MA710: Data Mining

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Supervised learning

training set

$$X = \begin{pmatrix} 1.1 & 2.2 \\ 6.7 & 0.5 \\ 2.4 & 9.3 \\ 1.5 & 0.0 \\ 0.5 & 3.5 \\ 5.1 & 9.7 \\ 3.7 & 7.8 \end{pmatrix} \qquad y = \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Target

test set

Categorical target variable (classification)

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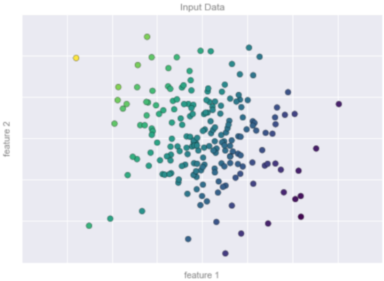
Numerical target variable (regression/prediction)



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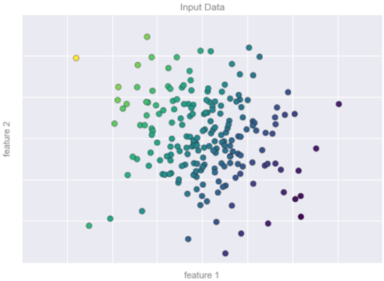
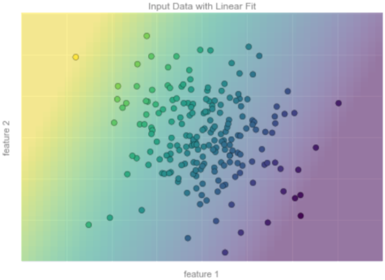
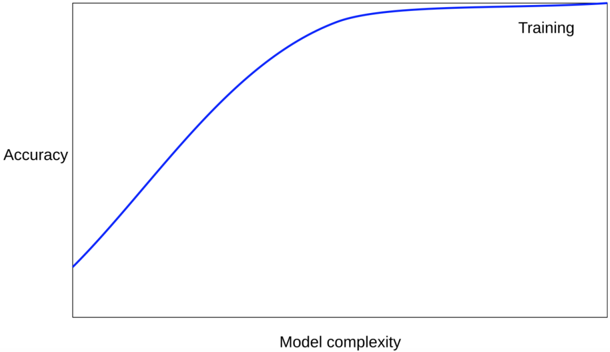




Overfitting and Underfitting



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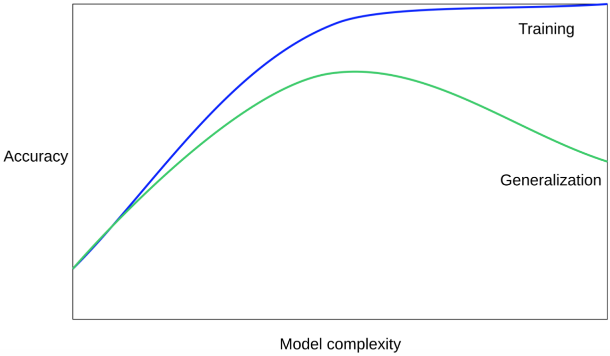

