Supervised Learning with Tabular Data

Gov 2018

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1. Regression with Continuous Outcome
   - OLS and Overfitting
   - Ridge
   - LASSO
   - Bias Variance Trade Off
   - Splines

Introduction

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- **Goal**
  - Supervised learning with continuous outcome categories
  - Bias-variance tradeoffs
  - Regularization
  - Flexible models to capture non-linearity

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Linear Regression

The linear regression model assumes that the regression function $\mathbb{E}(\mathbf{Y}|\mathbf{X})$ is linear in the sense that

$$f(\mathbf{X}) = \beta_0 + \sum_{k=1}^{K} X_k \beta_k$$

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$$f(\mathbf{X}) = \beta_0 + \sum_{k=1}^{K} X_k \beta_k$$

It minimizes the residual sum of squares.

$$\begin{aligned}\mathrm{RSS}(\beta) &= \sum_{i=1}^{N} (\underbrace{Y_i - f(x_i)}_{cost})^2 \\ &= \sum_{i=1}^{N} \left(Y_i - \beta_0 - \sum_{k=1}^{K} x_{ik} \beta_k \right)^2\end{aligned}$$

That is,

$$\hat{\beta} = \arg\min_{\beta} \left[(\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) \right]$$

Bias Variance Trade off

Let's consider fitting a higher order (linear) model on a given set of data:

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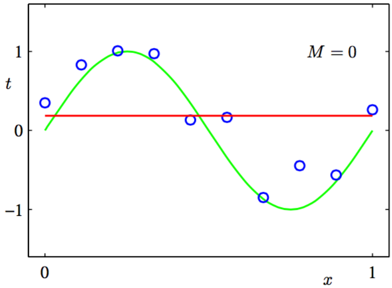
For example, if $M = 4$ we have:

$$Y = \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \beta 4 X^4 + \epsilon$$

The Bias-Variance Trade-off : $y = \sum_{m=0}^{M} \beta_m x^m$



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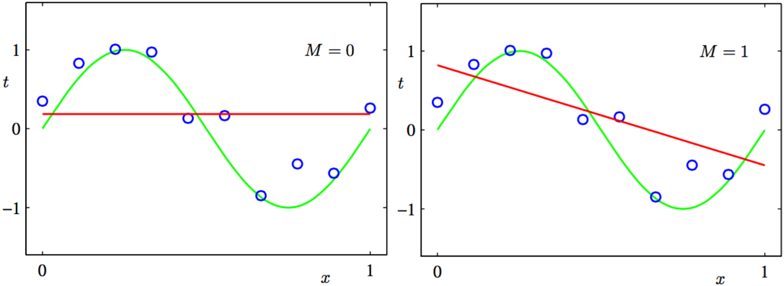

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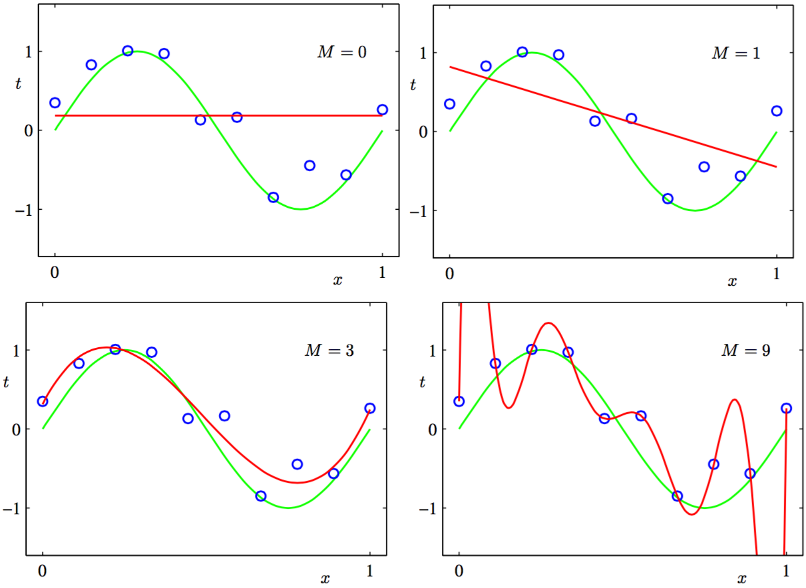

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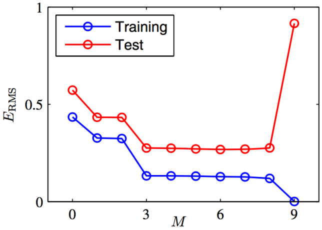

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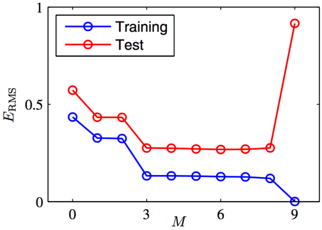

