x_{i1}) - \hat{f}_{k-1}(x_{i,k-1}) - \hat{f}_{k+1}(x_{i,k+1}) - ... - f_p(x_{ip})$$

- Run nonlinear regression with response $\tilde{y}_i$ and single input x_{ik}, to obtain the estimate of f_k. Update $\hat{f}_k$ by this estimate.
- Continue with the update of f_{k+1}. (If $k = p$ continue the update of f_1.)
- Repeat till convergence.

Pros and Cons of GAM

- It is nonlinear (potentially more accurate than linear if linear relation is not true)
- Additivity:
  - examine the effect of each x_j on the response y while holding all of the other variables fixed;
  - inference is possible;
  - the smoothness of the function f_j for the variable X_j can be summarized via degrees of freedom.
- Interactions are missed: add low-dimensional interaction functions of the form $f_{jk}(X_j, X_k)$.

GAM also work for generalized linear model

- In general we have

$$E(Y|X) = g(f_1(X_1) + ... + f_p(X_p))$$

  where g is known link function.
- For example, for logistic GAM:

$$P(Y = 1|X) = \frac{\exp(f_1(X_1) + ... + f_p(X_p))}{1 + \exp(f_1(X_1) + ... + f_p(X_p))}$$