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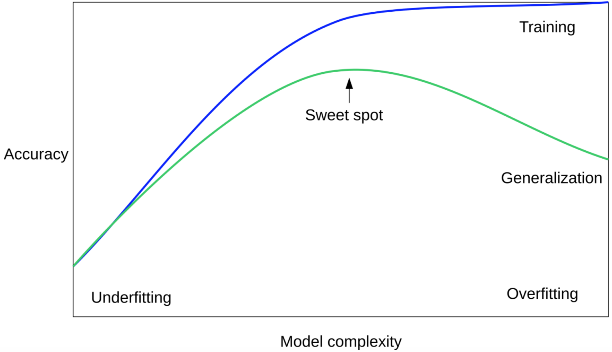
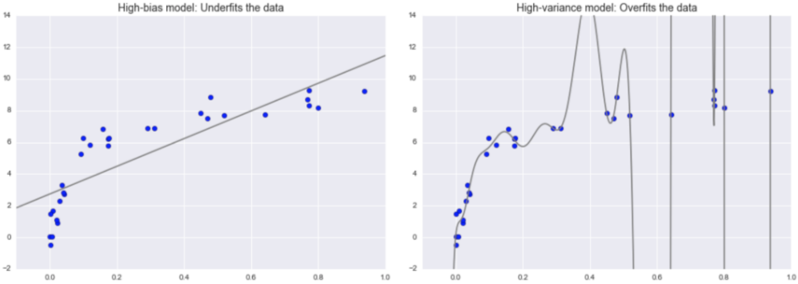
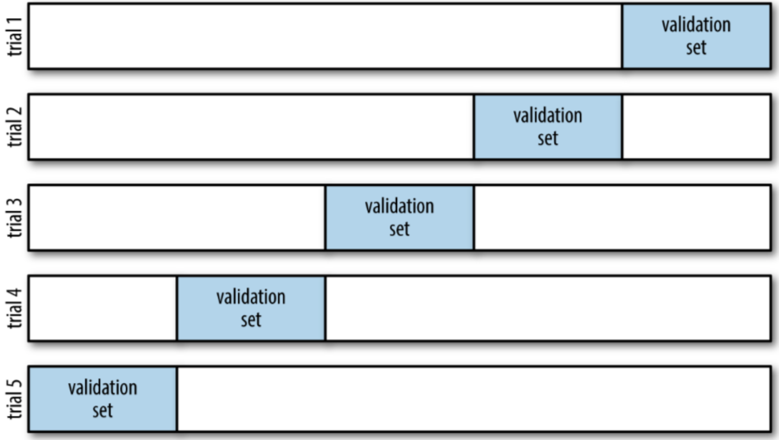
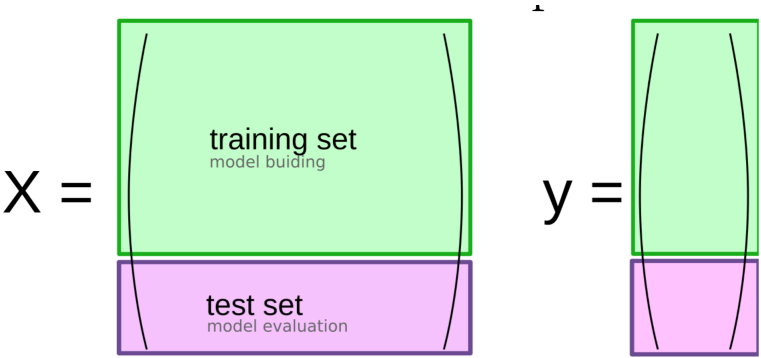



High-bias model: Underfits the data
High-variance model: Overfits the data
14
12
10
8
6
4
2
0
−2
0.0
0.2
0.4
0.6
0.8
1.0


Learning Curve Schematic
training score
validation score
High Variance
Good Fit
model score
training set size

Cross validation

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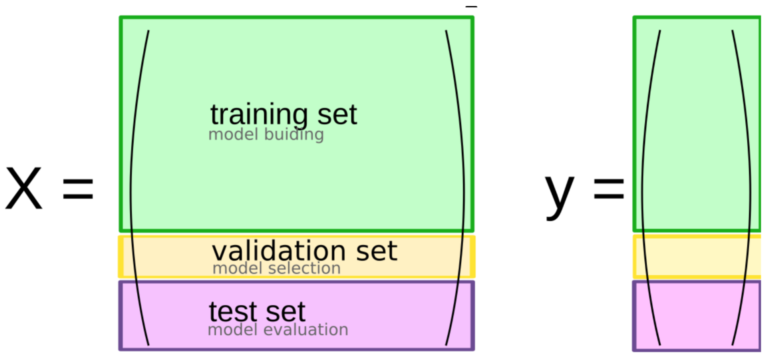
training set
model buiding
test set
model evaluation
y =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training set
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Supervised learning methods

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- very rigid, doesn't work for modeling complicated relations in data