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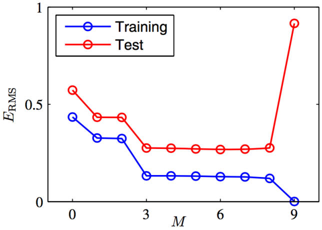

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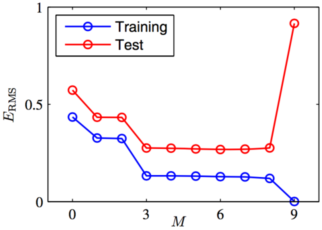

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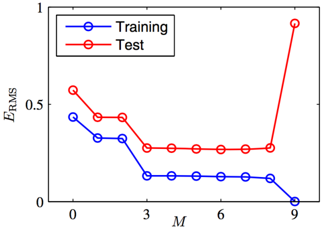

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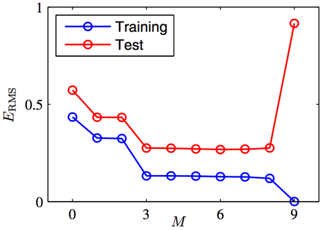

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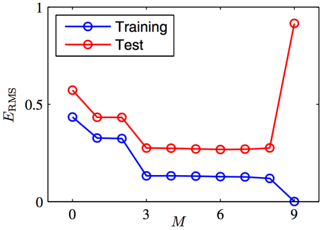

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- Flexible models are very good at “explaining” outliers
- We want to penalize models that are too flexible (preference for simpler theories) while allowing for model flexibility if the data demands it

In-sample MSE vs. Out-of-sample MSE?

By construction, OLS will do well for in-sample MSE

- When $n >> k$, it will probably do well in a stable environment (i.e., observations all from the same data-generating process and effects are strong)
- When $n << k$, out-of-sample MSE might be really bad, because nothing prevents flexible models from chasing outliers (finding spurious effects)

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Two reasons why we might not be satisfied with the least squares estimates

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Two reasons why we might not be satisfied with the least squares estimates

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2. **Interpretation:** We often include a long list of independent variables (a kitchen sink regression) $\rightarrow$ unparsimonious, difficult to interpret

Ridge Regression

- The objective:

$$\min_{\beta} \left[(\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) + \lambda \sum_{k=1}^{K} \beta_k^2 \right]$$

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- Re-expressing the problem

$$\text{PRSS}(\lambda)=(\mathbf{y}-\mathbf{X}\beta)^T(\mathbf{y}-\mathbf{X}\beta)+\lambda\beta^T\beta$$

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To minimize the above equation, we solve for zero .

Continued

$$
\begin{aligned}
\frac{\partial}{\partial \beta}\left\{(\mathbf{y}-\mathbf{X}\beta)^T(\mathbf{y}-\mathbf{X}\beta)+\lambda\beta^T\beta\right\} &= 0\\
\frac{\partial}{\partial \beta}\left\{\mathbf{y}^T\mathbf{y}+\mathbf{X}\beta^T\mathbf{X}\beta-2(\mathbf{X}\beta^T)\mathbf{y}+\lambda\beta^T\beta\right\} &= 0\\
2(\mathbf{X}^T\mathbf{X})\beta-2(\mathbf{X}^T\mathbf{y})+2\lambda\beta &= 0\\
(\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})\beta &= (\mathbf{X}^T\mathbf{y})
\end{aligned}
$$

Continued

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$$2(\mathbf{X}^T\mathbf{X})\beta-2(\mathbf{X}^T\mathbf{y})+2\lambda\beta=0$$

$$(\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})\beta=(\mathbf{X}^T\mathbf{y})$$

$$\hat{\beta}^{\text{ridge}}=(\mathbf{X}^T\mathbf{X}+\lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y}$$

Intuition on Ridge

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- The objective function or Ridge regression minimizes both RSS and $\sum \beta^2$, at the same time.

How does RSS look for OLS?

Let's take an example of two dimensions, with no constant.

$$Y = \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

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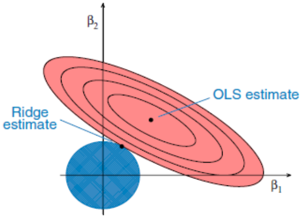
$$\begin{aligned}
\text{PRSS}_{\text{OLS}} &= \sum_{1}^{N} (y_i - \beta_1 x_{1i} - \beta_2 x_{2i})^2 \\
&= \sum_{1}^{N} a\beta_1^2 + b\beta_2^2 + c\beta_1\beta_2 + \text{constant}
\end{aligned}$$

This is how ellipse looks like on a 2 dimension coordinates!

