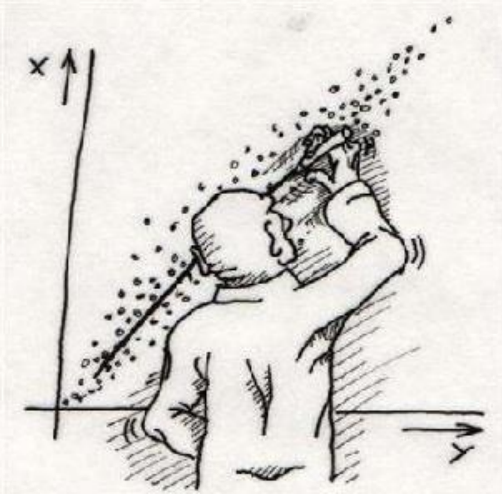
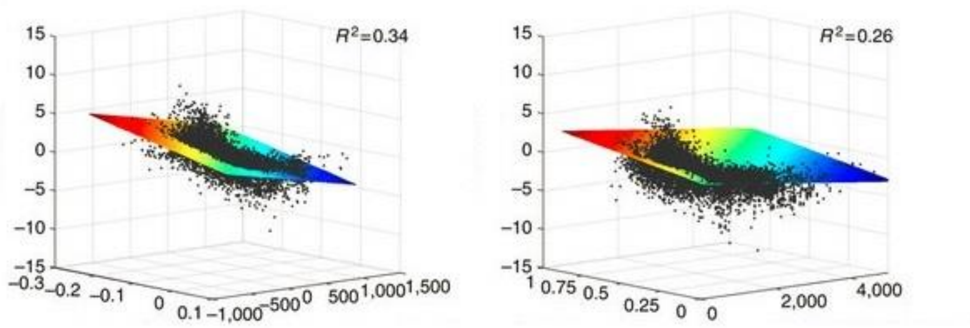
DATA 621 - Business Analytics and Data Mining





Meetup #4

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Nonlinear Regression

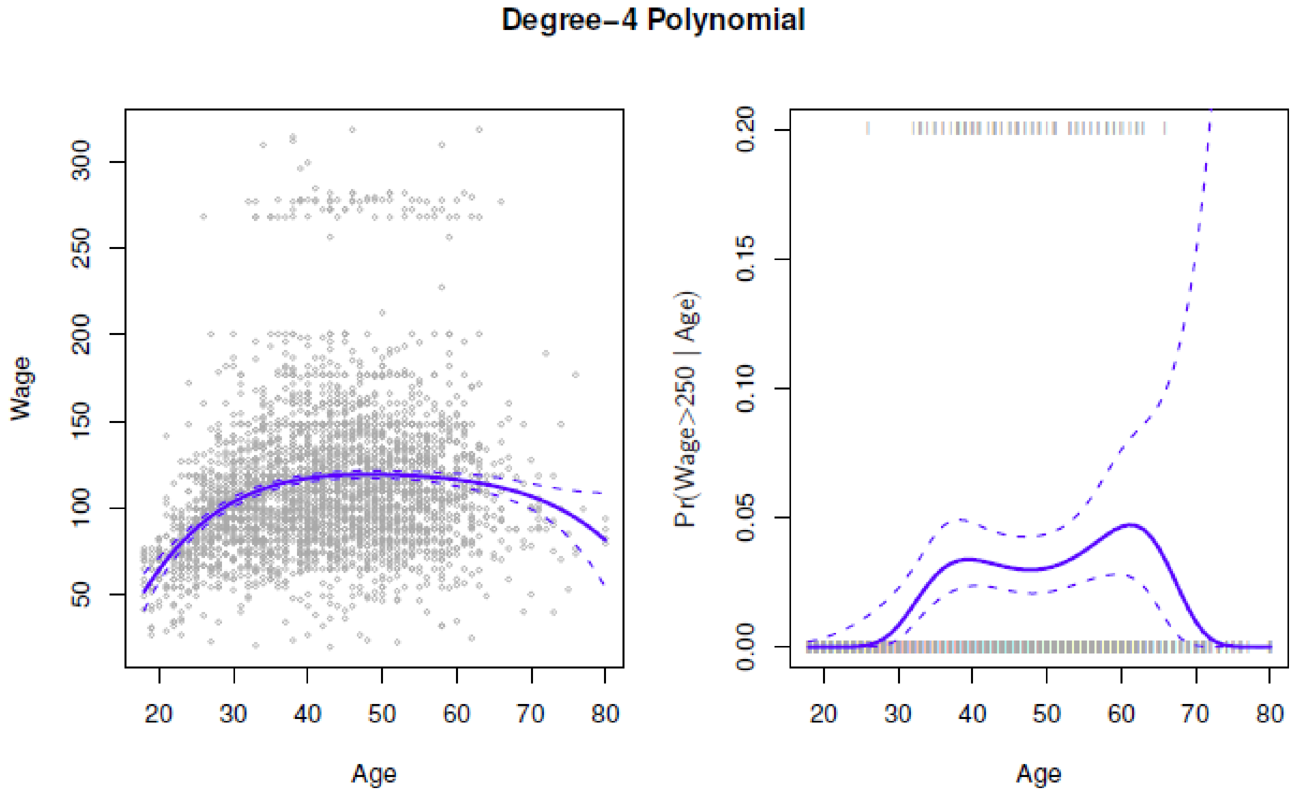
- The general linear model is linear in the regressors but not necessarily in the explanatory variables that generate these regressors.

