Regression 2

Welcome!

Machine Learning | Training and Testing

Overfitting

How do we check that we are not overfitting?

- · Data: labeled instances, e.g. emails marked spam/ham
 - · Training set
 - · Held out set
 - Test set
- Experimentation cycle
 - · Learn parameters (e.g. model probabilities) on training set
 - · Compute accuracy of test set
 - · Very important: never "peek" at the test set!
- Evaluation
 - · Accuracy: fraction of instances predicted correctly
- · Overfitting and generalization
 - · Want a classifier which does well on test data
 - Overfitting: fitting the training data very closely, but not generalizing well

Training Data

Held-Out Data

> Test Data

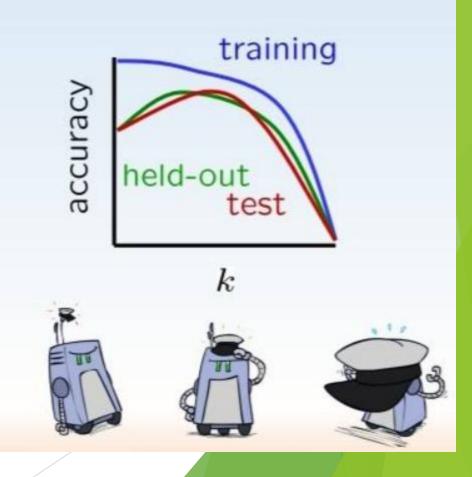


Machine Learning | Training and Testing | Parameter Estimation

Recap | Tuning

Tuning on Held-Out Data

- Now we've got two kinds of unknowns
 - Parameters: the probabilities P(X|Y), P(Y)
 - Hyperparameters: e.g. the amount / type of smoothing to do, k, α
- What should we learn where?
 - Learn parameters from training data
 - Tune hyperparameters on different data
 - · Why?
 - For each value of the hyperparameters, train and test on the held-out data
 - Choose the best value and do a final test on the test data



Mean Squared Error (MSE)

$$\blacktriangleright MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2$$

Root Mean Squared Error (RMSE)

$$\blacktriangleright \text{ RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \widehat{y}_i)^2}$$

Mean Absolute Error (MAE)

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|$$

Mean Absolute Percentage Error (MAPE)

$$MAPE = \frac{100\%}{n} \sum_{i=1}^{n} \left| \frac{y_i - \widehat{y_i}}{y_i} \right|$$

The R² Formula

$$R^{2} = 1 - \frac{\sum_{i=1}^{n} (y_{i} - \widehat{y}_{i})^{2}}{\sum_{i=1}^{n} (y_{i} - \overline{y})^{2}}$$

Adjusted R-squared

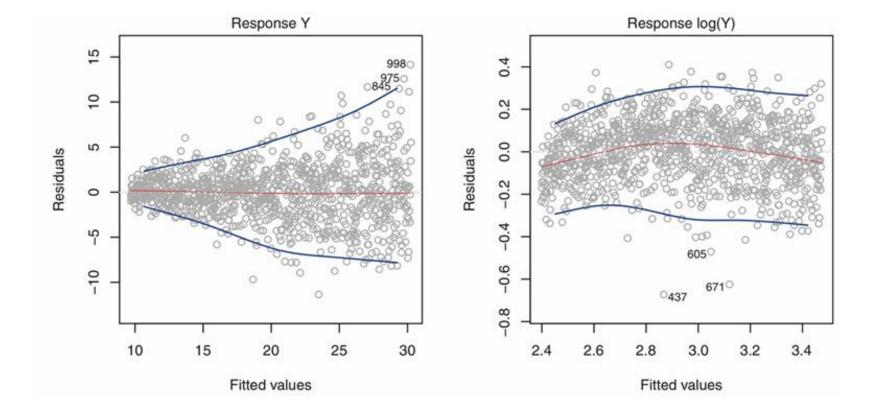
$$\overline{R^2} = 1 - (1 - R^2) \cdot \frac{n - 1}{n - k - 1}$$