Ridge Plot



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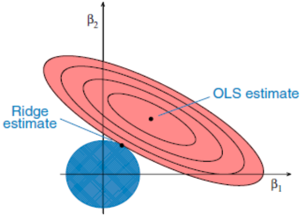

- The ellipses correspond to the contours of residual sum of squares (RSS): the inner ellipse has smaller RSS, and RSS is minimized at ordinal least square (OLS) estimates.

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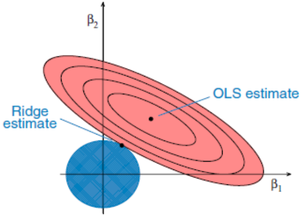

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$$\sum_{j=1}^{p} = \beta_j^2 < C$$

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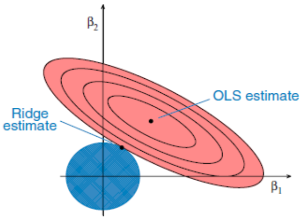

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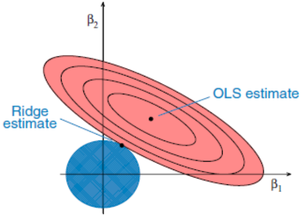

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- We are trying to minimize the ellipse size and circle simultanously in the ridge regression.
- The ridge estimate is given by the point at which the ellipse and the circle touch.

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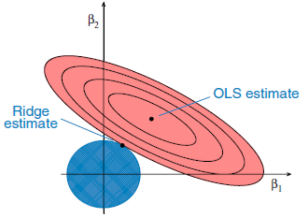

- There is a trade-off between the penalty term and RSS.

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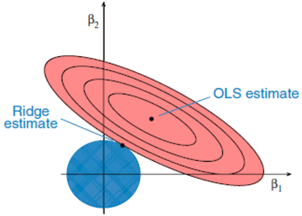

- There is a trade-off between the penalty term and RSS.
- Maybe a large β would give you a better residual sum of squares but then it will push the penalty term higher.

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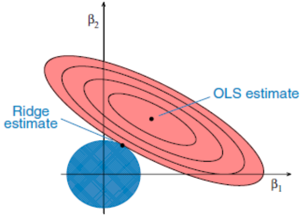

- There is a correspondence between $\frac{1}{\lambda}$ and C.

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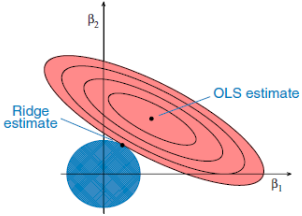

- There is a correspondence between $\frac{1}{\lambda}$ and C.
- The larger the λ is, the more you prefer the β_j's close to zero.

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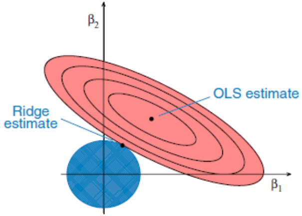

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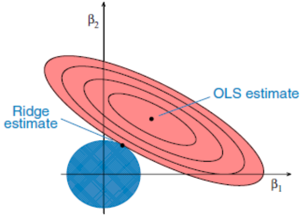

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- And the other extreme as λ approaches infinity, you set all the β's to zero.

Ridge Regression: Another Perspective

Suppose you first transform each $\mathbf{x}_i$ into a more complicated $\mathbf{z}_i$, so that your $\mathbf{X}$ matrix is now a (wider) $\mathbf{Z}$ matrix. You now want to solve for the ridge coefficients β

Ridge Regression: Another Perspective

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Taking the derivative and setting it to zero:

$$0 = \sum_{i=1}^{N} 2(\beta^\top \mathbf{z}_i - y_i)\mathbf{z}_i + 2\lambda\beta$$

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Ridge Regression: Another Perspective

Now let's go back to the objective function and rewrite it.

$$
\begin{aligned}
\text{PRSS}(\lambda) &= (\mathbf{Z}\beta - \mathbf{y})^\top(\mathbf{Z}\beta - \mathbf{y}) + \lambda\beta^\top\beta \\
&= (\beta^\top\mathbf{Z}^\top - \mathbf{y}^\top)(\mathbf{Z}\beta - \mathbf{y}) + \lambda\beta^\top\beta \\
&= \beta^\top\mathbf{Z}^\top\mathbf{Z}\beta - 2\beta^\top\mathbf{Z}^\top\mathbf{y} + \mathbf{y}^\top\mathbf{y} + \lambda\beta^\top\beta \\
&= \left(\gamma^\top\mathbf{Z}\right)\mathbf{Z}^\top\mathbf{Z}\left(\mathbf{Z}^\top\gamma\right) - 2\left(\gamma^\top\mathbf{Z}\right)\mathbf{Z}^\top\mathbf{y} + \mathbf{y}^\top\mathbf{y} + \lambda\left(\gamma^\top\mathbf{Z}\right)\left(\mathbf{Z}^\top\gamma\right)
\end{aligned}
$$