- However, there are nonlinear regression methods that offer a lot of flexibility, without losing the ease and interpretability of parametric models:
  - Polynomial regression
  - Step functions
  - Regression splines

Polynomial Regression

- Replace the standard linear model with a polynomial function:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \ldots + \beta_d x_i^d + \epsilon_i$$



Polynomial Regression (cont.)

- For large enough degree *d*, a polynomial regression allows us to produce an extremely non-linear curve.
- We do this by creating new variables $X_1 = X$, $X_2 = X^2$, etc. and then treat as multiple OLS linear regression.
- In general, we are not really interested in the coefficients, but instead the fitted function values at any value x_0:

$$\hat{f}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0 + \hat{\beta}_2 x_0^2 + \hat{\beta}_3 x_0^3 + \hat{\beta}_4 x_0^4$$

Polynomial Regression (cont.)

- Since $\hat{f}(x_0)$ is a linear function of the $\hat{\beta}_j$, we can get a simple expression for *pointwise variances* $\mathrm{Var}[\hat{f}(x_0)]$ at any value of x_0.

- It is unusual to use *d* greater than 3 or 4 because for large values of *d*, the polynomial curve can become overly flexible and can take on very strange shapes.

- Note that we can also use cross-validation to choose *d*.

Step Functions

- Using polynomial functions of the features as predictors in a linear model imposes a *global* structure on the non-linear function of X.

- To avoid imposing such a global structure, we can create transformations of a variable by cutting the variable into distinct regions.

- In particular, we use *step functions* to break the range of X into bins, where we fit a different constant in each bin.

Step Functions (cont.)

- This amounts to converting a continuous variable into an *ordered categorical variable*.
- In greater detail, we create cutpoints (or knots) c_1, c_2,….,c_K in the range of X and then construct $K + 1$ new variables:

$$\begin{array}{lcl} C_0(X) & = & I(X < c_1), \\ C_1(X) & = & I(c_1 \leq X < c_2), \\ C_2(X) & = & I(c_2 \leq X < c_3), \\ & \vdots & \\ C_{K-1}(X) & = & I(c_{K-1} \leq X < c_K), \\ C_K(X) & = & I(c_K \leq X), \end{array}$$

where $I(.)$ is an *indicator function* that returns a 1 if the condition is true and 0 otherwise.

Step Functions (cont.)

- Note that for any value of *X*, $C_0(X) + C_1(X) + \ldots + C_K(X) = 1$, since *X* must be exactly in one of the *K* + 1 intervals.

