Prediction

Utrecht University Winter School: Regression in R

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Outline

Prediction

So far, we've focused primarily on inferences about the estimated regression coefficients.

- Asking questions about how $\mathbf{X}$ is related to Y

We can also use linear regression for *prediction*.

- Given a new observation, X_m, what outcome value, $\hat{Y}_m$, does our model attribute to the mth observation?

Prediction Example

To fix ideas, let's reconsider the *diabetes* data and the following model:

$$Y_{LDL} = \beta_0 + \beta_1 X_{BP} + \beta_2 X_{gluc} + \beta_3 X_{BMI} + \varepsilon$$

Training this model on the first $N = 400$ patients' data produces the following fitted model:

$$\hat{Y}_{LDL} = 22.135 + 0.089 X_{BP} + 0.498 X_{gluc} + 1.48 X_{BMI}$$

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$$\hat{Y}_{LDL} = 22.135 + 0.089 X_{BP} + 0.498 X_{gluc} + 1.48 X_{BMI}$$

Suppose a new patient presents with $BP = 121$, $gluc = 89$, and $BMI = 30.6$. We can predict their LDL score by:

$$\begin{aligned} \hat{Y}_{LDL} &= 22.135 + 0.089(121) + 0.498(89) + 1.48(30.6) \\ &= 122.463 \end{aligned}$$

Prediction with Centered X Variables

Suppose we fit the preceding model with BP centered at 90, $gluc$ centered at 100, and BMI centered at 30.

- We'd get the following fitted model:

$$\hat{Y}_{LDL} = 124.289 + 0.089X_{BP.90} + 0.498X_{gluc.100} + 1.48X_{BMI.30}$$

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Now, let's generate predictions for our patient with $BP = 121$, $gluc = 89$, and $BMI = 30.6$:

$$\begin{aligned}\hat{Y}_{LDL} &= 124.289 + 0.089(121) + 0.498(89) + 1.48(30.6) \\ &= 224.617\end{aligned}$$

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To get the correct prediction, we need to plug-in the centered X values:

$$\begin{aligned}\hat{Y}_{LDL} &= 124.289 + 0.089(121 - 90) + 0.498(89 - 100) + 1.48(30.6 - 30) \\ &= 122.463\end{aligned}$$

Interval Estimates for Prediction

To quantify uncertainty in our predictions, we want to use an appropriate interval estimate.

- Two flavors of interval are applicable to predictions:
  1. Confidence intervals for $\hat{Y}$
  2. Prediction intervals for a specific observation

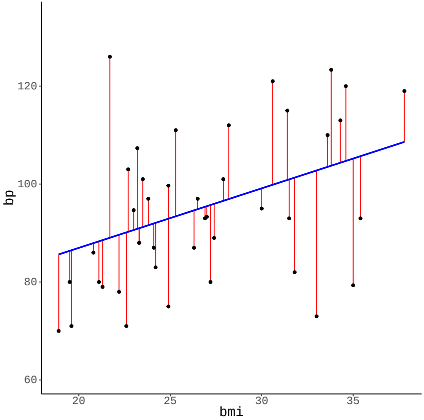
- CIs for $\hat{Y}$ give a likely range (in the sense of coverage probability and "confidence") for the true conditional mean of Y, $\mu_{Y|X^*}$.
  - They only account for uncertainty in the estimated regression coefficients, $\{\hat{\beta}_0, \hat{\beta}_p\}$.

- Prediction intervals give a likely range (in the same sense as CIs) for future outcome values, Y^*.
  - They also account for the regression errors, ε.

Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

$$Y_{BP} = \hat{\beta}_0 + \hat{\beta}_1 X_{BMI} + \hat{\varepsilon}$$

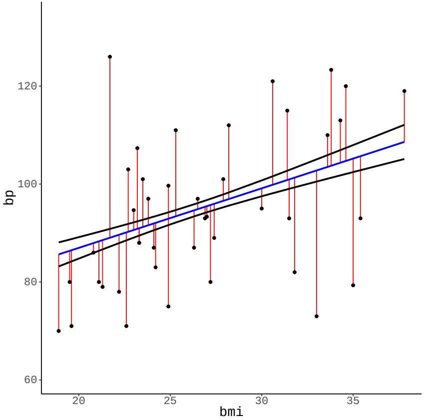


Confidence vs. Prediction Intervals

Let's visualize the predictions from a simple model:

$$Y_{BP} = \hat{\beta}_0 + \hat{\beta}_1 X_{BMI} + \hat{\varepsilon}$$

- CIs for $\hat{Y}$ ignore the errors, ε.
    - They only care about the best-fit line, $\beta_0 + \beta_1 X_{BMI}$.



