3. Overfitting

Ludwig Krippahl

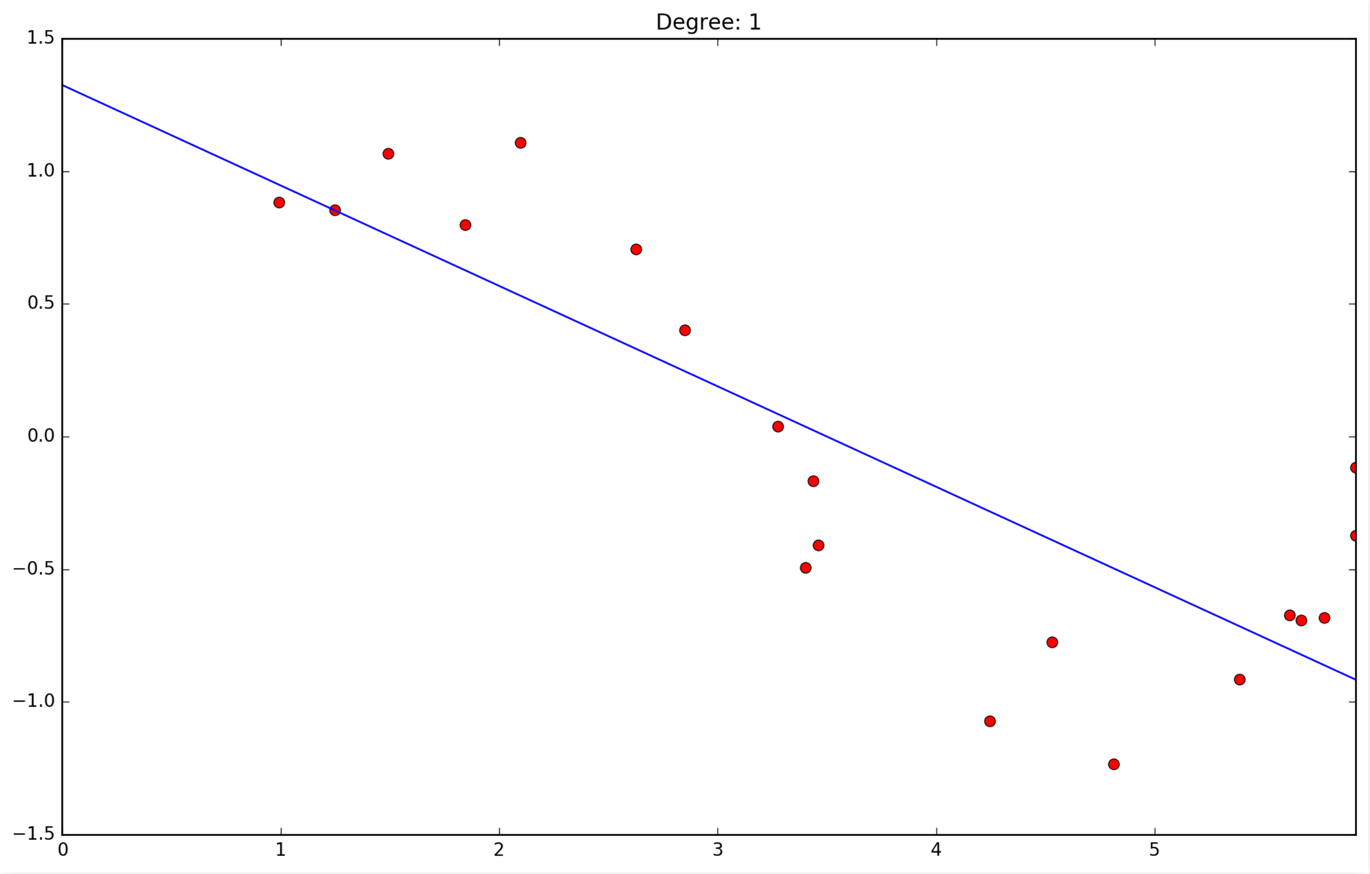
Summary

- Errors
  - How to estimate the true error
- Overfitting and how to avoid it
  - How to select the best model
  - Regularization: reduce overfitting in training

Last Lecture

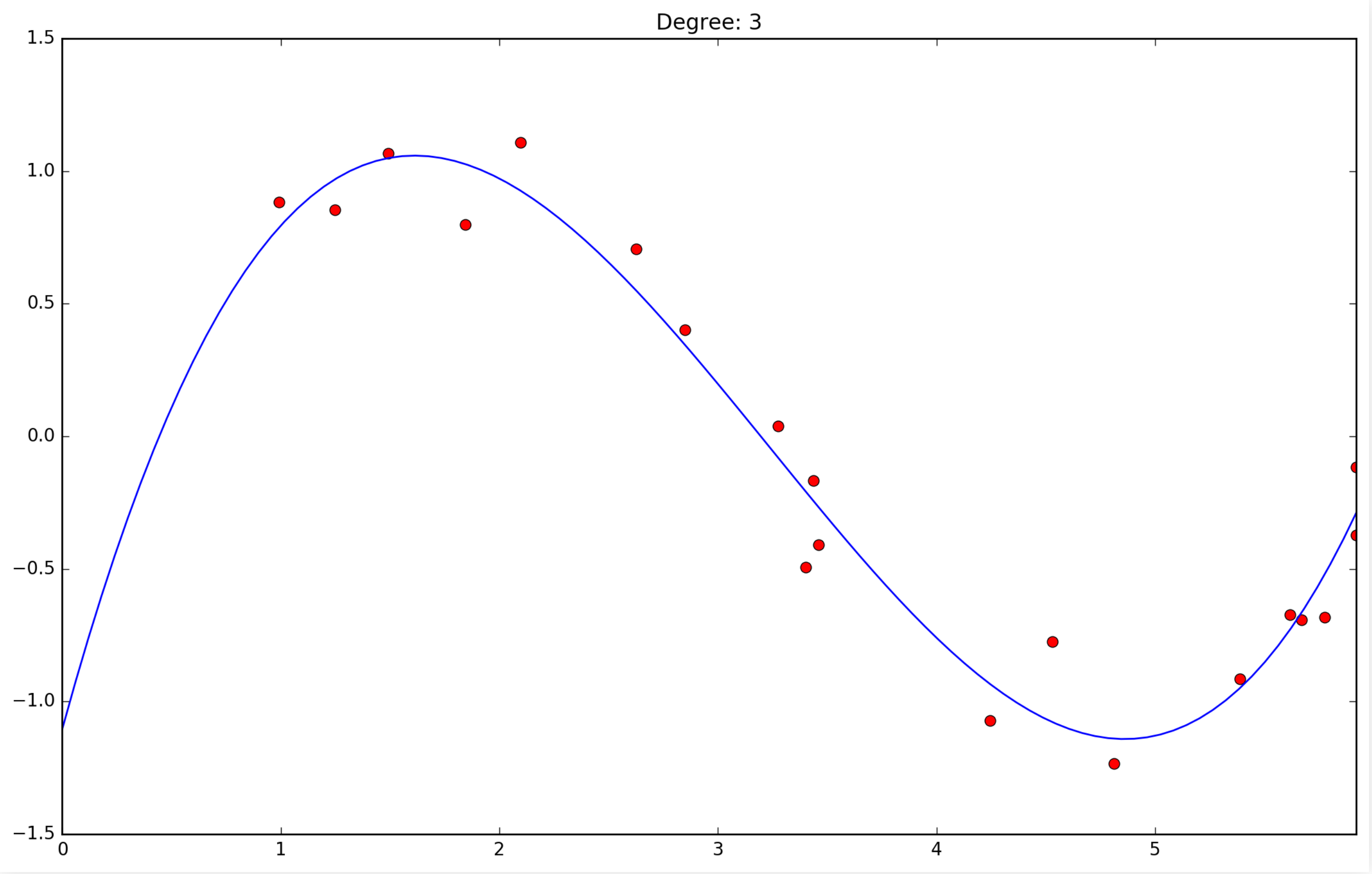
- Model fitting: find hypothesis by optimization
  - (max likelihood, least mean squares in linear regression)
- More powerful models in higher dimensions
  - Nonlinear transformation for new features
- Problem of overfitting:
  - The hypothesis we obtain fits the training data too much
  - Sacrifices performance outside the training data