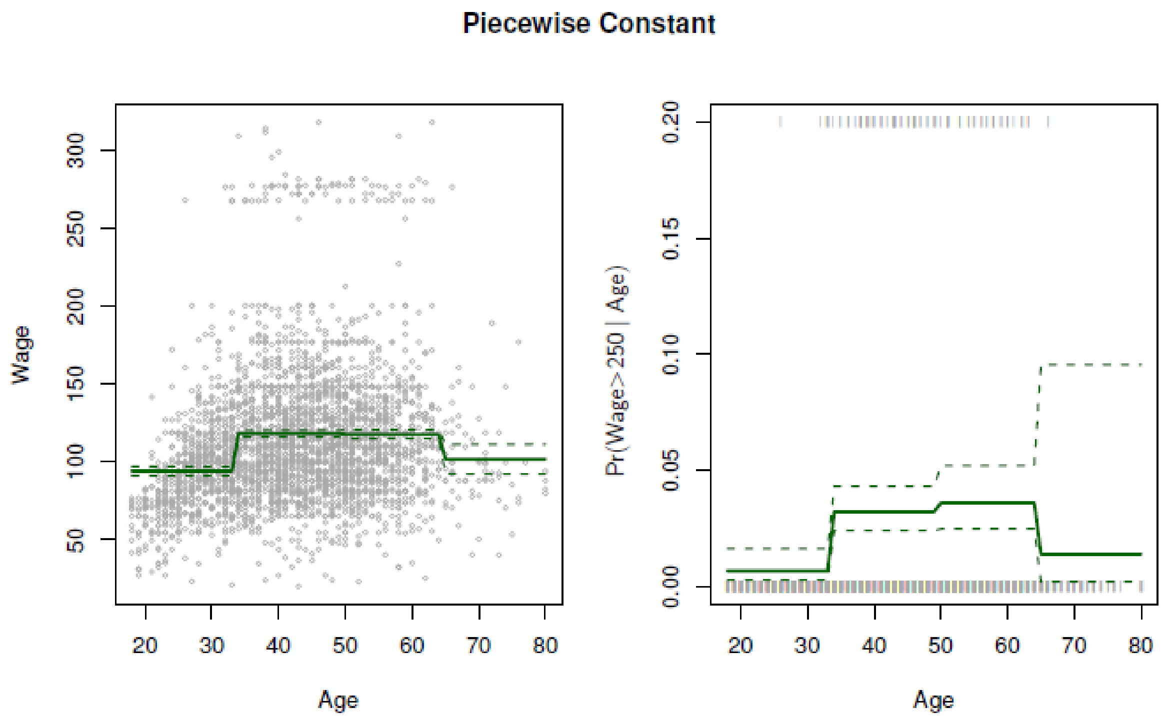
- We then use OLS estimation to fit a linear model using these *K* + 1 new variables:

- For a given value of *X*, at most one of C_1, C_2,…,C_K can be non-zero.

- β_j represents the average increase in the response for *X* in $c_j \leq X \leq c_{j+1}$ relative to $X < c_1$.

Step Functions (cont.)

$$C_1(X) = I(X < 35), \quad C_2(X) = I(35 \leq X < 50), \ldots, C_3(X) = I(X \geq 65)$$



- Unless there are natural breakpoints in the predictors, piece-wise constant functions can miss the action.

Basis Functions

- Polynomial and piece-wise constant regression models are special cases of a *basis function* approach.

- The idea is to have at hand a family of functions or transformations that can be applied to a variable X: $b_1(X),\ldots,b_K(X)$

- Instead of fitting a linear model in X, we fit the following model:

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \beta_3 b_3(x_i) + \ldots + \beta_K b_K(x_i) + \epsilon_i$$

- Note that the basis functions $b_1(.),\ldots,b_K(.)$ are fixed and known.

Basis Functions (cont.)

- For polynomial regression, the basis functions are $b_j(x_i) = x_i^j$

- For piece-wise constant functions, the basis functions are
$$b_j(x_i) = I(c_j \leq x_i \leq c_{j+1})$$

- Note that we can use OLS to estimate the unknown regression coefficients.

- Thus, all of the inference tools for linear models (standard errors, F-statistics, etc.) are available in this setting.

Regression Splines

- Regression splines are a flexible class of basis functions that extend upon the polynomial regressions and piece-wise constant regression approaches.
- They involve dividing the range of *X* into *K* distinct regions; within each region, a polynomial function is fit to the data.
- These polynomials are constrained so that they join *smoothly* at the region boundaries (or *knots*).
- Provided that the interval is divided into enough regions, this can produce an extremely flexible it.

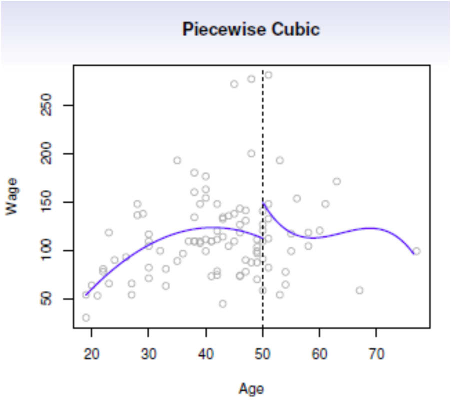
Piecewise Polynomials

- Instead of fitting a high-degree polynomial over the entire range of *X*, *piece-wise polynomial regression* involves fitting separate low-degree polynomials over different regions of *X*.