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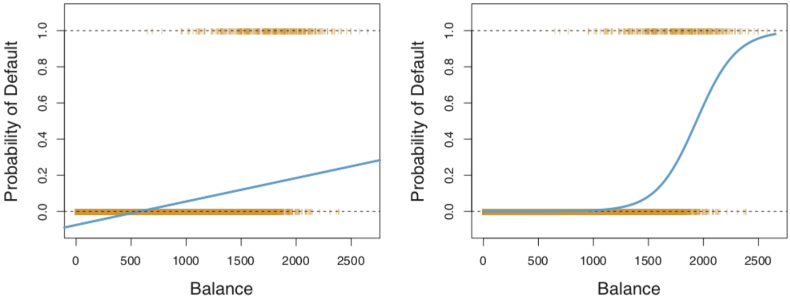
Example (linear regression on left, logistic regression on right):



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- depends on hyperparameter k, an integer

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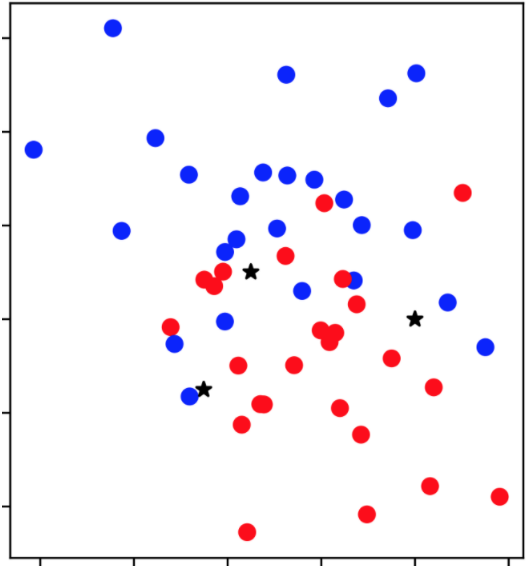

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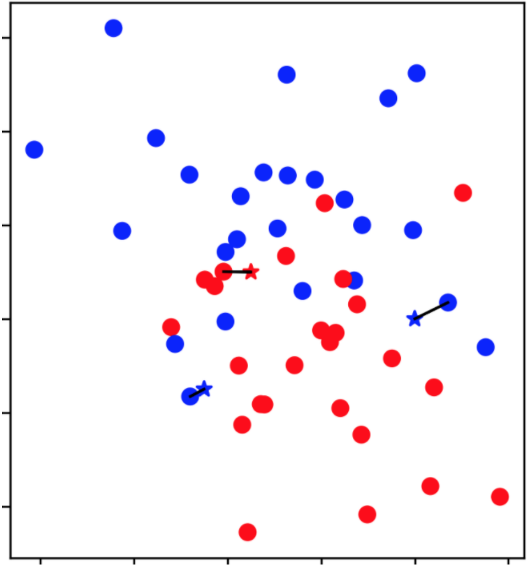

k=1

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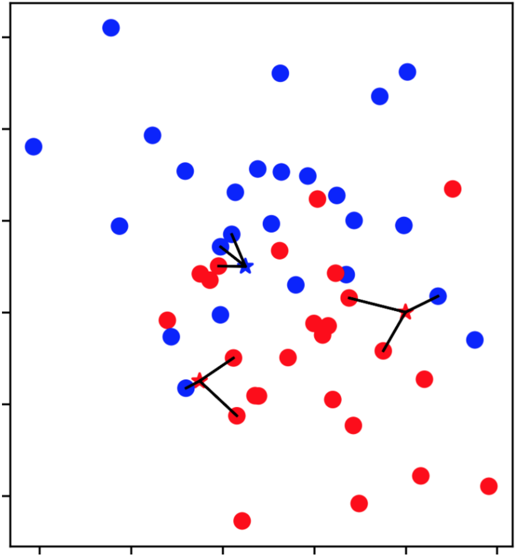