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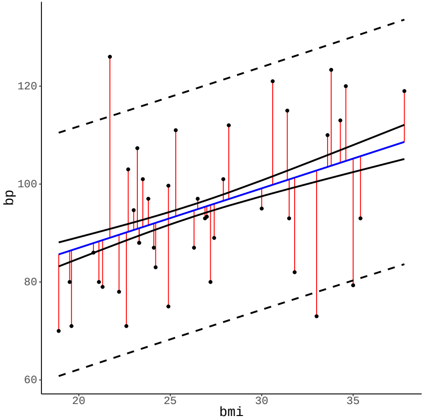
- CIs for $\hat{Y}$ ignore the errors, ε.
  - They only care about the best-fit line, $\beta_0 + \beta_1 X_{BMI}$.
- Prediction intervals are wider than CIs.
  - They account for the additional uncertainty contributed by ε.



Interval Estimates Example

Going back to our hypothetical "new" patient, we get the following 95% interval estimates:

$$95\% CI_{\hat{Y}_{LDL}} = [115.599; 129.327]$$

$$95\% PI = [66.559; 178.368]$$

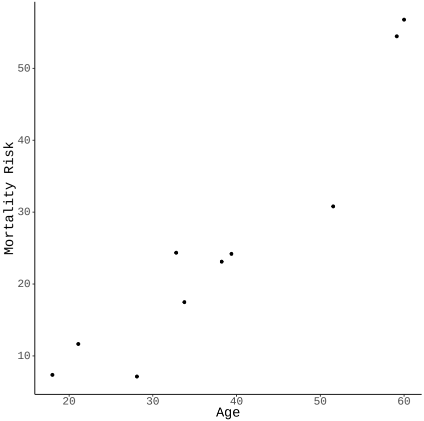
- We can be 95% confident that the average *LDL* of patients with $BP = 121$, $gluc = 89$, and $BMI = 30.6$ will be somewhere between 115.599 and 129.327.

- We can be 95% confident that the *LDL* of a specific patient with $BP = 121$, $gluc = 89$, and $BMI = 30.6$ will be somewhere between 66.559 and 178.368.

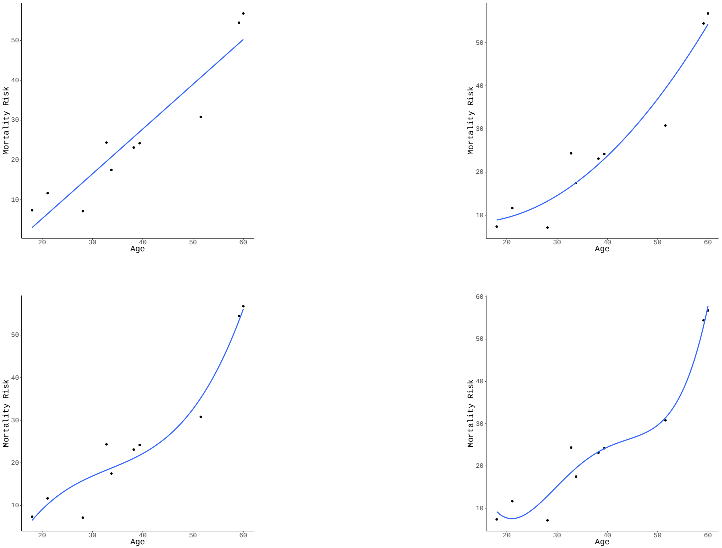
Evaluating Predictive Performance

How do we assess "good" prediction?

- Can we simply find the model that best predicts the data used to train the model?
- What are we trying to do when building a predictive model?
- Can we quantify this objective with some type of fit measure?



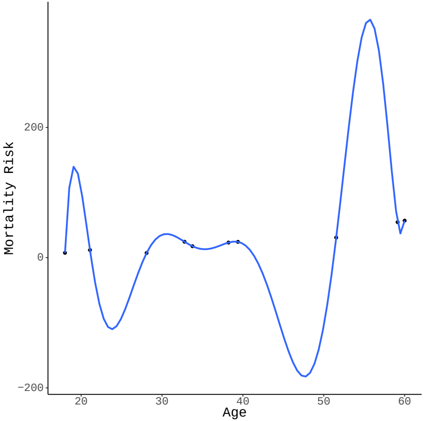
Different Possible Models



Over–fitting

We can easily go too far.

- Enough polynomial terms will exactly replicate any data.
- Is this what we're trying to do?
- What kind of issues arise in the extreme case?



Consequences of Over–fitting

Should we be pleased to be able to perfectly predict mortality risk?

- Is our model useful?
- What happens if we try to apply our fitted model to new data?