- Here, the beta coefficients differ in different parts of the range of *X*; the points where the coefficients change are called *knots*.

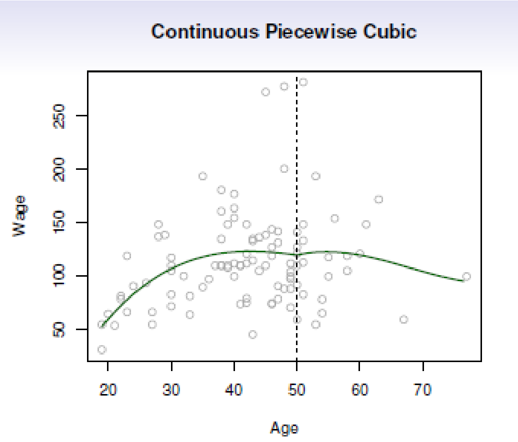
- Example: A piecewise cubic polynomial with a single knot at a point *c* takes the following form:

$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \epsilon_i & \text{if } x_i < c; \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \epsilon_i & \text{if } x_i \geq c. \end{cases}$$



Piecewise Polynomials (cont.)

- Each of the polynomial functions can be fit using OLS applied to simple functions of the original predictor.



- Using more knots leads to a more flexible piecewise polynomial.

- If general, if we place K different knots through the range of X, then we end up fitting $K + 1$ different polynomials.

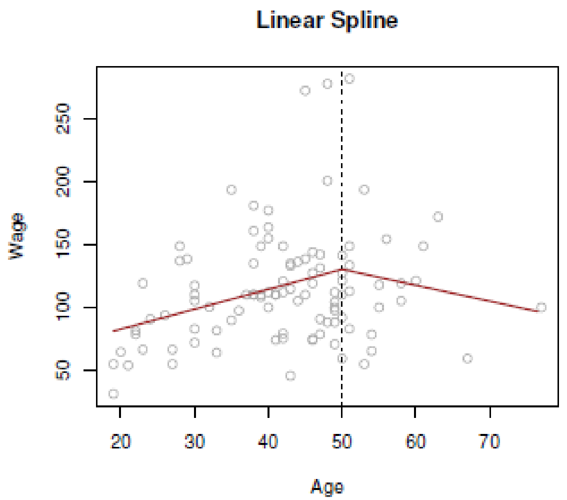
- It is better to add *constraints* to the polynomials (e.g., continuity). *Splines* have the maximum amount of continuity

Regression Splines (cont.)

- Each constraint that we impose effectively frees up one degree of freedom, by reducing the complexity of the resulting piecewise polynomial fit.

- The general definition of a degree-d spline is that it is a piecewise degree-d polynomial, with continuity in derivatives up to degree $d - 1$ at each knot.

- Thus, a **linear spline** is obtained by fitting a line in each region of the predictor space defined by the knots, requiring continuity at each knot.



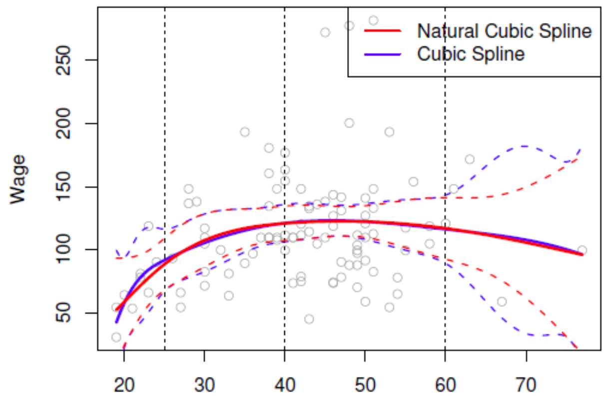
Regression Splines (cont.)

- A *natural spline* is a regression spline with additional boundary constraints.

- The function is required to be linear at the boundary (in the region where *X* is smaller than the smallest knot, or larger than the largest knot).

- This additional constraint means that natural splines generally produce more stable estimates at the boundaries.

- A *natural cubic spline* extrapolates linearly beyond the knots.



Regression Splines (cont.)

Choosing the Location of Knots

- The regression spline is most flexible in regions that contain a lot of knots, because in those regions the polynomial coefficients can change rapidly.

- One option is to place more knots in places where we feel the function might vary most rapidly, and to place fewer knots where it seems more stable.

- In practice, it is common to place knots in a uniform fashion. For example, one strategy is to decide K, the number of knots, and then place them at appropriate quantiles of the observed X.

Regression Splines (cont.)