Last Lecture

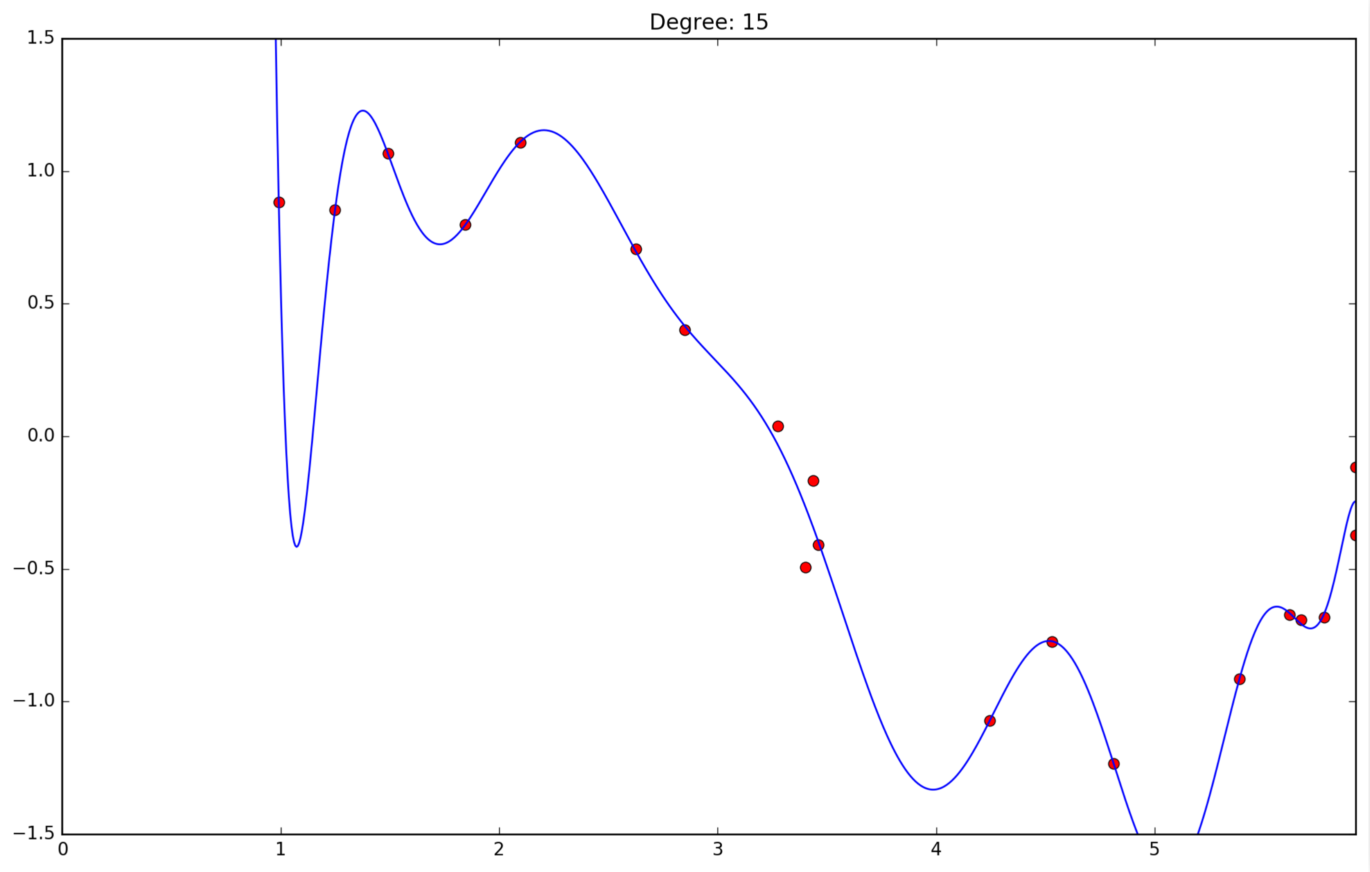


Overfitting

Last Lecture



Last Lecture



Errors

Measuring Errors

- Goal of regression: Find $g(\theta, X) : X \rightarrow Y$ based on $\left\{(x^1, y^1), \ldots, (x^n, y^n)\right\}$ to predict y for any example of $\mathcal{U}$
- Training Error: measured in the training set
- Problem: not a good indicator of the error for new examples

• Training set is used to adjust θ to minimize error

• This makes training error a biased estimate

Problem:

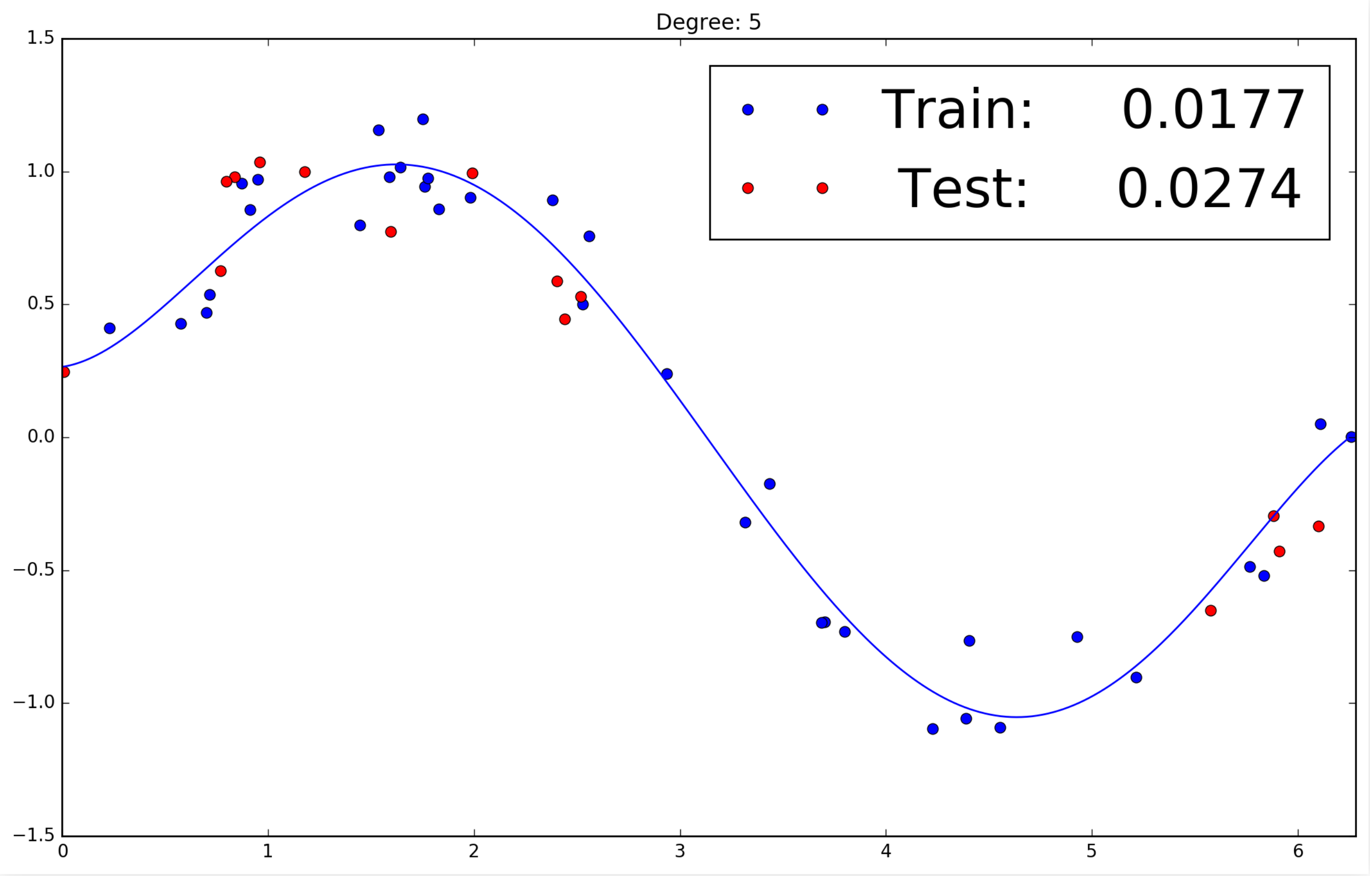
- How to estimate performance for $\mathcal{U}$?

Solution:

- Measure error outside the training set (estimate true error)

