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Articles - Regression Analysis

Nonlinear Regression Essentials in R: Polynomial and Spline Regression Models

kassambara | *11/03/2018* | *1149* | *Comments (4)* | *Regression Analysis*

In some cases, the true relationship between the outcome and a predictor variable might not be linear.

There are different solutions extending the linear regression model (Chapter @ref(linear-regression)) for capturing these nonlinear effects, including:

- **Polynomial regression**. This is the simple approach to model non-linear relationships. It add polynomial terms or quadratic terms (square, cubes, etc) to a regression.
- **Spline regression**. Fits a smooth curve with a series of polynomial segments. The values delimiting the spline segments are called **Knots**.
- **Generalized additive models** (GAM). Fits spline models with automated selection of knots.

In this chapter, you'll learn how to compute non-linear regression models and how to compare the different models in order to choose the one that fits the best your data.

The RMSE and the R2 metrics, will be used to compare the different models (see Chapter @ref(linear regression)).

Recall that, the RMSE represents the model prediction error, that is the average difference the observed outcome values and the predicted outcome values. The R2 represents the squared correlation between the observed and predicted outcome values. The best model is the model with the lowest RMSE and the highest R2.

Contents:

Loading Required R packages

- `tidyverse` for easy data manipulation and visualization
- `caret` for easy machine learning workflow

```
library(tidyverse)
library(caret)
theme_set(theme_classic())
```

Preparing the data

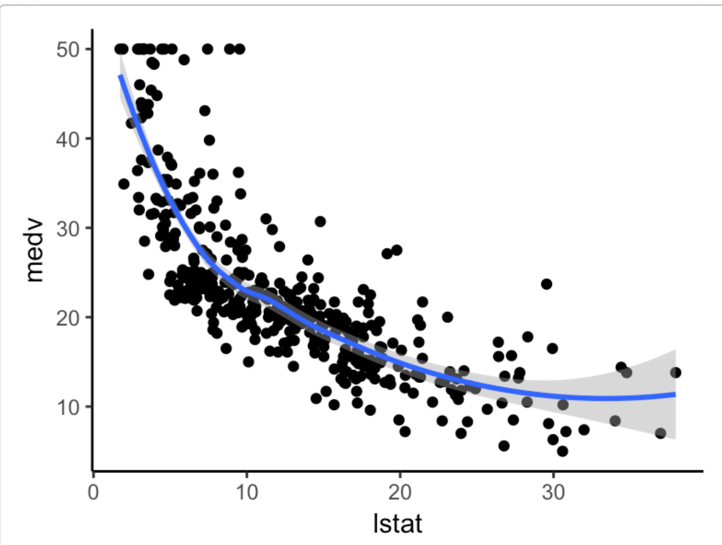
We'll use the `Boston` data set [in `MASS` package], introduced in Chapter @ref(regression-analysis), for predicting the median house value (`mdev`), in Boston Suburbs, based on the predictor variable `lstat` (percentage of lower status of the population).

We'll randomly split the data into training set (80% for building a predictive model) and test set (20% for evaluating the model). Make sure to set seed for reproducibility.

```
# Load the data
data("Boston", package = "MASS")
# Split the data into training and test set
set.seed(123)
training.samples <- Boston$medv %>%
  createDataPartition(p = 0.8, list = FALSE)
train.data  <- Boston[training.samples, ]
test.data <- Boston[-training.samples, ]
```

First, visualize the scatter plot of the `medv` vs `lstat` variables as follow:

```
ggplot(train.data, aes(lstat, medv) ) +
  geom_point() +
  stat_smooth()
```



✔ The above scatter plot suggests a non-linear relationship between the two variables

In the following sections, we start by computing linear and non-linear regression models. Next, we'll compare the different models in order to choose the best one for our data.

Linear regression {linear-reg}

The standard linear regression model equation can be written as `medv = b0 + b1*lstat`.