Choosing the Number of Knots

- One option is to try out different numbers of knots and see which produces the best looking curve.
- However, a more objective approach is to use cross-validation.
- The procedure is repeated for different number of knots *K*; then the value of *K* giving the smallest RSS is chosen.
- Splines allow us to place more knots, and hence flexibility, over regions where the function *f* seems to be changing rapidly, and fewer knots where *f* appears more stable.

Nonparametric Regression

- The nonparametric regression approach is to choose a function *f* from some smooth family of functions.
- We do need to make some assumptions about *f* – that it has some degree of smoothness and continuity. However, these restrictions are far less limiting than the parametric way.
- Unlike parametric models, nonparametric models do not have a formulaic way of describing the relationship between the predictors and the response; this often needs to be done graphically.
- However, the nonparametric approach is more flexible, assumes far less (and so is less liable to make bad mistakes), and is particularly useful when little past experience is available to know the appropriate form for a parametric model.

Smoothing Splines

- We create regression splines by specifying a set of knots, producing a sequence of basis functions, and then use OLS to estimate the spline coefficients.

- What we really want is a function *g* that makes RSS small and *smooth*. Thus, consider the following criterion for fitting a smooth function *g*(*x*) to some data (known as a *smoothing spline*):

$$\underset{g \in \mathcal{S}}{\text{minimize}} \sum_{i=1}^{n} (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

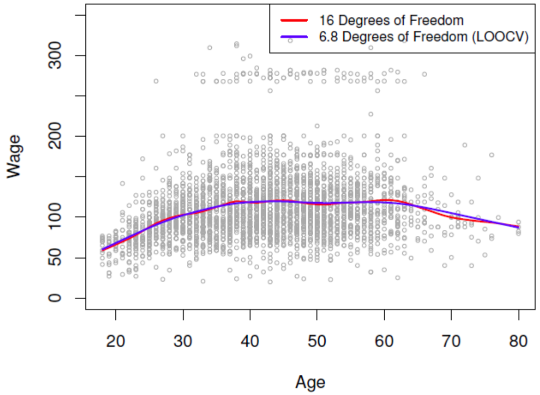
where λ is a nonnegative tuning parameter.

Smoothing Splines (cont.)

- The first term is a loss function (RSS), which tries to make $g(x)$ match the data at each x_i.
- The second term is a *roughness penalty* and controls how wiggly $g(x)$ is; this is modulated by the tuning parameter λ.
- The larger the value of λ, the smoother g will be. The smaller the value of λ, the more wiggly the function.
- As $\lambda \rightarrow \infty$, the function $g(x)$ becomes linear.

Smoothing Splines (cont.)

- It turns out that the solution is a natural cubic spline, with a knot at every unique value of x_i.
- The tuning parameter λ controls the level of roughness (i.e., the effective degrees of freedom).
- Smoothing splines avoid the knot-selection issue, leaving a single λ to be chosen.
- We use LOOCV to find λ!!



Local Regression

- *Local regression* is a different approach for fitting flexible non-linear functions, which involves computing the fit at a target point x_0 using only the nearby training observations.

- It is a *memory-based* procedure because we need all the training data each time we wish to compute a prediction.

- The *span* plays a role like that of the tuning parameter λ in smoothing splines; it controls the flexibility of the non-linear fit.

Local Regression (cont.)

- The smaller the value of the span s, the more *local* and wiggly will be our fit.
- A very large value of s will lead to a global fit to the data using all of the training observations.
- We can use cross-validation to choose s or specify it directly.
- Another choice to be made includes how to define the weighting function K, and whether to fit a linear, constant, or quadratic regression.

Local Regression (cont.)

Algorithm 7.1 *Local Regression At* $X = x_0$

1. Gather the fraction $s = k/n$ of training points whose x_i are closest to x_0.
2. Assign a weight $K_{i0} = K(x_i, x_0)$ to each point in this neighborhood, so that the point furthest from x_0 has weight zero, and the closest has the highest weight. All but these k nearest neighbors get weight zero.
3. Fit a *weighted least squares regression* of the y_i on the x_i using the aforementioned weights, by finding $\hat{\beta}_0$ and $\hat{\beta}_1$ that minimize

$$\sum_{i=1}^{n} K_{i0}(y_i - \beta_0 - \beta_1 x_i)^2. \tag{7.14}$$

4. The fitted value at x_0 is given by $\hat{f}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0$.

Local Regression (cont.)

- With a sliding weight function, we fit separate linear fits over the range of *X* by weighted least squares.