k=3

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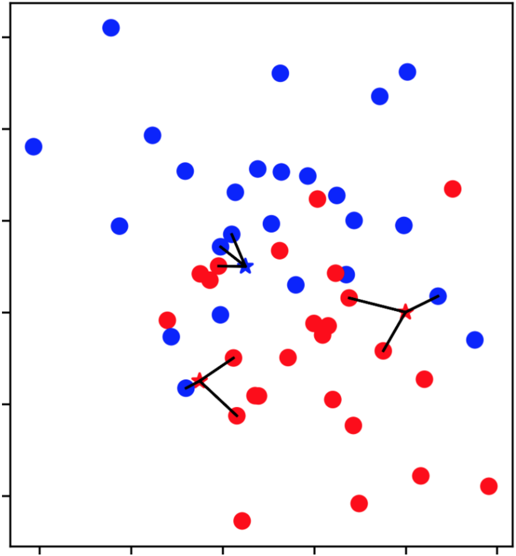

k=3

Smaller *k* value means more local-influenced and complex model (large *k* averages things out more, essentially blurring the data)

Unsupervised learning

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- Cluster analysis
- Dimension reduction (such as PCA)

k-means clustering:

k-means clustering algorithm:

1. Start with k initial clusters (user chooses k).
2. At every step, each record is reassigned to the cluster with the "closest" centroid.
3. Recompute the centroids of clusters that lost or gained a record, and repeat Step 2.

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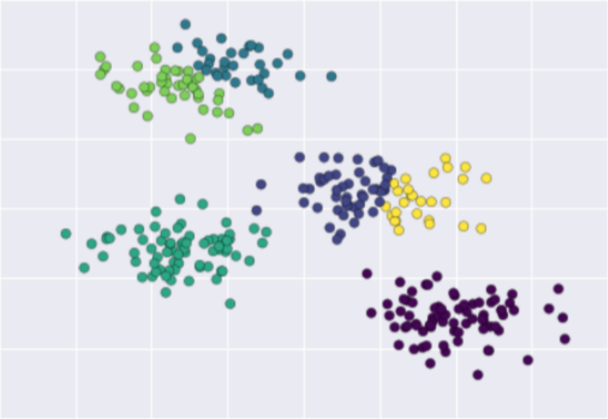
How to choose k? Maybe contextual knowledge, or you can try to interpret the clusters, or you can try an *elbow chart* (such as overall average within-cluster distance), but often it is hard.

Here the number of k was chosen poorly:



Chapter 2.3

Steps in Data Mining

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10. Deploy the model.

Chapter 2.4

```
> housing.df <- read.csv("DMBA-R-datasets/WestRoxbury.csv", header = TRUE)
> dim(housing.df)  # find the dimension of data frame
[1] 5802   14
> head(housing.df)  # show the first six rows
  TOTAL.VALUE  TAX LOT.SQFT YR.BUILT GROSS.AREA LIVING.AREA FLOORS ROOMS BEDROOMS FULL.BATH HALF.BATH KITCHEN FIREPLACE REMODEL
1       344.2 4330     9965     1880       2436        1352      2     6        3         1         1       1         0    None
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Often we'll need to convert categorical variables into binary dummy variables (one-hot encoding):

```
> library(fastDummies)
> new.df <- dummy_cols(housing.df,remove_first_dummy=T,remove_selected_columns=T)
> head(new.df)
  TOTAL.VALUE  TAX LOT.SQFT YR.BUILT GROSS.AREA LIVING.AREA FLOORS ROOMS BEDROOMS FULL.BATH HALF.BATH KITCHEN FIREPLACE REMODEL_Old REMODEL_Recent
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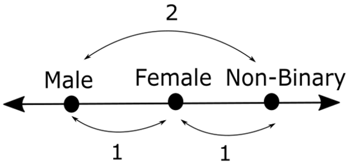

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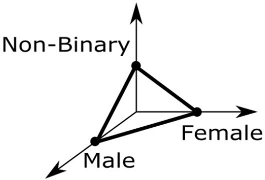

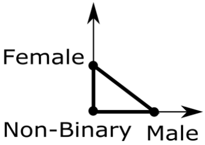

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In R, you normalize with the function `rescale()` from the `scales` package, and you standardize with the function `scale()`.

When normalizing/standardizing, you should compute the translation and scaling factors from the **training** data alone then apply them to the other data sets (to avoid "leakage").