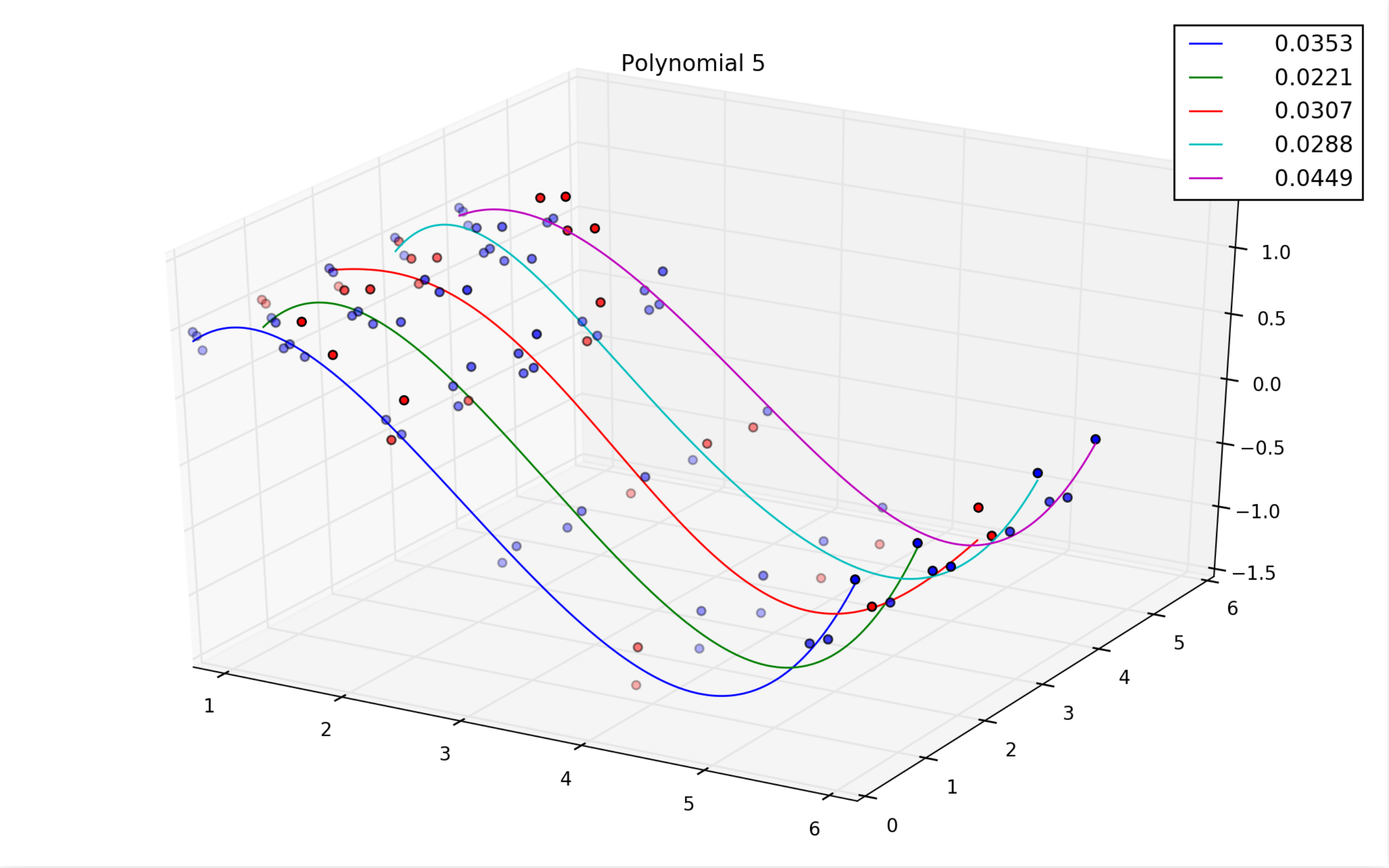
Measure error outside the training set

- Split the data: training set and test set to estimate true error



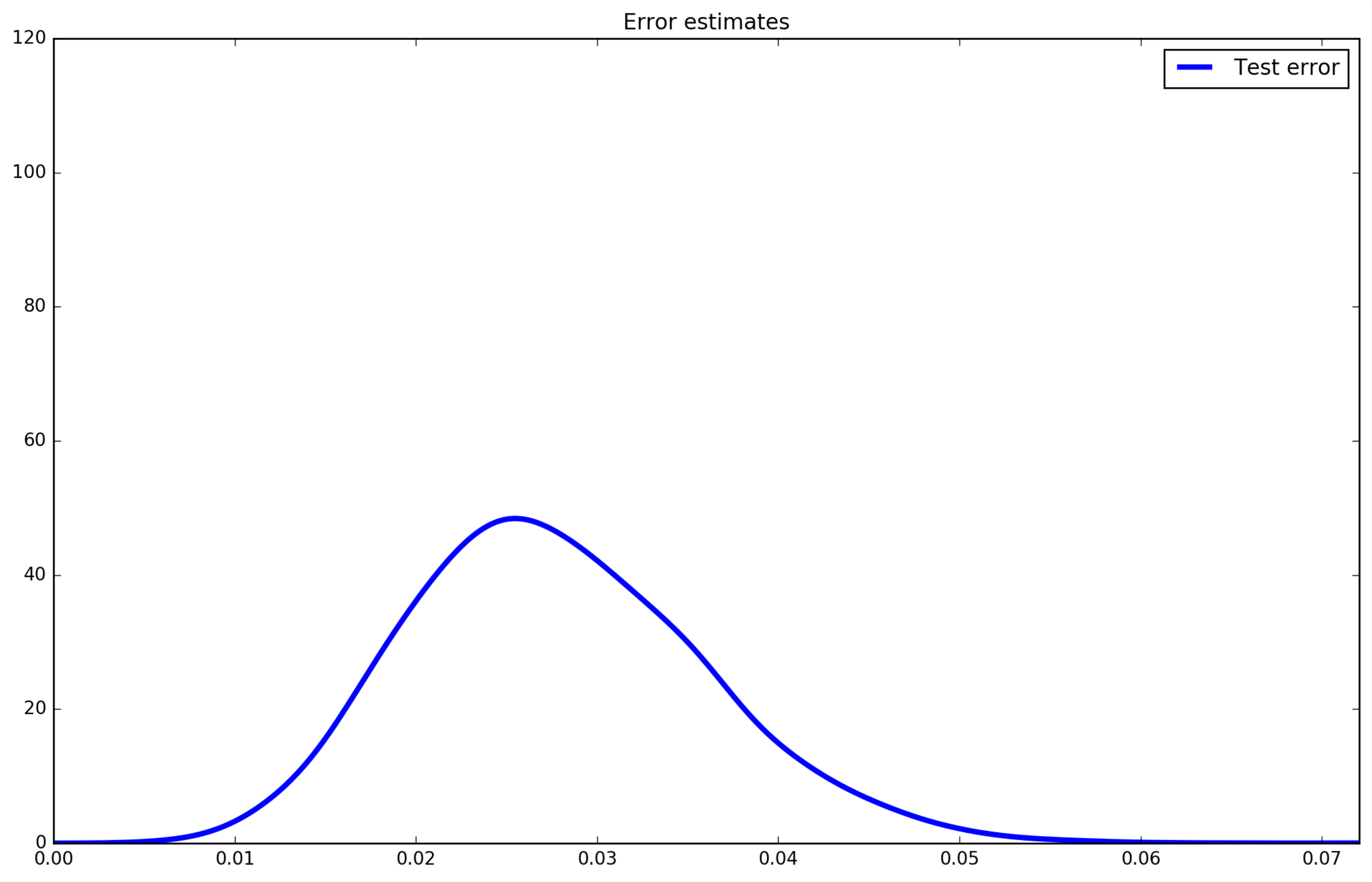
Note: estimate is stochastic.

- We estimate the true error; we cannot measure it



Errors

- The $\boxed{\text{Test Error}}$ is an unbiased $\boxed{\text{estimate}}$ of the $\boxed{\text{True Error}}$



Errors

Measurable Errors

- Training error: error measured in the training data and used to fit the parameters.

- Also Empirical Error or Sample Error

- Test error: error measured on the test data to estimate the true error.

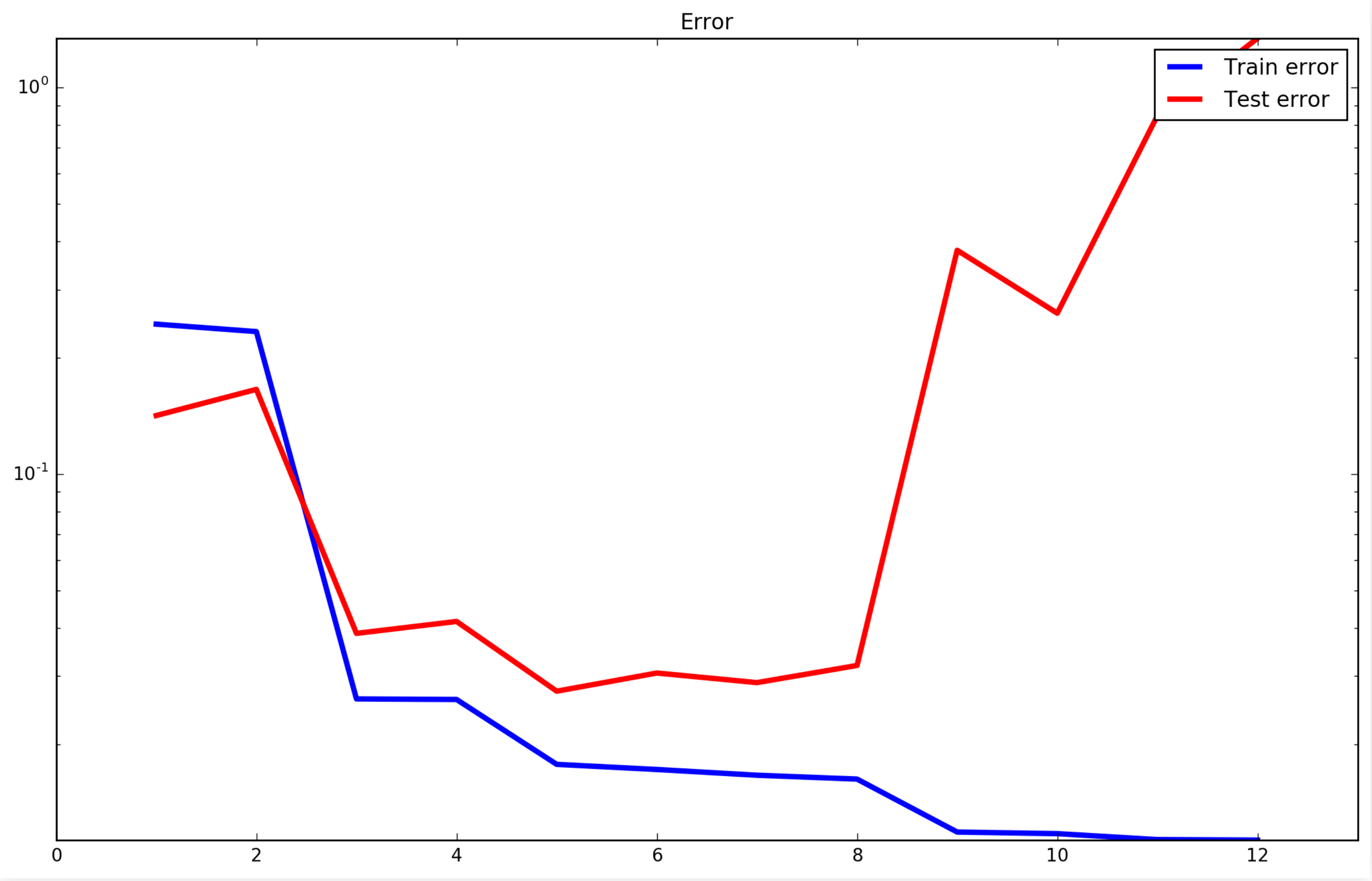
Unmeasurable Errors

- True error: expected error for all $\mathcal{U}$.
- Generalization error: difference between True Error and Training error