Continued

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Continued

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Taking the derivative w.r.t. γ and setting it to zero:

$$0 = 2\mathbf{K}\mathbf{K}\gamma - 2\mathbf{K}\mathbf{y} + 2\lambda\mathbf{K}\gamma$$
$$\gamma = (\mathbf{K} + \lambda\mathbf{I})^{-1}\,\mathbf{y}$$

and we can plug this back in to find the coefficients of interest, β

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LASSO : Least Absolute Shrinkage and Selection Operator

- Limitations of OLS
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- Lasso
  - The objective:

$$\min_{\beta} \left[\frac{1}{2}(y - X\beta)^T (y - X\beta) + \lambda \sum_{k=1}^{K} \mid \beta_k \mid \right] \tag{1}$$

- The first term in this objective function is the residual sum of a squares.
- The second term has two components: the tuning parameter λ, indexed by sample size, and the penalty term $|\widetilde{\beta}|$.

Lasso with a single covariate

- Take as observed data an outcome Y_i for $i \in \{1, 2, \ldots, N\}$, and a single observed covariate, X_i with associated parameter β^o. We assume the data are generated as

$$Y_i = X_i\beta^o + \epsilon_i$$

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- For simplicity: we scale $\frac{1}{N}\sum_{i=1}^{N} X_i = \frac{1}{N}\sum_{i=1}^{N} Y_i = 0$ and $\sum_{i=1}^{N} X_i^2 = N - 1$, so X_i has sample standard deviation one.

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- We assume the error is mean-zero, equivariant, and that all fourth moments of $[Y_i, X_i]$ exist.

Continued

- Under the setup, we will denote the least squares estimate as

$$\widehat{\beta}^{LS} = \frac{\sum_{i=1}^{N} Y_i X_i}{\sum_{i=1}^{N} X_i^2} = \frac{\sum_{i=1}^{N} Y_i X_i}{N-1}$$

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- Let's consider LASSO in the case with a single covariate.

$$\widehat{\beta}^L = \arg\min_{\widetilde{\beta}} \frac{1}{2} \sum_{i=1}^{N} (Y_i - X_i \widetilde{\beta})^2 + \lambda |\widetilde{\beta}|$$

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Continued

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\beta &= \frac{XY - \lambda}{X^2} \\
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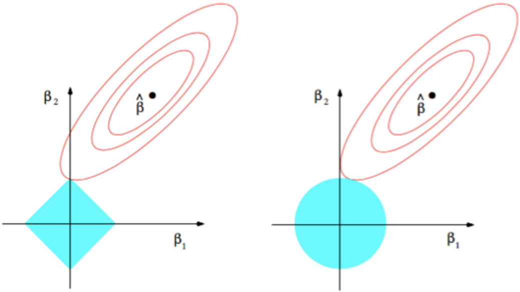
- For those variables with a relatively small OLS coefficient, we shrink them to zero.
- Rest of the variables, we shrink the size.

Lasso Plot

Similarly, Lasso plot consists of a square, because we minimize the RSS and absolute value of coefficients.

Question: Try drawing in R:

$$|\beta_1| + |\beta_2| \leq C$$



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  - Prediction accuracy
  - Interpretation with sparsity

- Disadvantages
  - LASSO won't work when there are a lot of variables that actually matter (ridge works better in that case)
  - With high collinearity, the LASSO arbitrarily selects only one among highly correlated variables (fine if goal is prediction)
  - You will get a completely different coefficient estimate "chosen" by LASSO with a slightly different sample, but predictions will be similar
  - This is why you need to be really careful about interpreting coefficients (remember that LASSO aims to optimally predict out-of-sample)

Statistical Inference with LASSO

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2. Covariance test: Lockhart, Taylor, Tibshirani (2014)
   - p-value for each variable as it is added to lasso model

Oracle Inequality (Optional)

- The single-parameter least squares estimator achieves predictive error

$$E\left\{\frac{1}{N}\sum_{i=1}\left(X_i(\widehat{\beta}^{LS}-\beta^o)\right)^2\right\}=\sigma^2/N.$$

  A LASSO estimator satisfies the Oracle Inequality if it achieves a prediction rate similar to that of the OLS estimator, were the true model known in advance.

- Oracle Inequality in the Single-Parameter Case
  An estimator satisfies the Oracle Inequality if

$$\frac{1}{N}\sum_{i=1}\left(X_i\left(\widehat{\beta}^L(\lambda_N)-\beta^o\right)\right)^2\leq C\frac{\sigma^2}{N}$$

  with a high probability for some constant $C>0$.