Chapter 2.5

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Chapter 2.6

After we preprocess then partition, we can build a model (supervised learning). Here's an example with linear regression:

Chapter 2.6

Training data:

```
reg <- lm(TOTAL_VALUE ~ ., data = housing.df, subset = train.rows)
tr.res <- data.frame(train.data$TOTAL_VALUE, reg$fitted.values, reg$residuals)
head(tr.res)
```

Partial Output

```
> head(tr.res)
     train.data.TOTAL_VALUE reg.fitted.values reg.residuals
3651                  371.6          371.5818   0.018235205
359                   299.4          299.4014  -0.001431463
1195                  294.5          294.4762   0.023835688
1024                  249.4          249.4029  -0.002874472
3984                  505.5          505.5246  -0.024612237
2227                  410.5          410.5323  -0.032339156
```

Validation data:

```
pred <- predict(reg, newdata = valid.data)
vl.res <- data.frame(valid.data$TOTAL_VALUE, pred, residuals =
          valid.data$TOTAL_VALUE - pred)
head(vl.res)
```

Partial Output

```
> head(vl.res)
   valid.data.TOTAL_VALUE     pred    residuals
1                   344.2 344.2388 -0.038842075
14                  575.0 575.0025 -0.002509638
16                  298.2 298.2107 -0.010697442
17                  313.1 313.0764  0.023567596
18                  344.9 344.8719  0.028111825
19                  330.7 330.7222 -0.022234883
```

Chapter 2.6 and 5.2

Performance metrics:

```
library(forecast)
# compute accuracy on training set
accuracy(reg$fitted.values, train.data$TOTAL_VALUE)

# compute accuracy on prediction set
pred <- predict(reg, newdata = valid.data)
accuracy(pred, valid.data$TOTAL_VALUE)
```

Partial Output

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE         MAE          MPE       MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

> accuracy(pred, valid.data$TOTAL_VALUE)
               ME     RMSE      MAE      MPE     MAPE
Test set 90.86934 161.5043 118.6455 15.14207 24.45668
```

Chapter 2.6 and 5.2

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE        MAE          MPE       MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

> accuracy(pred, valid.data$TOTAL_VALUE)
               ME     RMSE      MAE      MPE     MAPE
Test set 90.86934 161.5043 118.6455 15.14207 24.45668
```

ME: Mean Error

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE        MAE          MPE       MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

> accuracy(pred, valid.data$TOTAL_VALUE)
               ME     RMSE      MAE      MPE     MAPE
Test set 90.86934 161.5043 118.6455 15.14207 24.45668
```

ME: Mean Error

RMSE: Root Mean Squared Error

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE        MAE          MPE        MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

> accuracy(pred, valid.data$TOTAL_VALUE)
               ME     RMSE      MAE      MPE     MAPE
Test set 90.86934 161.5043 118.6455 15.14207 24.45668
```

ME: Mean Error
RMSE: Root Mean Squared Error
MAE: Mean Absolute Error

Chapter 2.6 and 5.2

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE        MAE          MPE       MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

> accuracy(pred, valid.data$TOTAL_VALUE)
               ME     RMSE      MAE      MPE     MAPE
Test set 90.86934 161.5043 118.6455 15.14207 24.45668
```

ME: Mean Error

RMSE: Root Mean Squared Error

MAE: Mean Absolute Error

MPE: Mean Percentage Error

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE        MAE          MPE       MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

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```

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Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

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```

ME: Mean Error
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To see if outliers are playing a role, look at the distribution of the residuals.

```
> accuracy(reg$fitted.values, train.data$TOTAL_VALUE)
                   ME       RMSE        MAE          MPE       MAPE
Test set 1.388101e-16 0.02268016 0.01956465 5.193036e-06 0.00528389

> accuracy(pred, valid.data$TOTAL_VALUE)
               ME     RMSE      MAE      MPE     MAPE
Test set 90.86934 161.5043 118.6455 15.14207 24.45668
```

ME: Mean Error
RMSE: Root Mean Squared Error
MAE: Mean Absolute Error
MPE: Mean Percentage Error
MAPE: Mean Absolute Percentage Error

To see if outliers are playing a role, look at the distribution of the residuals.

Always good to compare a model against the *naive baseline/benchmark*, which for regression is the average value of the target variable across the training data.