Overfitting

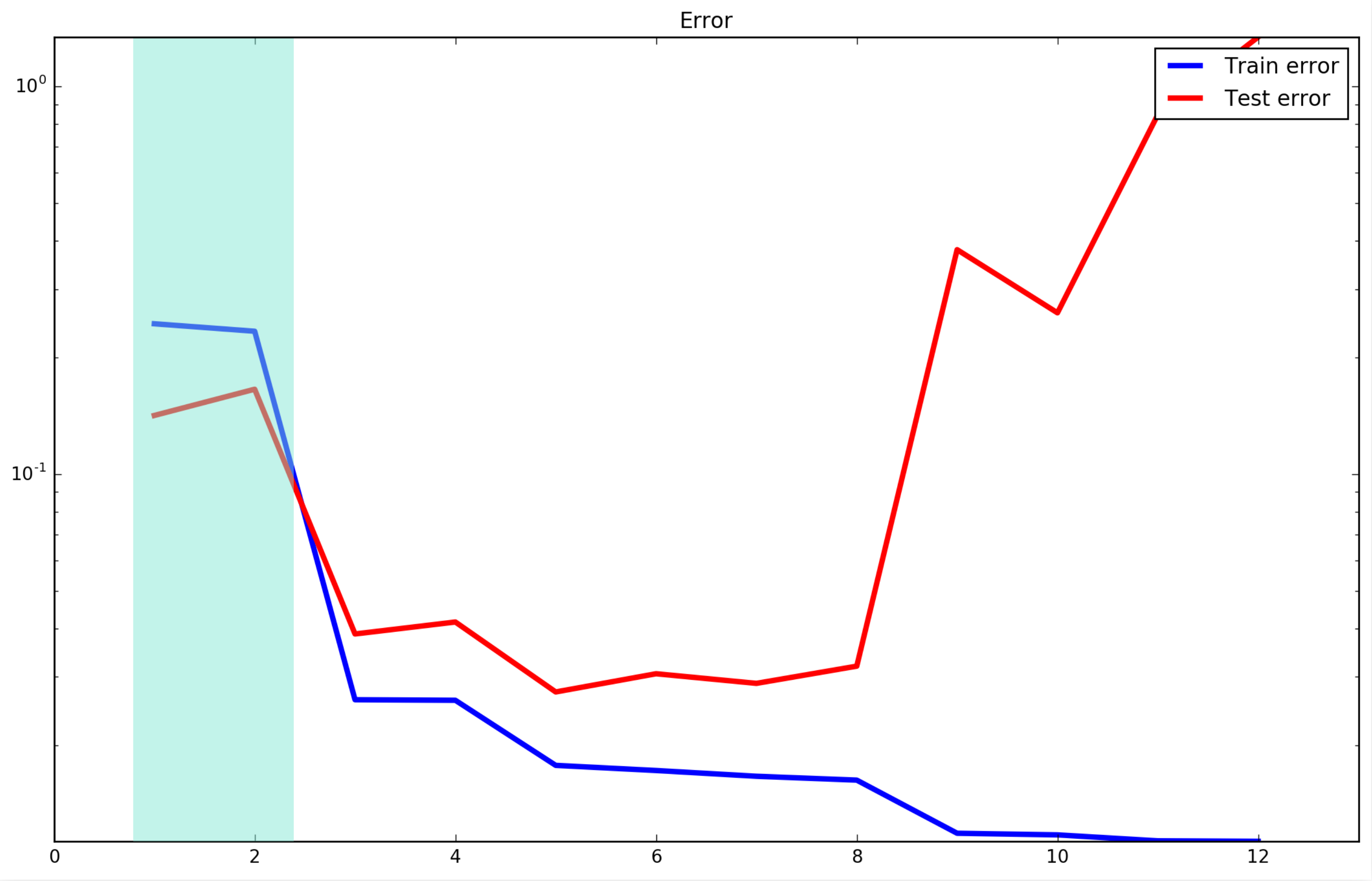
Overfitting

- Increasing power, training error and test error eventually diverge:



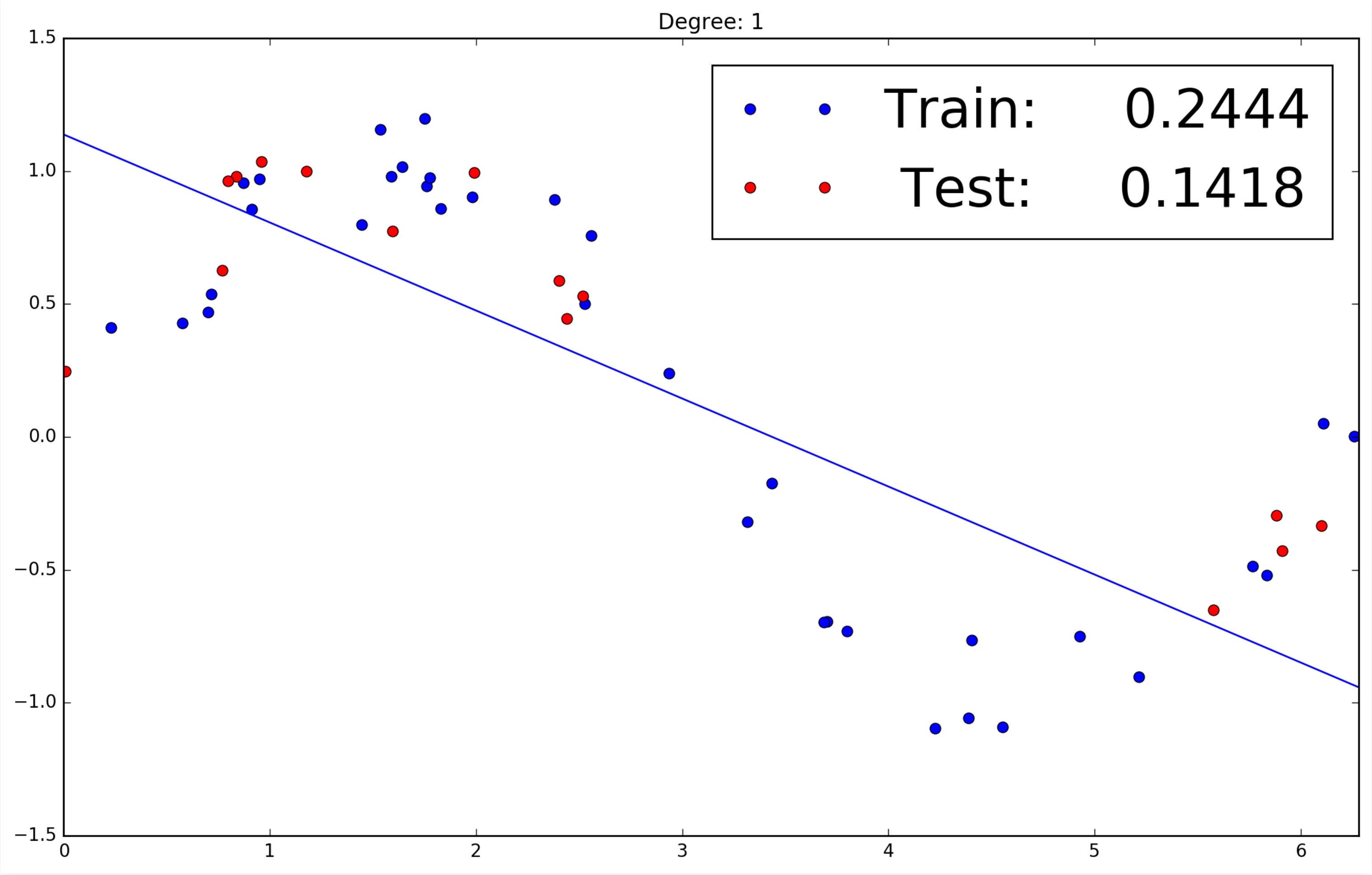
Overfitting

- Underfitting: Error mostly because model cannot fit the data



Overfitting

- Underfitting example



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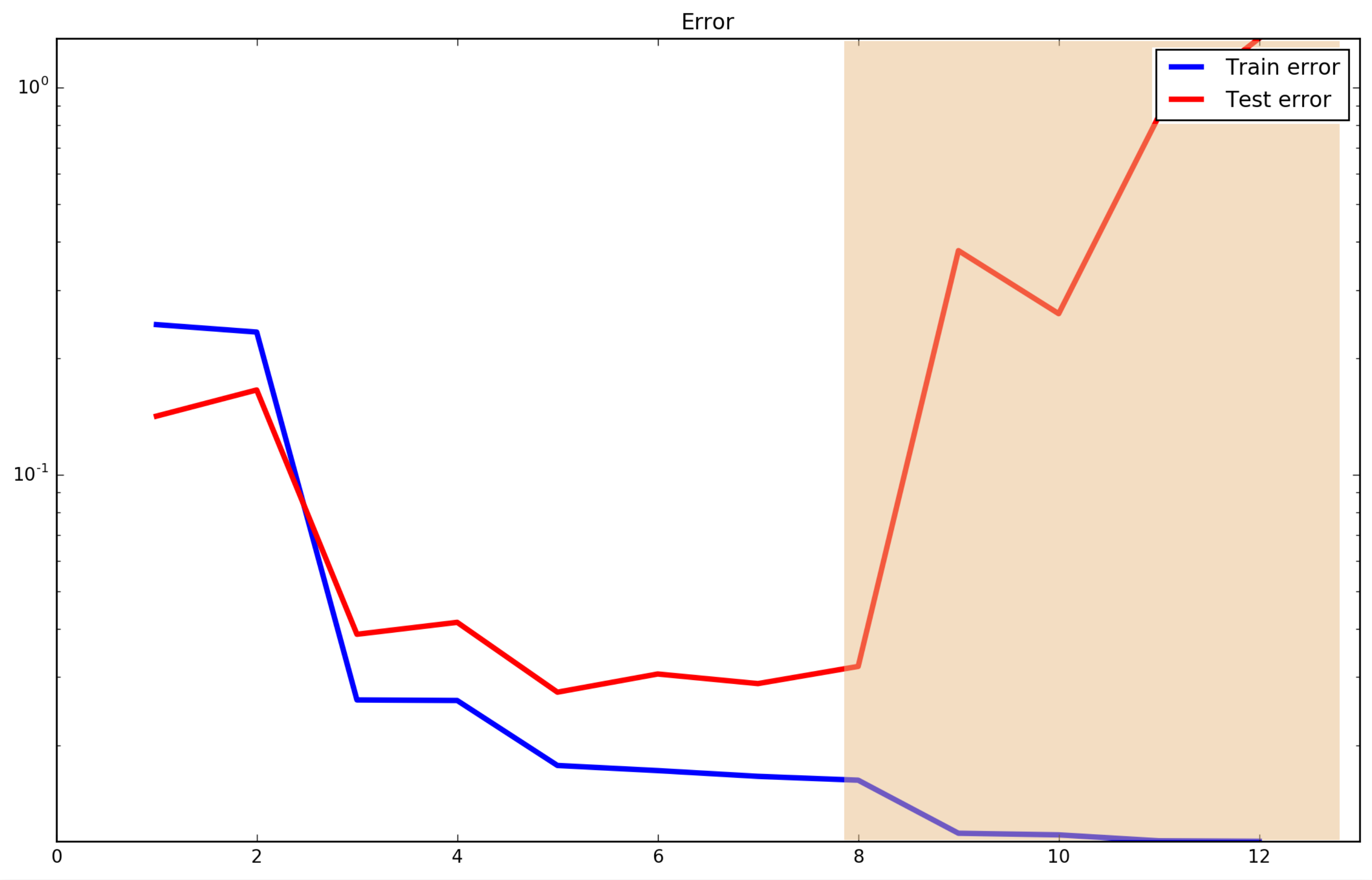
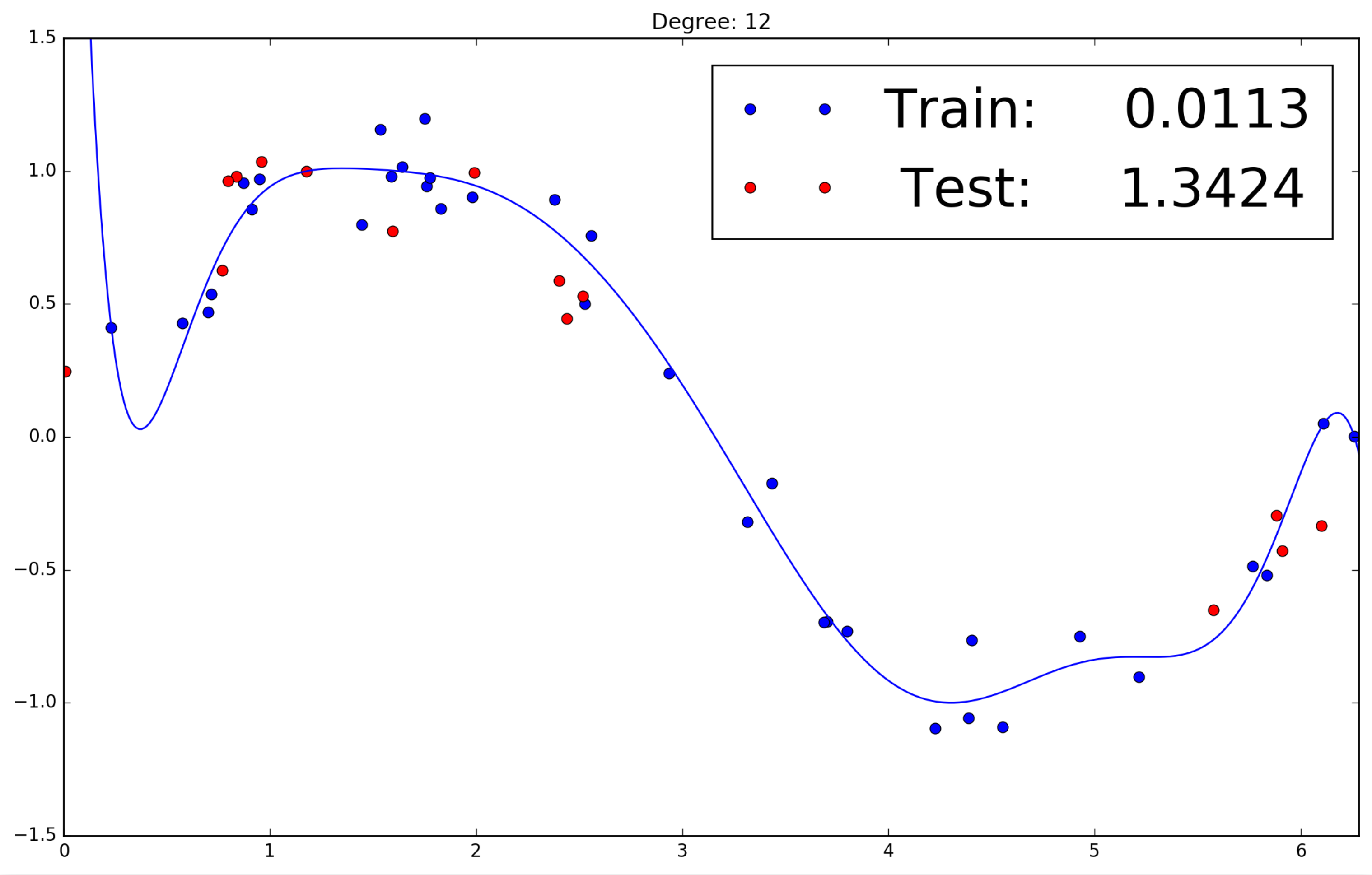
Overfitting