Compute linear regression model:

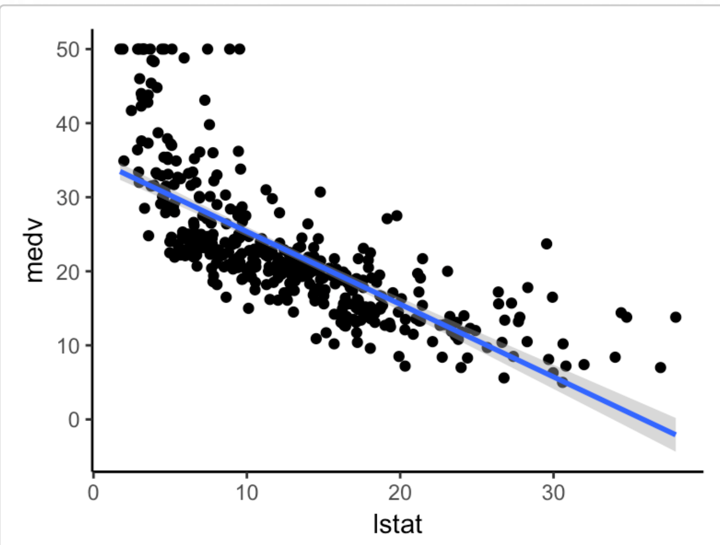
```
# Build the model
model <- lm(medv ~ lstat, data = train.data)
# Make predictions
predictions <- model %>% predict(test.data)
```

```
# Model performance
data.frame(
  RMSE = RMSE(predictions, test.data$medv),
  R2 = R2(predictions, test.data$medv)
)
```

```
##   RMSE    R2
## 1 6.07 0.535
```

Visualize the data:

```
ggplot(train.data, aes(lstat, medv) ) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ x)
```



Polynomial regression

The polynomial regression adds polynomial or quadratic terms to the regression equation as follow:

$$medv = b0 + b1 * lstat + b2 * lstat^2$$

In R, to create a predictor x^2 you should use the function `I()`, as follow: `I(x^2)`. This raise x to the power 2.

The polynomial regression can be computed in R as follow:

```
lm(medv ~ lstat + I(lstat^2), data = train.data)
```

An alternative simple solution is to use this:

```
lm(medv ~ poly(lstat, 2, raw = TRUE), data = train.data)
```

```
##
## Call:
## lm(formula = medv ~ poly(lstat, 2, raw = TRUE), data = train.data)
##
## Coefficients:
##                 (Intercept)  poly(lstat, 2, raw = TRUE)1
##                      43.351                       -2.340
## poly(lstat, 2, raw = TRUE)2
##                       0.043
```

The output contains two coefficients associated with lstat : one for the linear term (lstat^1) and one for the quadratic term (lstat^2).

The following example computes a sixfth-order polynomial fit:

```
lm(medv ~ poly(lstat, 6, raw = TRUE), data = train.data) %>%
  summary()
```

```
##
## Call:
## lm(formula = medv ~ poly(lstat, 6, raw = TRUE), data = train.data)
##
## Residuals:
##    Min     1Q Median     3Q    Max
## -14.23  -3.24  -0.74   2.02  26.50
##
## Coefficients:
##                              Estimate Std. Error t value Pr(>|t|)
## (Intercept)                  7.14e+01   6.00e+00   11.90  < 2e-16 ***
## poly(lstat, 6, raw = TRUE)1 -1.45e+01   3.22e+00   -4.48  9.6e-06 ***
## poly(lstat, 6, raw = TRUE)2  1.87e+00   6.26e-01    2.98    0.003 **
## poly(lstat, 6, raw = TRUE)3 -1.32e-01   5.73e-02   -2.30    0.022 *
## poly(lstat, 6, raw = TRUE)4  4.98e-03   2.66e-03    1.87    0.062 .
## poly(lstat, 6, raw = TRUE)5 -9.56e-05   6.03e-05   -1.58    0.114
## poly(lstat, 6, raw = TRUE)6  7.29e-07   5.30e-07    1.38    0.170
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 5.28 on 400 degrees of freedom
## Multiple R-squared:  0.684,  Adjusted R-squared:  0.679
## F-statistic:  144 on 6 and 400 DF,  p-value: <2e-16
```