- Specifically, an estimator satisfies the Oracle Inequality if we can bound the loss function, with high probability, at a rate going to zero at $1/N$. We next show that if λ_N grows as $\sqrt{N}$, it will satisfiy the Oracle Inequality.
- Oracle Inequaltiy for the LASSO in the Single Parameter Case:

  For $\lambda_N = \sigma \times t \times \sqrt{(N-1)}$, the single-parameter LASSO estimator satistfies the Oracle Inequality

$$\frac{1}{N}\left\{\sum_{i=1}\left(X_i(\widehat{\beta}^L(\lambda_N)-\beta^o)\right)^2+\lambda_N\left|\widehat{\beta}^L(\lambda_N)-\beta^o\right|\right\}\leq\frac{20\sigma^2t^2}{N-1}$$

  with probability at least $1-2\exp\left\{-t^2/2\right\}$.
- Proof as the bonus question for Pset I

Variance and Bias Trade-off

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$$
\begin{aligned}
\text{MSE} &= \mathbf{E}\left((\hat{\beta}-\beta)^2\right) \\
&= \mathbf{E}\left((\underbrace{\hat{\beta}-\mathbf{E}(\hat{\beta})}_{A} + \underbrace{\mathbf{E}(\hat{\beta})-\beta}_{B})^2\right) \\
&= \mathbf{E}\left(A^2 + B^2 + 2AB\right) \\
&= \underbrace{\mathbf{E}\left((\hat{\beta}-\mathbf{E}(\hat{\beta}))^2\right)}_{\text{variance}} + \mathbf{E}\underbrace{\left(\mathbf{E}(\hat{\beta})-\beta)\right)^2}_{\text{bias}^2} + 2\mathbf{E}\left((\hat{\beta}-\mathbf{E}(\hat{\beta}))(\mathbf{E}(\hat{\beta})-\beta)\right)
\end{aligned}
$$

Variance and Bias

- Let's first take a look at the cross term.

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$$
\begin{aligned}
&\mathbf{E}\left((\hat{\beta} - \mathbf{E}(\hat{\beta}))(\mathbf{E}(\hat{\beta}) - \beta)\right) \\
&= \mathbf{E}\left(\hat{\beta}\mathbf{E}(\hat{\beta}) - \mathbf{E}(\hat{\beta})\mathbf{E}(\hat{\beta}) - \hat{\beta}\beta + \mathbf{E}(\hat{\beta})\beta\right) \\
&= \mathbf{E}(\hat{\beta})\mathbf{E}(\hat{\beta}) - \mathbf{E}(\hat{\beta})\mathbf{E}(\hat{\beta}) - \beta\mathbf{E}(\hat{\beta}) + \beta\mathbf{E}(\hat{\beta}) \\
&= 0
\end{aligned}
$$

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&= \underbrace{\mathbf{E}\left((\hat{\beta} - \mathbf{E}(\hat{\beta}))^2\right)}_{\text{variance}} + \underbrace{\left(\mathbf{E}(\hat{\beta}) - \beta\right)^2}_{\text{bias}^2}
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Piecewise Polynomials

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- One option: LASSO and ridge could be used to capture nonlinearities with predefined basis functions (e.g., $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2^2 + \beta_3 X_1 \cdot X_2 + \cdots + \beta_k X_1^k + \epsilon$)

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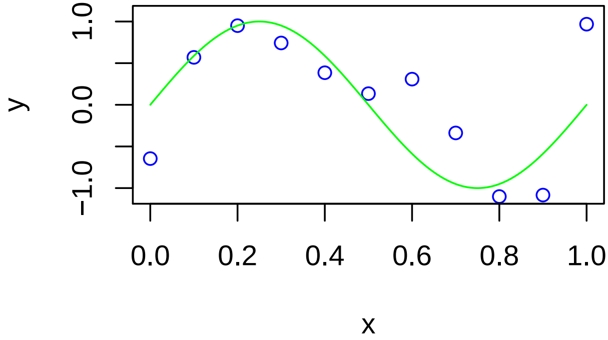
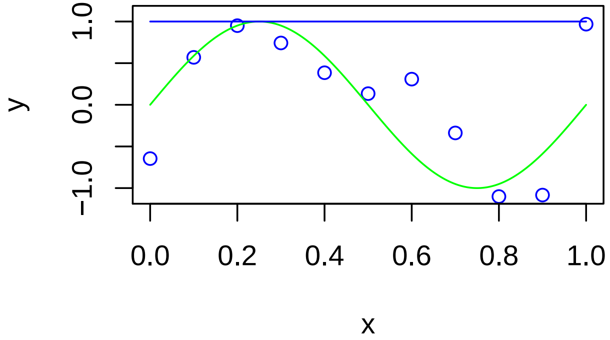
- Here, we consider basic splines
- Other options for capturing nonlinearity include weighted moving average and generalizations (LOESS)