- Overfitting: error mostly because model adapts too much



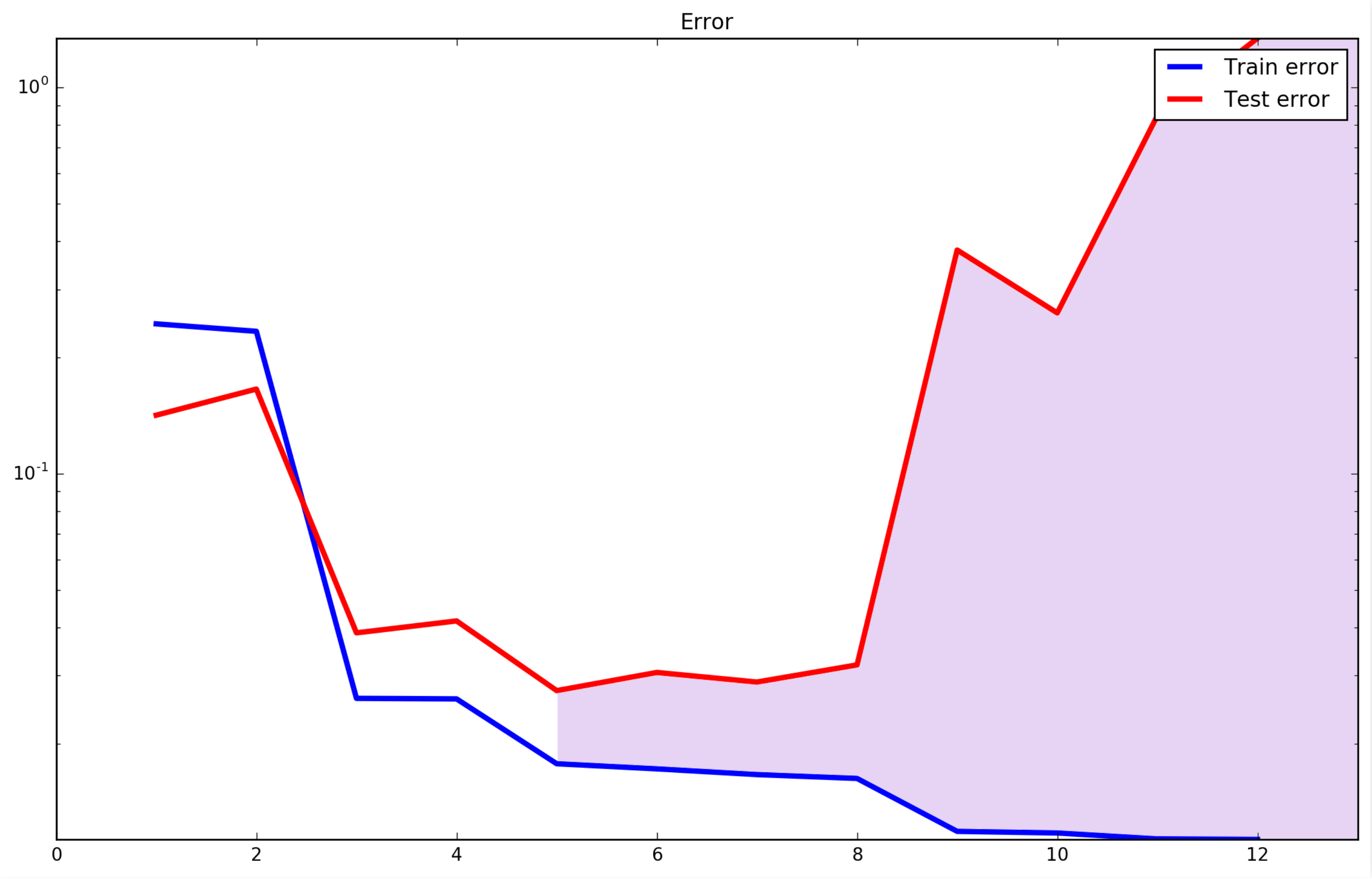
Overfitting

- Overfitting example



Overfitting

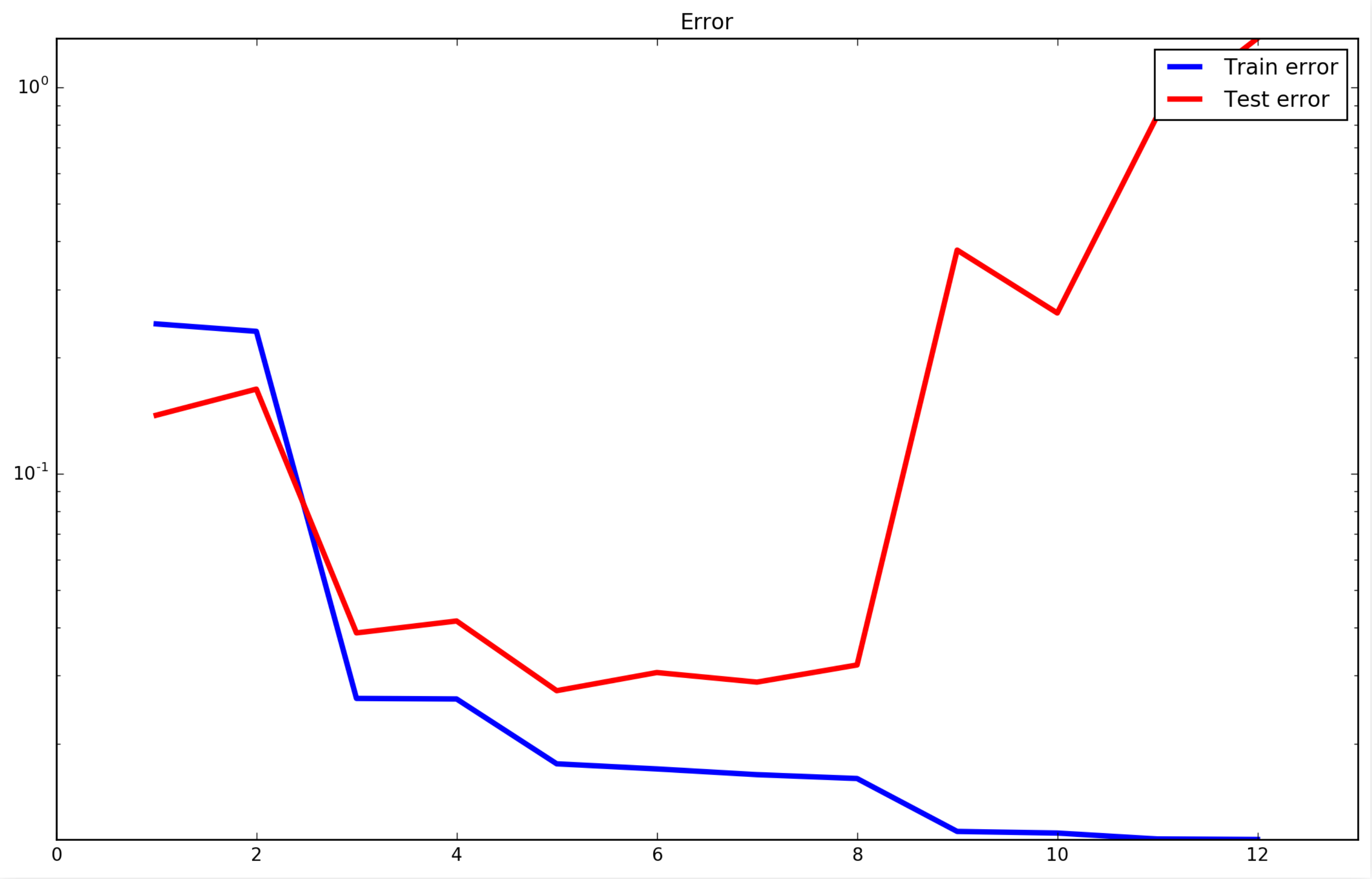
- Overfitting increases generalization error



Validation and Selection

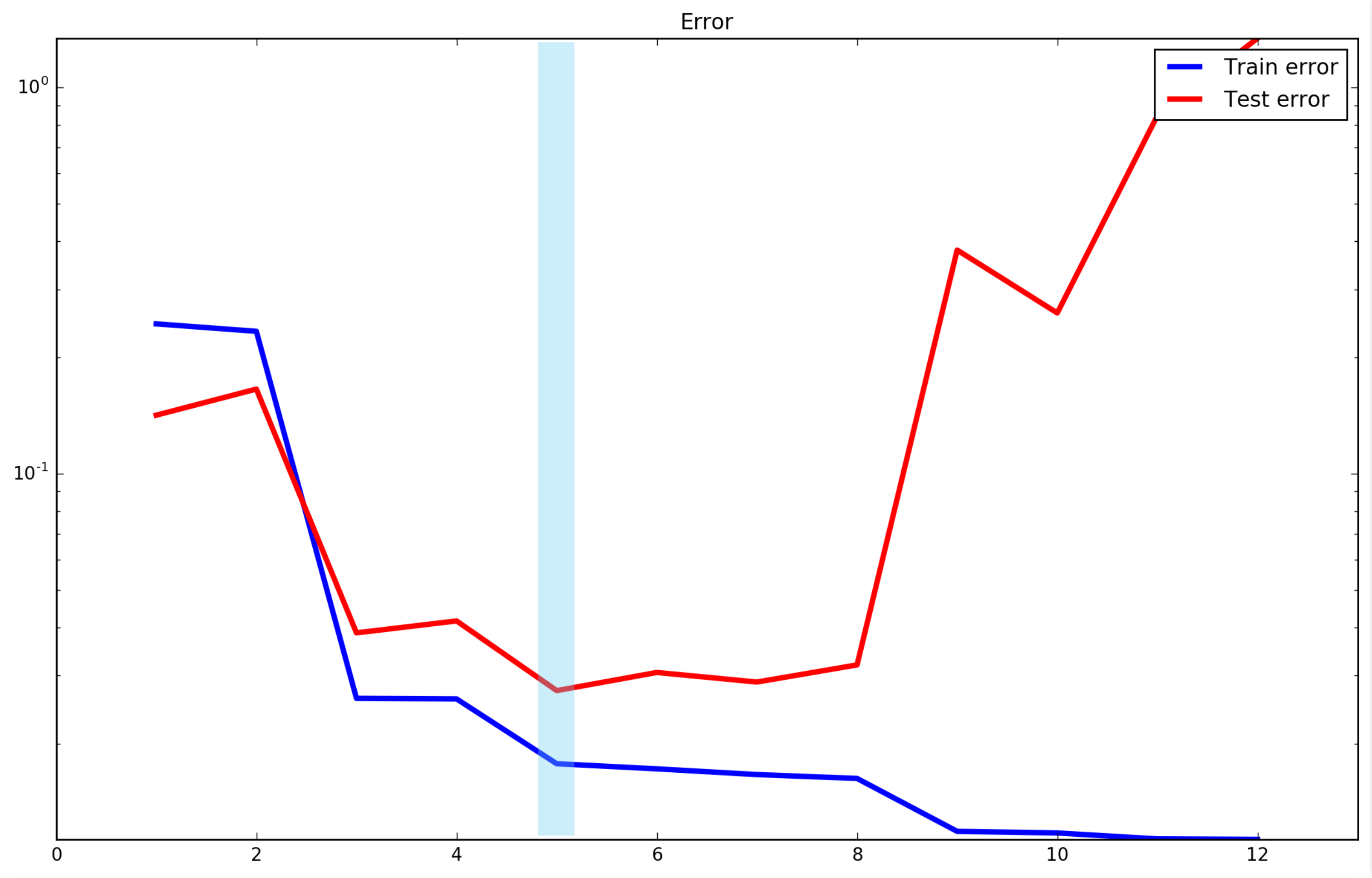
Validation and Selection

- Not all models are alike



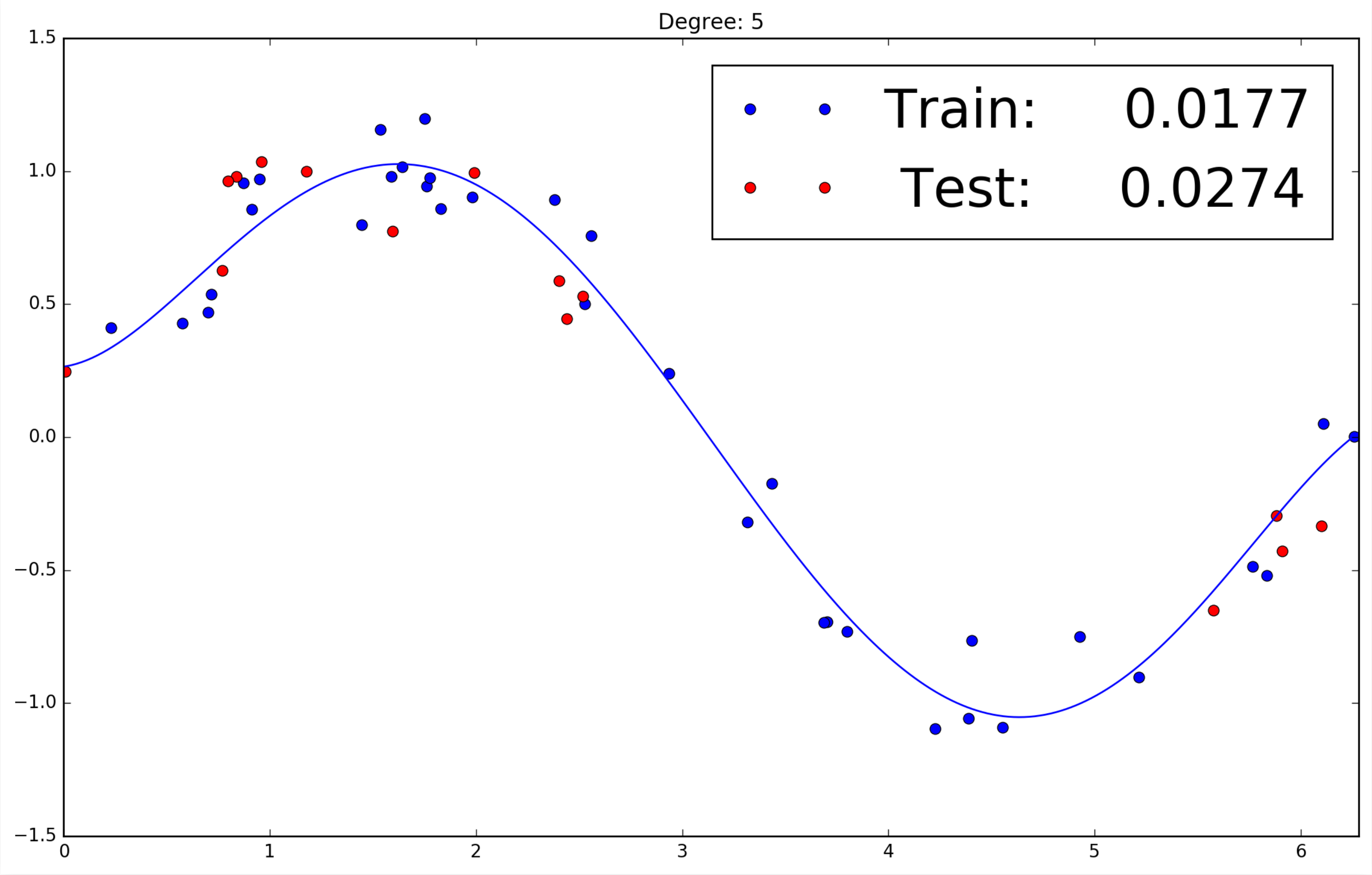
Validation and Selection

- Choose the lowest test error?