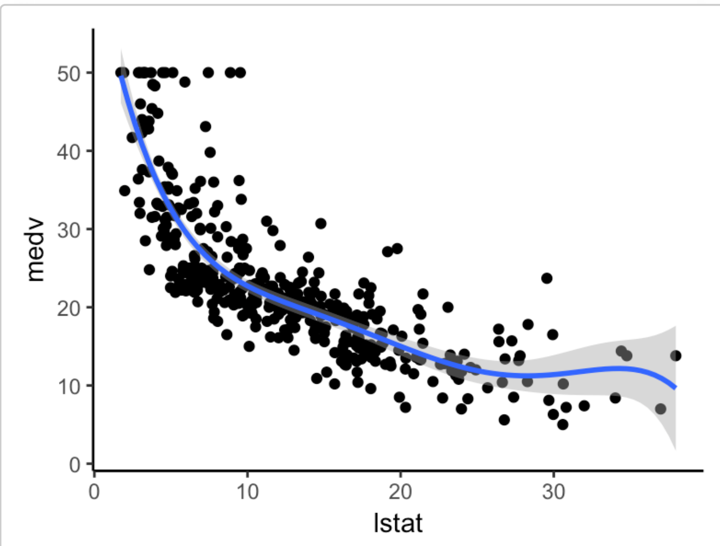
From the output above, it can be seen that polynomial terms beyond the fith order are not significant. So, just create a fith polynomial regression model as follow:

```
# Build the model
model <- lm(medv ~ poly(lstat, 5, raw = TRUE), data = train.data)
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance
data.frame(
  RMSE = RMSE(predictions, test.data$medv),
  R2 = R2(predictions, test.data$medv)
)
```

```
##   RMSE    R2
## 1 4.96 0.689
```

Visualize the fith polynomial regression line as follow:

```
ggplot(train.data, aes(lstat, medv) ) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ poly(x, 5, raw = TRUE))
```



Log transformation

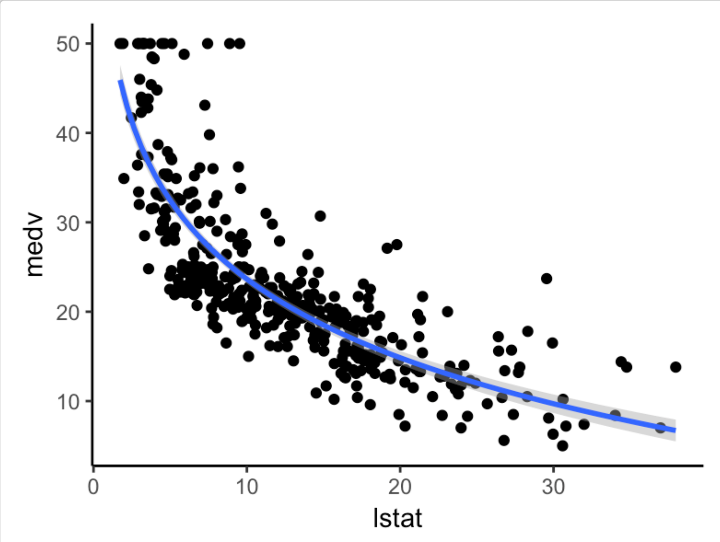
When you have a non-linear relationship, you can also try a logarithm transformation of the predictor variables:

```
# Build the model
model <- lm(medv ~ log(lstat), data = train.data)
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance
data.frame(
  RMSE = RMSE(predictions, test.data$medv),
  R2 = R2(predictions, test.data$medv)
)
```

```
##   RMSE    R2
## 1 5.24 0.657
```

Visualize the data:

```
ggplot(train.data, aes(lstat, medv) ) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ log(x))
```



Spline regression

Polynomial regression only captures a certain amount of curvature in a nonlinear relationship. An alternative, and often superior, approach to modeling nonlinear relationships is to use splines (P. Bruce and Bruce 2017).

Splines provide a way to smoothly interpolate between fixed points, called knots. Polynomial regression is computed between knots. In other words, splines are series of polynomial segments strung together, joining at knots (P. Bruce and Bruce 2017).

The R package `splines` includes the function `bs` for creating a b-spline term in a regression model.