Piecewise Polynomials



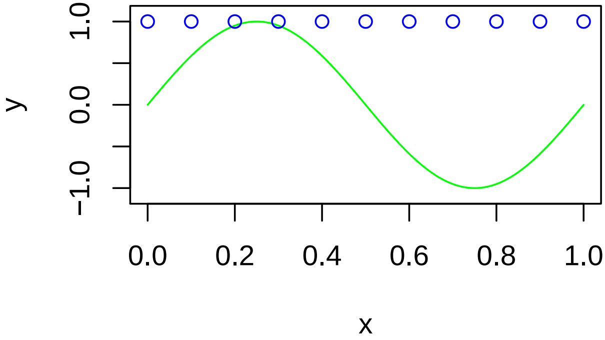
True DGP: $Y_i = \sin(2\pi X_i) + \varepsilon$

Piecewise Polynomials



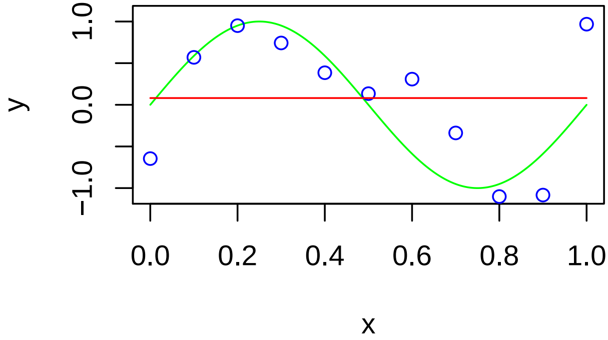
Consider the *constant* basis function $f_1(x) = 1$

Piecewise Polynomials



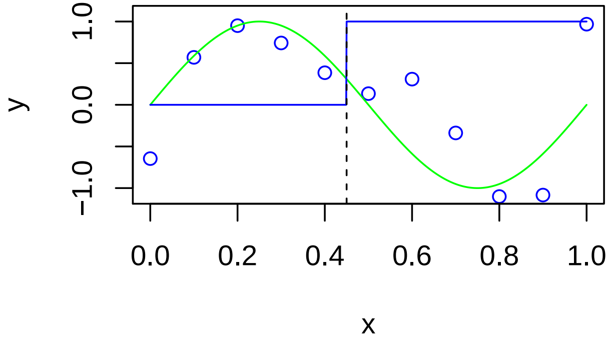
For observation i, this creates a feature $f_1(X_i)$. Prediction performance is not ideal.

Piecewise Polynomials



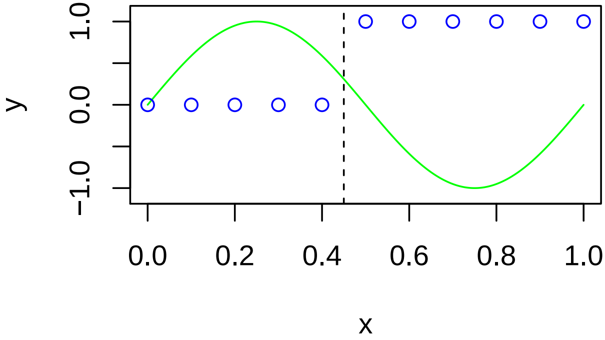
If one were to run a linear regression with $f(x)$ and y, you will get the red line. OLS is confused because $f(x) = 1$ always.

Piecewise Polynomials



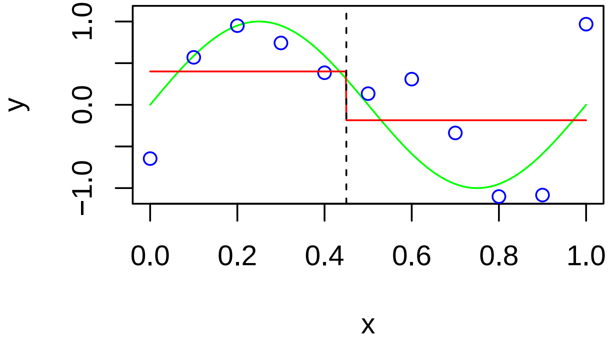
We could add a second *piecewise constant* basis function $f_2(x) = 1(x > \xi)$, with a discontinuity at some *knot*, ξ

Piecewise Polynomials



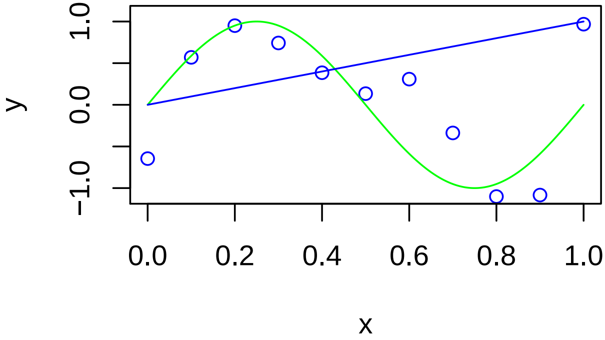
This would produce a second feature in the data matrix, prediction performance is slightly better.