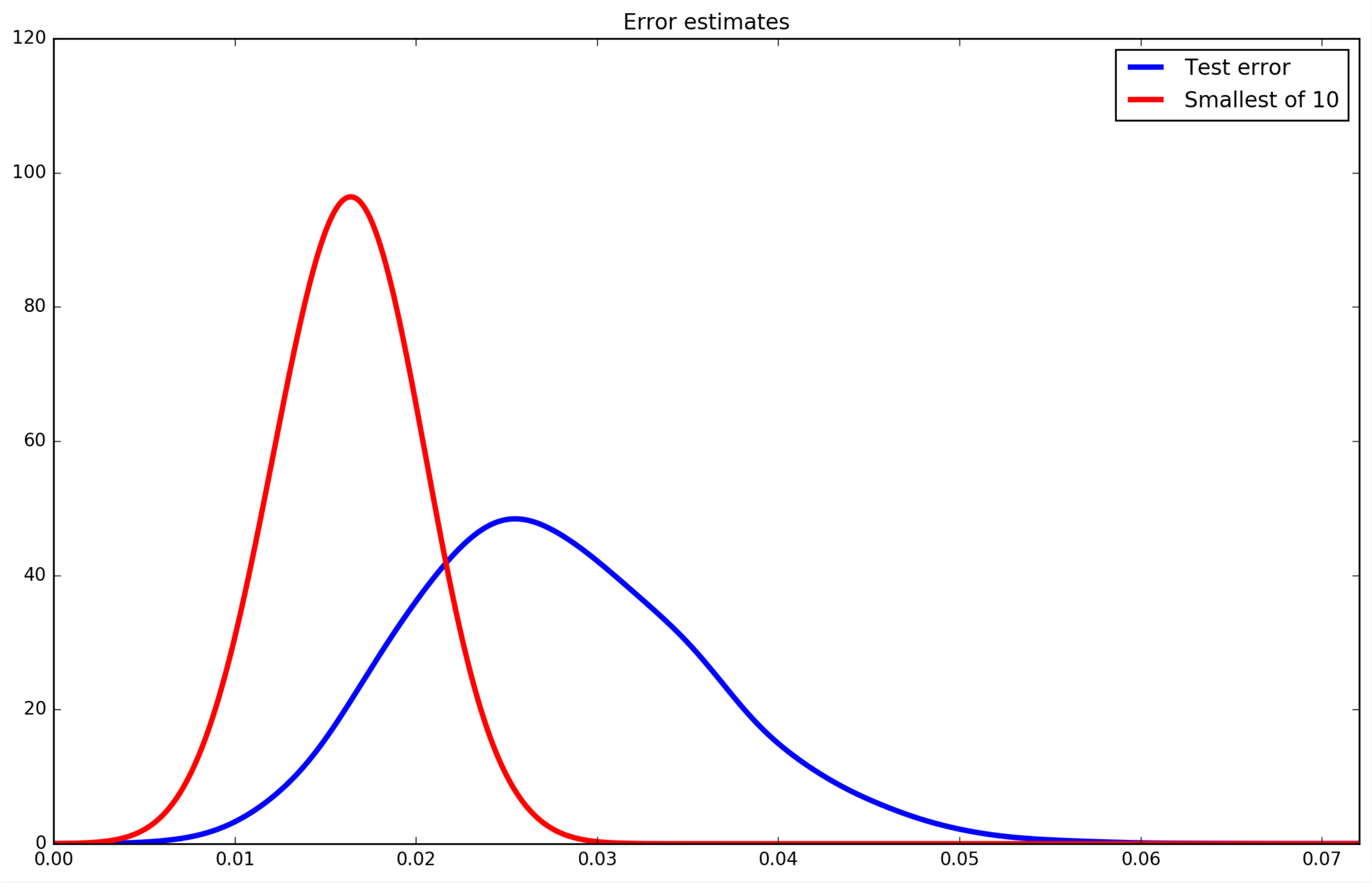
Validation and Selection

- Choose the lowest test error?



Validation and Selection

- Problem: choosing lowest makes test error biased.



Validation and Selection

Choosing best test error makes estimate biased

- We cannot use the test error to choose the best model
- This would no longer be a test error (it will be a biased estimate)

Solution: we need three sets

- Training set to fit parameters and choose the best hypothesis in each hypothesis class.
- Validation set to choose best hypothesis class (model).
- Test set to estimate true error of the final hypothesis.

Note: we'll see better ways of doing this. For now it's the idea that matters

Regularization

Regularization

Two ways of dealing with overfitting:

- Model Selection:
  - Pick model that best predicts outside training set (validation set).
- Regularization:
  - Change learning algorithm to reduce overfitting.

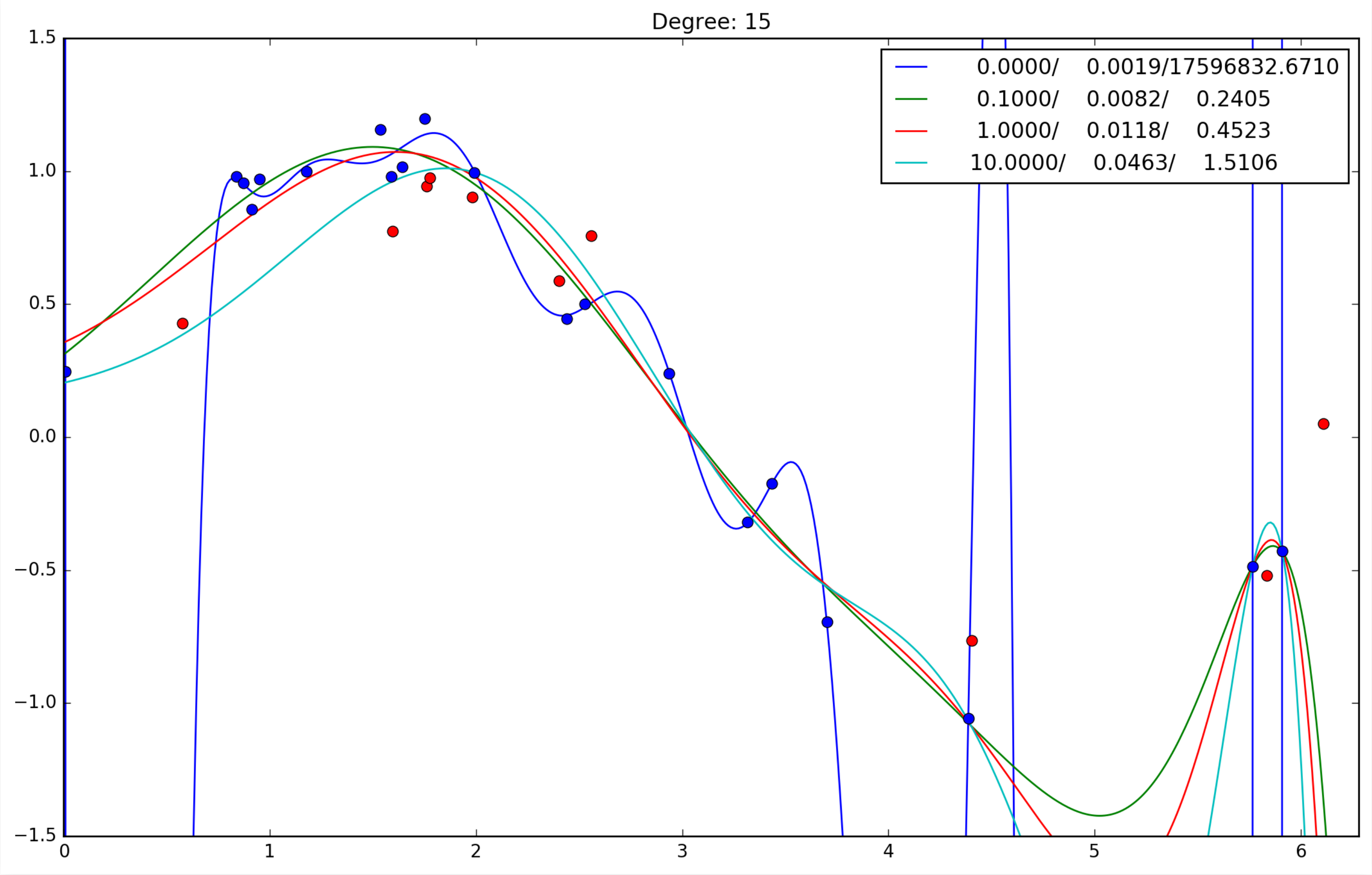
Regularization: modify training to reduce overfitting

- Example:
  - Add penalty as a function of the magnitude of the parameters.
- Ridge regression:

$$J(\theta) = \sum_{t=1}^{n} \left[y^t - g(x^t|\theta)\right]^2 + \lambda \sum_{j=1}^{m} \theta_j^2$$

Regularization

- Degree 15, different λ values.