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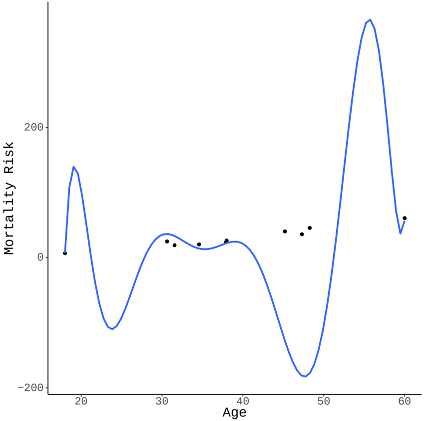
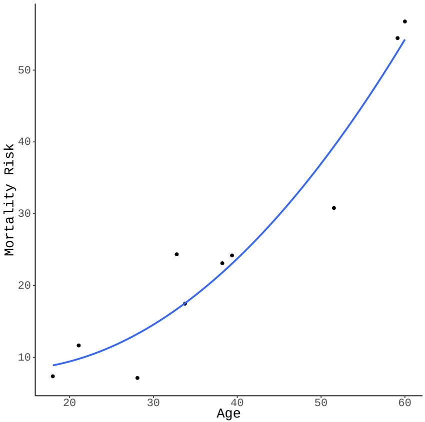
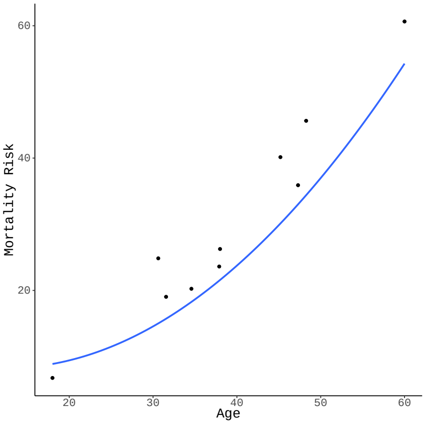


Correct Fit

Let's try something a bit more reasonable.





A Sensible Goal

Our goal is to train a model that can best predict *new data*.

- The predictive performance on the training data is immaterial.
- We can always fit the training data arbitrarily well.
- Fit to the training data will always be at-odds with fit to future data.

This conflict is the driving force behind the *bias-variance trade-off*

Model Fit for Prediction

When assessing predictive performance, we will most often use the *mean squared error* (MSE) as our criterion.

$$
\begin{aligned}
MSE &= \frac{1}{N} \sum_{n=1}^{N} \left(Y_n - \hat{Y}_n \right)^2 \\
&= \frac{1}{N} \sum_{n=1}^{N} \left(Y_n - \hat{\beta}_0 - \sum_{p=1}^{P} \hat{\beta}_p X_{np} \right)^2 \\
&= \frac{RSS}{N}
\end{aligned}
$$

Training vs. Test MSE

The MSE on the preceding slide (i.e., the only MSE we've considered, so far) is computing entirely from training data.

- *Training MSE*

What we want is a measure of fit to new, *testing* data.

- *Test MSE*
- Given M new observations $\{Y_m, X_{m1}, X_{m2}, \ldots, X_{mP}\}$, and a fitted regression model, $f(\mathbf{X})$, defined by the coefficients $\{\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \ldots, \hat{\beta}_P\}$, the *Test MSE* is given by:

$$MSE = \frac{1}{M} \sum_{m=1}^{M} \left(Y_m - \hat{\beta}_0 - \sum_{p=1}^{P} \hat{\beta}_p X_{mp} \right)^2$$

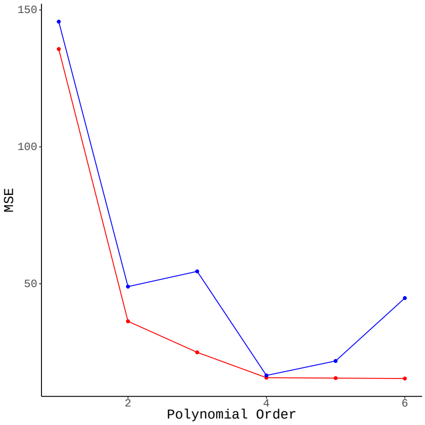
Training vs. Test MSE

Training MSE will always decrease in response to increased model complexity.

- Note the red line in the plot.

Test MSE will reach a minimum at some “optimal” level of model complexity.

- Further complicating the model will increase Test MSE.
- Note the blue line.



Training vs. Testing MSE

At the end of our model building example, we compared the following two models:

$$Y_{BP} = \beta_0 + \beta_1 X_{age} + \beta_2 X_{LDL} + \beta_3 X_{HDL} + \beta_4 X_{BMI} + \varepsilon \quad (1)$$

$$Y_{BP} = \beta_0 + \beta_1 X_{age} + \beta_2 X_{BMI} + \varepsilon \quad (2)$$

- The ΔR^2 test suggested that the loss in fit between Model 1 and Model 2 was trivial.
- The AIC and BIC both suggested that Model 2 should be preferred over Model 1.
- The training MSE values suggested that Model 1 should be preferred.