Piecewise Polynomials



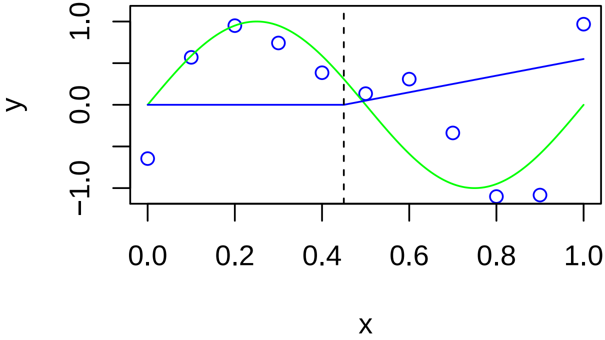
With this expanded basis set, a richer set of approximating functions could be constructed from $\beta_1 f_1(x) + \beta_2 f_2(x)$. The one that minimizes MSE is plotted in red here.

Piecewise Polynomials



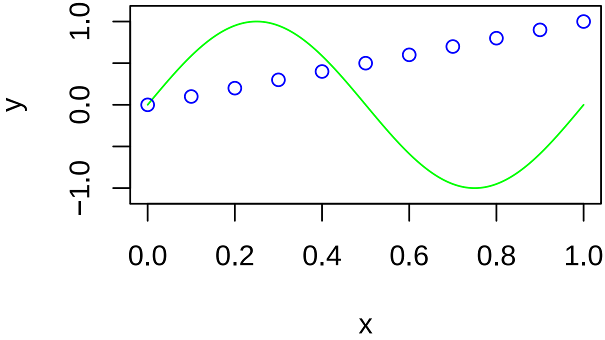
Higher order basis functions can be added, e.g. the linear function $g_1(x) = x$...

Piecewise Polynomials



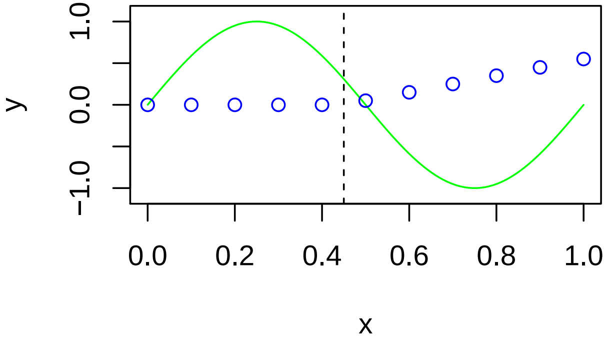
... or the continuous and piecewise linear $g_2(x) = (x - \xi) \cdot 1(x > \xi)$

Piecewise Polynomials



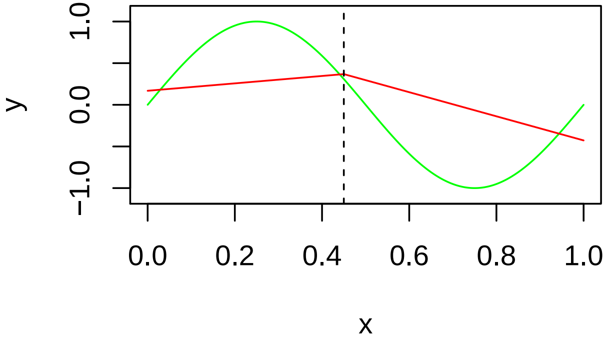
OLS will predict the points like this.

Piecewise Polynomials



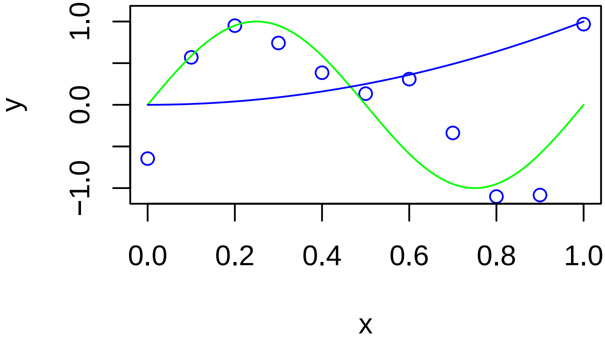
Piecewise function will predict the points like this.