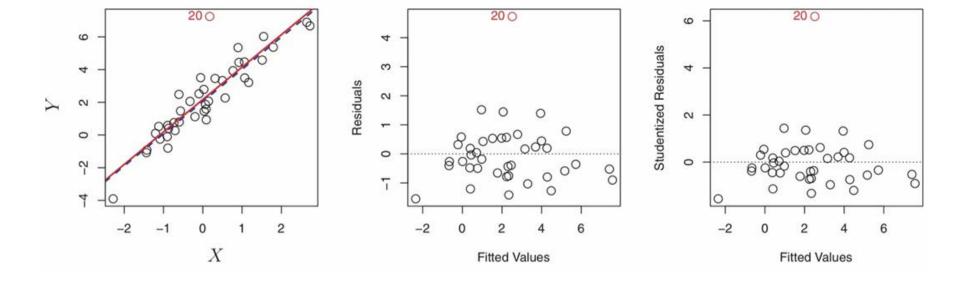
Bayesian Information Criterion (BIC)

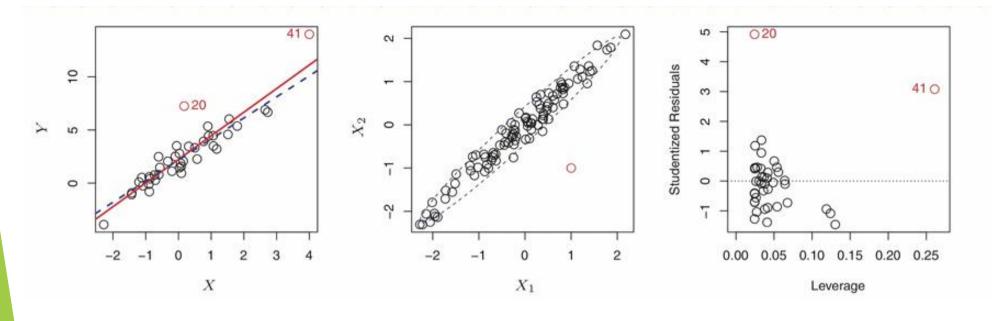
$$\blacktriangleright \quad \text{BIC} = \ln(n) \cdot k - 2\ln(\hat{L})$$

$$\hat{L} = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \hat{y_i})^2}{2\sigma^2}\right)$$

Regression Problems!







Gradient descent

$$w^{(t+1)} = w^{(t)} + \alpha \sum_{i=1}^{n} (y_i - w^{(t)^{\mathsf{T}}} x_i) x_i$$

Code example!

Machine Learning | Neural Network | Training

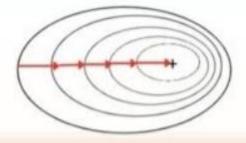
Gradient Descents

Example

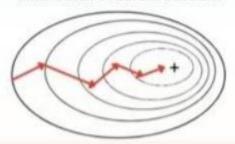
If you have 1000 training examples and are using:

- Batch gradient descent: 1 epoch = 1 iteration (all 1000 examples used for one update)
- Mini-batch gradient descent with batch size 100: 1 epoch = 10 iterations
- Stochastic gradient descent: 1 epoch = 1000 iterations

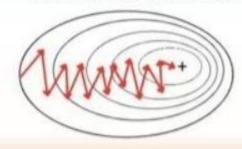
Batch Gradient Descent



Mini-Batch Gradient Descent



Stochastic Gradient Descent



Machine Learning | Neural Network | Training Gradient Descents

Method	Data Used	Speed	Stability	Memory Usage	Convergence
Batch	All data	Slowest	Most stable	Highest	Smooth, deterministic
Stochastic	1 example	Fastest per step	Least stable	Lowest	Noisy, may oscillate
Mini- Batch	Small subset	Fast	Moderate	Moderate	Moderate noise