You need to specify two parameters: the degree of the polynomial and the location of the knots. In our example, we'll place the knots at the lower quartile, the median quartile, and the upper quartile:

```
knots <- quantile(train.data$lstat, p = c(0.25, 0.5, 0.75))
```

We'll create a model using a cubic spline (degree = 3):

```
library(splines)
# Build the model
knots <- quantile(train.data$lstat, p = c(0.25, 0.5, 0.75))
model <- lm (medv ~ bs(lstat, knots = knots), data = train.data)
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance
data.frame(
  RMSE = RMSE(predictions, test.data$medv),
```

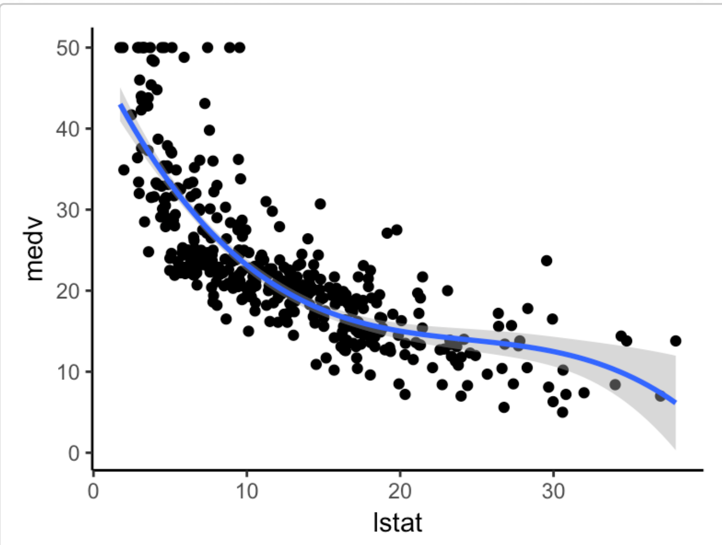
```
  R2 = R2(predictions, test.data$medv)
)
```

```
##   RMSE    R2
## 1 4.97 0.688
```

Note that, the coefficients for a spline term are not interpretable.

Visualize the cubic spline as follow:

```
ggplot(train.data, aes(lstat, medv) ) +
  geom_point() +
  stat_smooth(method = lm, formula = y ~ splines::bs(x, df = 3))
```



Generalized additive models

Once you have detected a non-linear relationship in your data, the polynomial terms may not be flexible enough to capture the relationship, and spline terms require specifying the knots.

Generalized additive models, or GAM, are a technique to automatically fit a spline regression. This can be done using the `mgcv` R package:

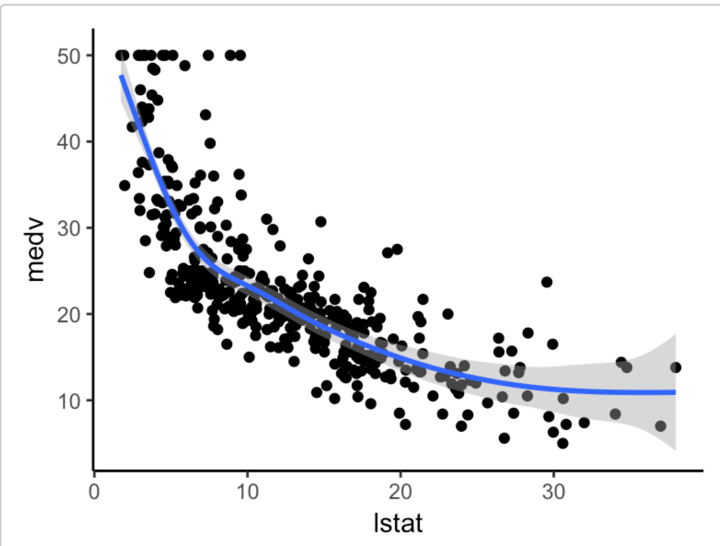
```
library(mgcv)
# Build the model
model <- gam(medv ~ s(lstat), data = train.data)
# Make predictions
predictions <- model %>% predict(test.data)
# Model performance
data.frame(
  RMSE = RMSE(predictions, test.data$medv),
  R2 = R2(predictions, test.data$medv)
)
```

```
##   RMSE    R2
## 1 5.02 0.684
```

The term `s(lstat)` tells the `gam()` function to find the "best" knots for a spline term.

Visualize the data:

```
ggplot(train.data, aes(lstat, medv) ) +
  geom_point() +
  stat_smooth(method = gam, formula = y ~ s(x))
```



Comparing the models

From analyzing the RMSE and the R2 metrics of the different models, it can be seen that the polynomial regression, the spline regression and the generalized additive models outperform the linear regression model and the log transformation approaches.

Discussion

This chapter describes how to compute non-linear regression models using R.