Piecewise Polynomials



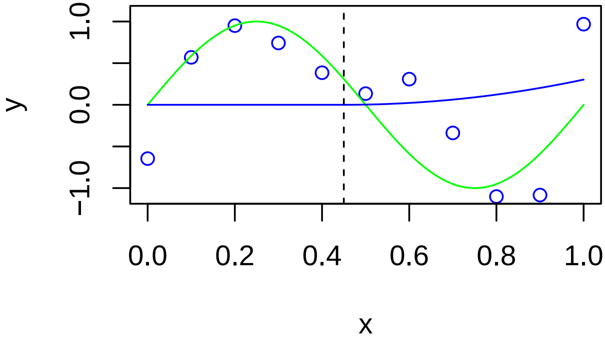
From $f(x) = 1$, $g_1(x) = x$, and $g_2(x) = (x - \xi) \cdot 1(x > \xi)$, many approximating functions of the form $\alpha f(x) + \beta_1 g_1(x) + \beta_2 g_2(x)$ can be constructed for the true conditional expectation—all of which are continuous, but have discontinuous first derivatives.

Piecewise Polynomials



Further basis functions $h_1(x) = x^2$ and $h_2(x) = (x - \xi)^2 \cdot 1(x > \xi)$ and the corresponding features

Piecewise Polynomials



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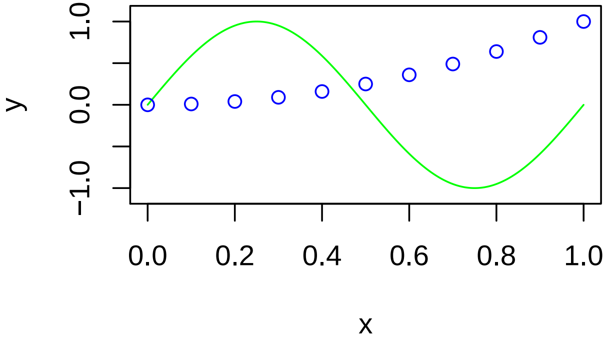

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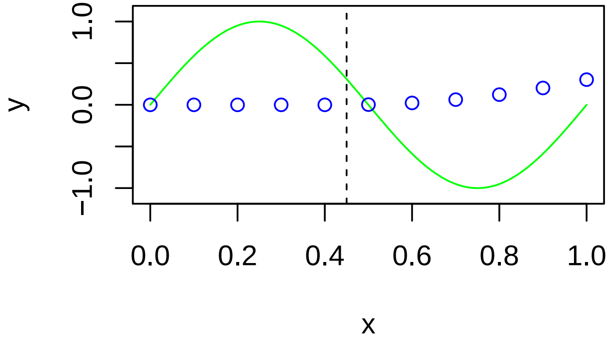

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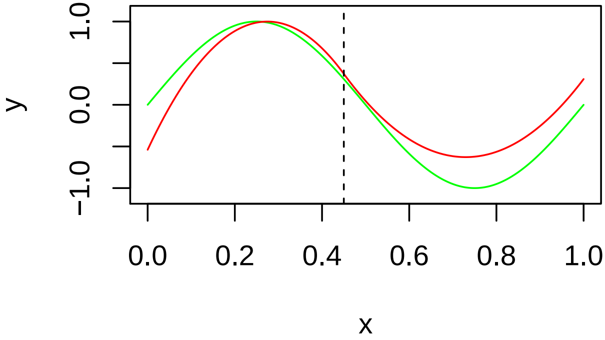

An function of the form $\alpha f(x) + \beta g(x) + \gamma_1 h_1(x) + \gamma_2 h_2(x)$. Observe that it is both continuous and has a continuous first derivative.

Cubic Splines

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  - The basis set consists of $f_0(x) = x^0$, $f_1(x) = x^1$, $f_2(x) = x^2$, and piecewise cubic terms $f_3(x) = x^3$, $f_k(x) = (x - \xi_k)^3 1(x > \xi_k)$, $\cdots$

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- *Natural* cubic splines force the outermost regions to be linear

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  - The basis set consists of $f_0(x) = x^0$, $f_1(x) = x^1$, $f_2(x) = x^2$, and piecewise cubic terms $f_3(x) = x^3$, $f_k(x) = (x - \xi_k)^3 1(x > \xi_k)$, $\cdots$
  - Many knots can be used: spaced equally, at quantiles of X, etc.
- *Natural* cubic splines force the outermost regions to be linear

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  - Many knots can be used: spaced equally, at quantiles of X, etc.
- *Natural* cubic splines force the outermost regions to be linear (reduces overfitting near the boundary, where there are no additional knots to constrain)

Cubic Smoothing Splines

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where z sweeps over all possible values that X_i can take on (what happens to this integral outside the outermost knots?)