What happens when we do the comparison based on testing MSE instead of training MSE?

Training vs. Test MSE

```r
set.seed(235711)

## Read in the data:
dataDir <- "../../../data/"
dDat    <- readRDS(paste0(dataDir, "diabetes.rds"))

## Split data into training and testing sets:
ind  <- sample(1 : nrow(dDat))
dat0 <- dDat[ind[1 : 400], ]   # Training data
dat1 <- dDat[ind[401 : 442], ] # Testing data

## Fit the models:
outF <- lm(bp ~ age + bmi + ldl + hdl, data = dat0)
outR <- lm(bp ~ age + bmi, data = dat0)

## Compute training MSEs:
trainMseF <- MSE(y_pred = predict(outF), y_true = dat0$bp)
trainMseR <- MSE(y_pred = predict(outR), y_true = dat0$bp)
```

Training vs. Test MSE

```r
## Compute testing MSEs:
testMseF <- MSE(y_pred = predict(outF, newdata = dat1),
                y_true = dat1$bp)
testMseR <- MSE(y_pred = predict(outR, newdata = dat1),
                y_true = dat1$bp)
```

Compare the two approaches:

	Full	Restricted
Train	147.72	148.44
Test	141.25	138.02

Table: MSE Values

Cross–Validation

To train a model that best predicts new data, we can use *cross-validation* to evaluate the expected predictive performance on new data.

1. Split the sample into two, disjoint sub-samples
    - *Training* data
    - *Testing* data
2. Estimate a candidate model, $f(\mathbf{X})$, on the training data.
3. Check the predictive performance of $\hat{f}(\mathbf{X})$ on the testing data.

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We can use this idea to select the best model from a pool of candidate models, $\mathcal{F} = \{f_1(X), f_2(X), \ldots, f_J(X)\}$

1. Repeat Steps 2 and 3 for all candidate models in $\mathcal{F}$.

2. Pick the $\hat{f}_j(\mathbf{X})$ that best predicts the testing data.

Different Flavors of Cross-Validation

In practice, the split-sample cross-validation procedure describe above can be highly variable.

- The solution is highly sensitive to the way the sample is split because each model is only training once.

Split-sample cross-validation can also be wasteful.

- We don't need to set aside an entire chunk of data for validation.

In most cases, we will want to employ a slightly more complex flavor of cross-validation:

- *K-fold cross-validation*

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1. Partition the data into K disjoint subsets $C_k = C_1, C_2, \ldots, C_K$.

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    - For each training replication, collapse $K - 1$ partitions into a set of training data, and use this training data to estimate the model.
    - Compute the test MSE for the kth partition, MSE_k, by using subset C_k as the test data for the kth fitted model.

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   - Compute the test MSE for the kth partition, MSE_k, by using subset C_k as the test data for the kth fitted model.
3. Compute the overall K-fold cross-validation error as:

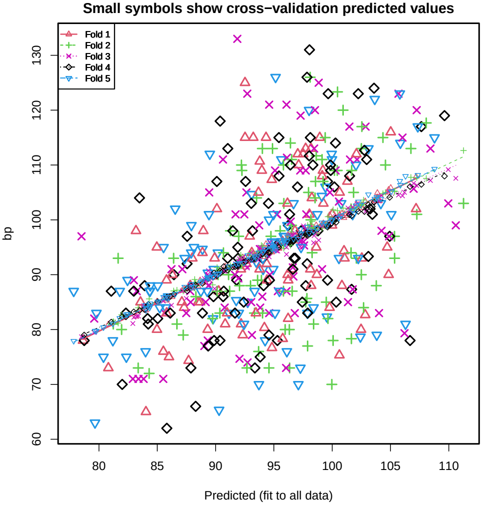
$$CVE = \sum_{k=1}^{K} \frac{N_k}{N} MSE_k,$$

Applying K–Fold CV to our Example

```r
cvOutF <- CVlm(data = diabetes,
               form.lm = outF,
               m = 5,
               printit = FALSE,
               seed = 235711)
```

```r
## Estimated CVE:
attr(cvOutF, "ms")

[1] 150.8718
```



Applying K-Fold CV to our Example

```r
cvOutR <- CVlm(data = diabetes,
               form.lm = outR,
               m = 5,
               printit = FALSE,
               seed = 235711)
```

```r
## Estimated CVE:
attr(cvOutR, "ms")
```

```
[1] 149.6954
```