References

Bruce, Peter, and Andrew Bruce. 2017. *Practical Statistics for Data Scientists*. O'Reilly Media.

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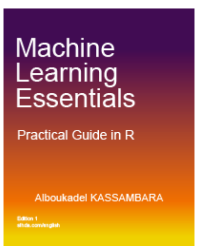

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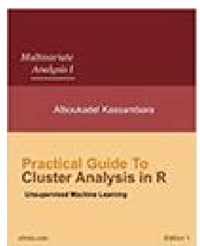

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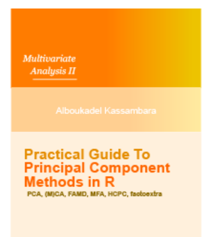

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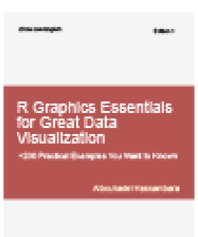

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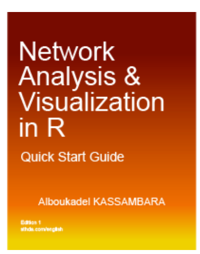

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Visitor 03/23/2018 at 14h33

Visitor

lm(medv ~ lstat + I(lstat^2), data = train.data) and lm(medv ~ poly(lstat, 2), data = train.data) , as it is said that can be used anyways, but the output is different. Why is it so?

#400

kassambara 03/25/2018 at 23h45

Administrator

Hi,

Thank for your comment. The article has been know updated. Please use, the argument raw = TRUE.

Code R : Copy to Clipboard

```
lm(formula = medv ~ poly(lstat, 2, raw = TRUE), data = train.data)
```

#402

tomer mann 05/12/2018 at 17h41

Member

thank you for another informative tutorial.
i have 2 questions:
regarding the question posted by visitor, when you calculate the ^2 polinomial, you use raw=TRUE. but for higher degrees polinomials, such as ^5, this argument is not used. why?and what is the meaning of raw=TRUE?
2. we keep comparing performances of model with predicting them on the test set , but to my understanding, we are not allowed to select models based on test set performances because than the test set becomes part of the training set in a way. is this true? and if so, how do you pick the best model? performance on the training set? other?
thank you!

#464

kassambara 05/19/2018 at 15h13
Administrator

Thank you for your comment.

1)

The article has been know updated to take your comment into account. You should use raw = TRUE, otherwise orthogonal polynomial regressions will be computed instead of the standard polynomial regression. See discussion on stack overflow

2)

When comparing model, the best model is defined as the model with lowest prediction error on a test set that has been not used to train the model.

#488

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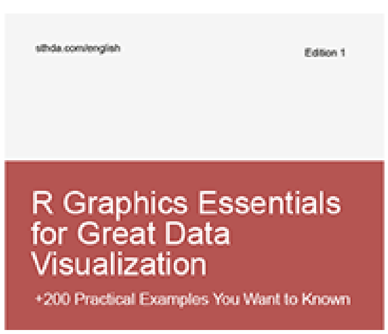

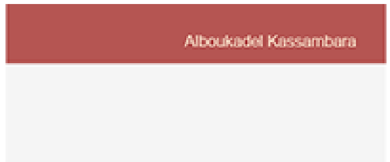

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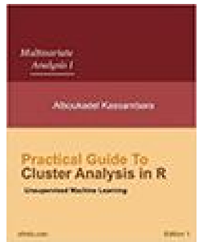

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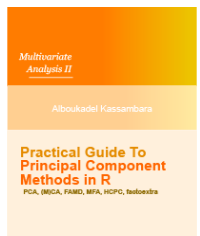

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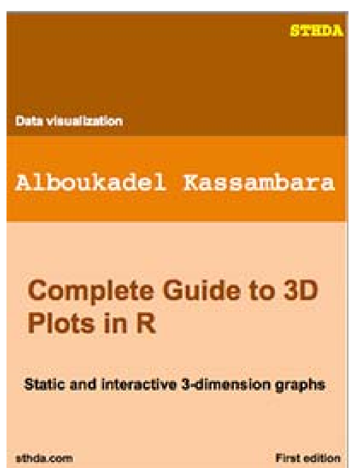

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Thank you, thank you!!!!

Pablo

By Visitor

By *visitor*

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