Example: GDP and Life Expectancy

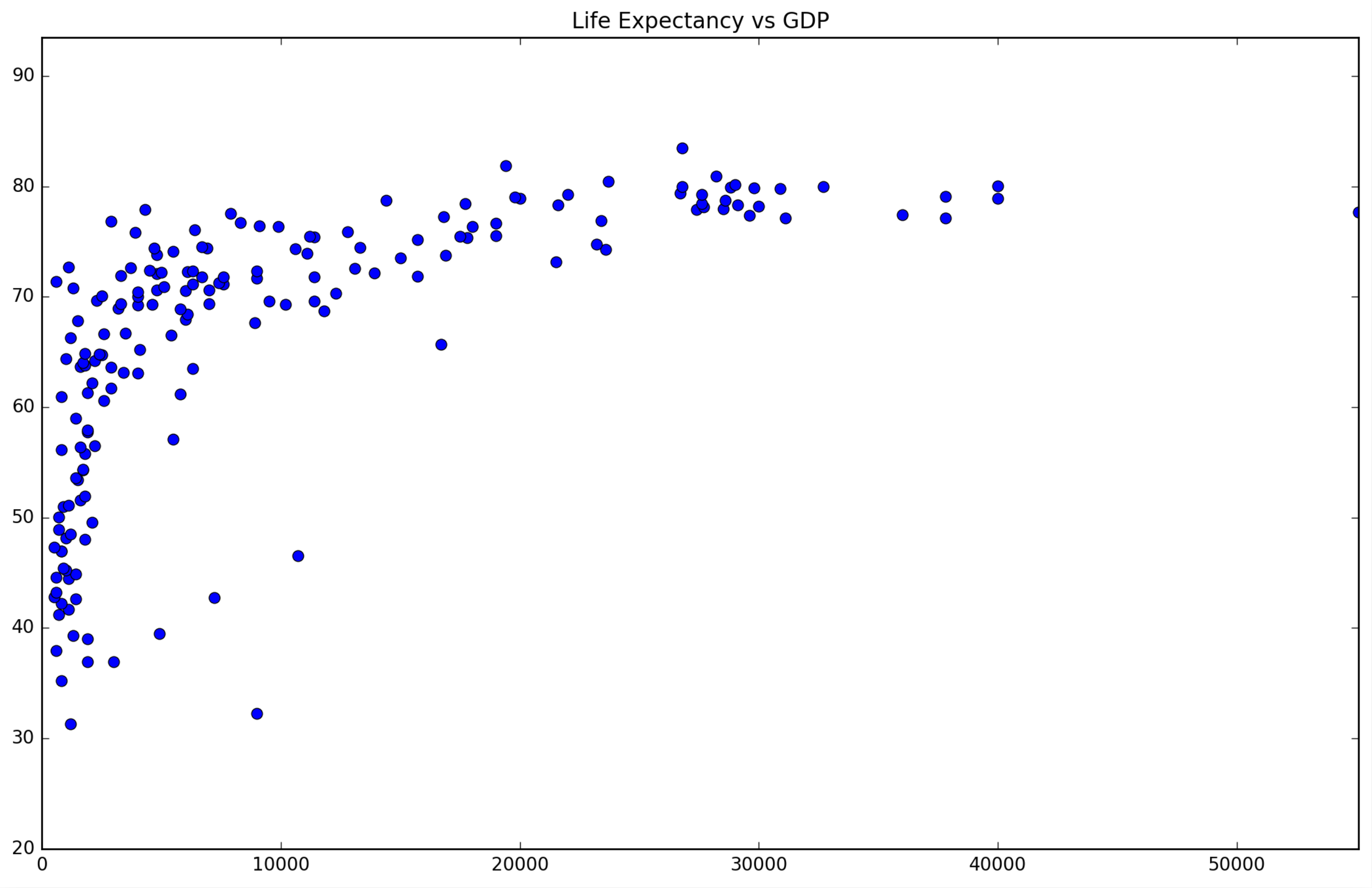
Example

- Data on Life Expectancy vs per capita GDP for 2003
  - http://www.indexmundi.com

```
1200    31.3
9000    32.26
800     35.25
3000    36.94
1900    36.96
600     37.98
...
```

Example

- Large range of values...



Example

Numerical problems

- Large differences in value magnitudes can cause problems.
  - Numerical instability
  - Finding parameters
  - Reproductibility of approach
- One simple solution:
  - Rescale values to 0..1
  - (We'll see more on this later)

Preparing the data

- Load the data, rescale and split

- Total 180 countries: 90 for training, 45 for validation, 45 for testing

```
import numpy as np

def random_split(data,test_points):
    """return two matrices splitting the data at random
    """
    ranks = np.arange(data.shape[0])
    np.random.shuffle(ranks)
    train = data[ranks>=test_points,:]
    test = data[ranks<test_points,:]
    return train,test

data = np.loadtxt('life_exp.csv',delimiter='\t')
scale=np.max(data,axis=0)
data=data/scale
train, temp = random_split(data, 90)
valid, test = random_split(temp, 45)
```

Find the best model (hypothesis class)

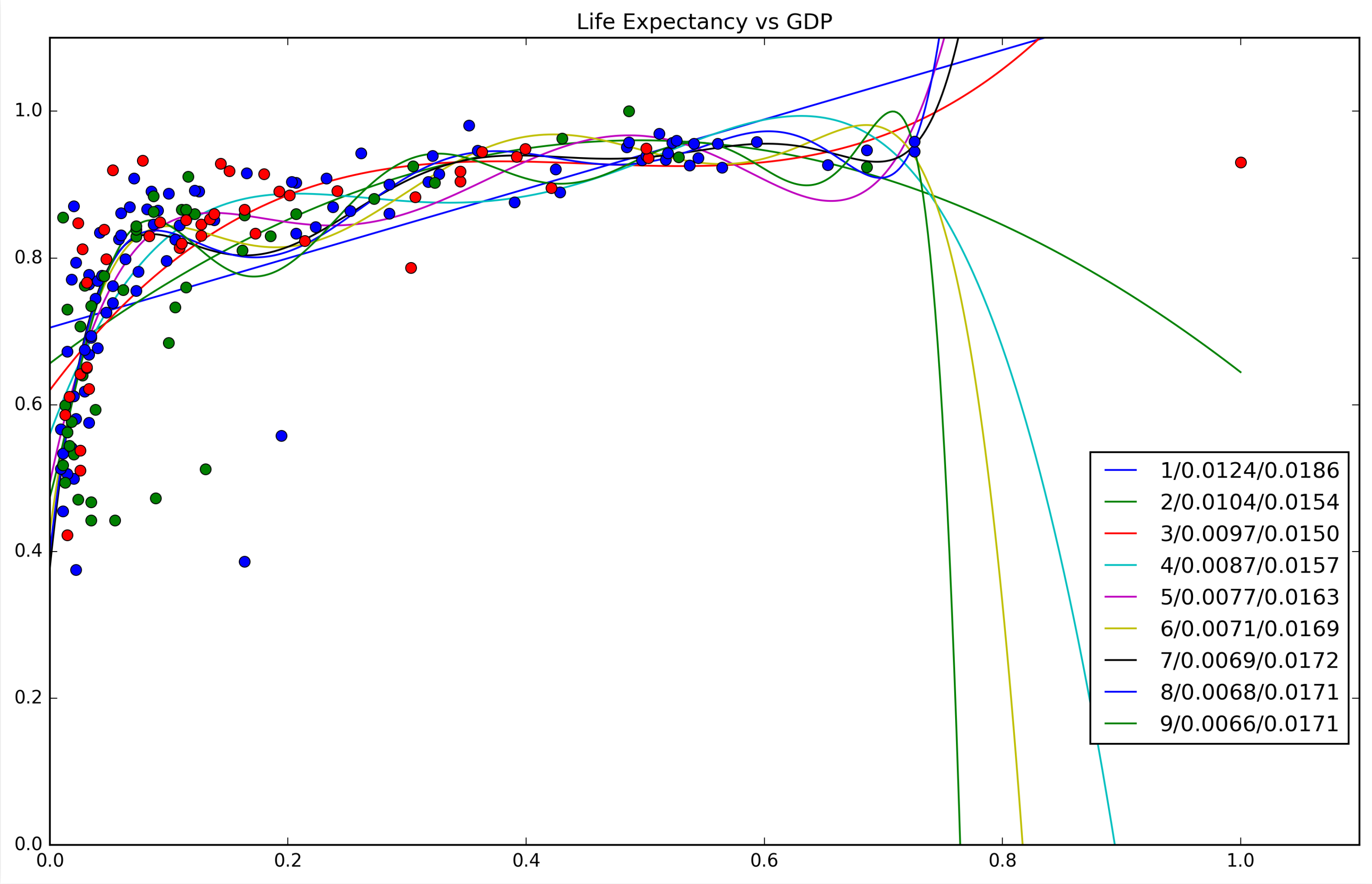
```
def mean_square_error(data,coefs):
    """Return mean squared error
           X on first column, Y on second column
    """
    pred = np.polyval(coefs,data[:,0])
    error = np.mean((data[:,1]-pred)**2)
    return error

best_err = 10000000 # very large number
for degree in range(1,9):
    coefs = np.polyfit(train[:,0],train[:,1],degree)
    valid_error = mean_square_error(valid,coefs)
    if valid_error < best_err:
        best_err = valid_error
        best_coef = coefs
        best_degree = degree

test_error = mean_square_error(test,best_coef)
print(best_degree,test_error)
```

Example

- Selecting the best hypothesis



Example

Selecting the best hypothesis:

- Degree 3, Validation error:0.0150
- Note: error estimates depend on the (random) split

- Maybe we should average them? Later...

Example

Regularization

- Different approach: use a high degree polynomial (degree 10)
- But regularize the fit (with ridge regression)

$$J(\theta) = \sum_{t=1}^{n} \left[y^t - g(x^t|\theta)\right]^2 + \lambda \sum_{j=1}^{m} \theta_j^2$$

In practice:

- The Scikit-learn library has a Ridge class to do ridge regression
- It's a linear model, but we can work with that by adding the necessary terms to our data

• Remember polynomial regression from last lecture

Example

- Loading and expanding the data to x^{10}

```
def expand(data,degree):
    """expands the data to a polynomial of specified degree"""
    expanded = np.zeros((data.shape[0],degree+1))
    expanded[:,0]=data[:,0]
    expanded[:,-1]=data[:,-1]
    for power in range(2,degree+1):
        expanded[:,power-1]=data[:,0]**power
    return expanded

orig_data = np.loadtxt('life_exp.csv',delimiter='\t')
scale=np.max(orig_data, axis=0)
orig_data=orig_data/scale
data = expand(orig_data,10)
train, temp = random_split(data, 90)
valid, test = random_split(temp, 45)
```

Example

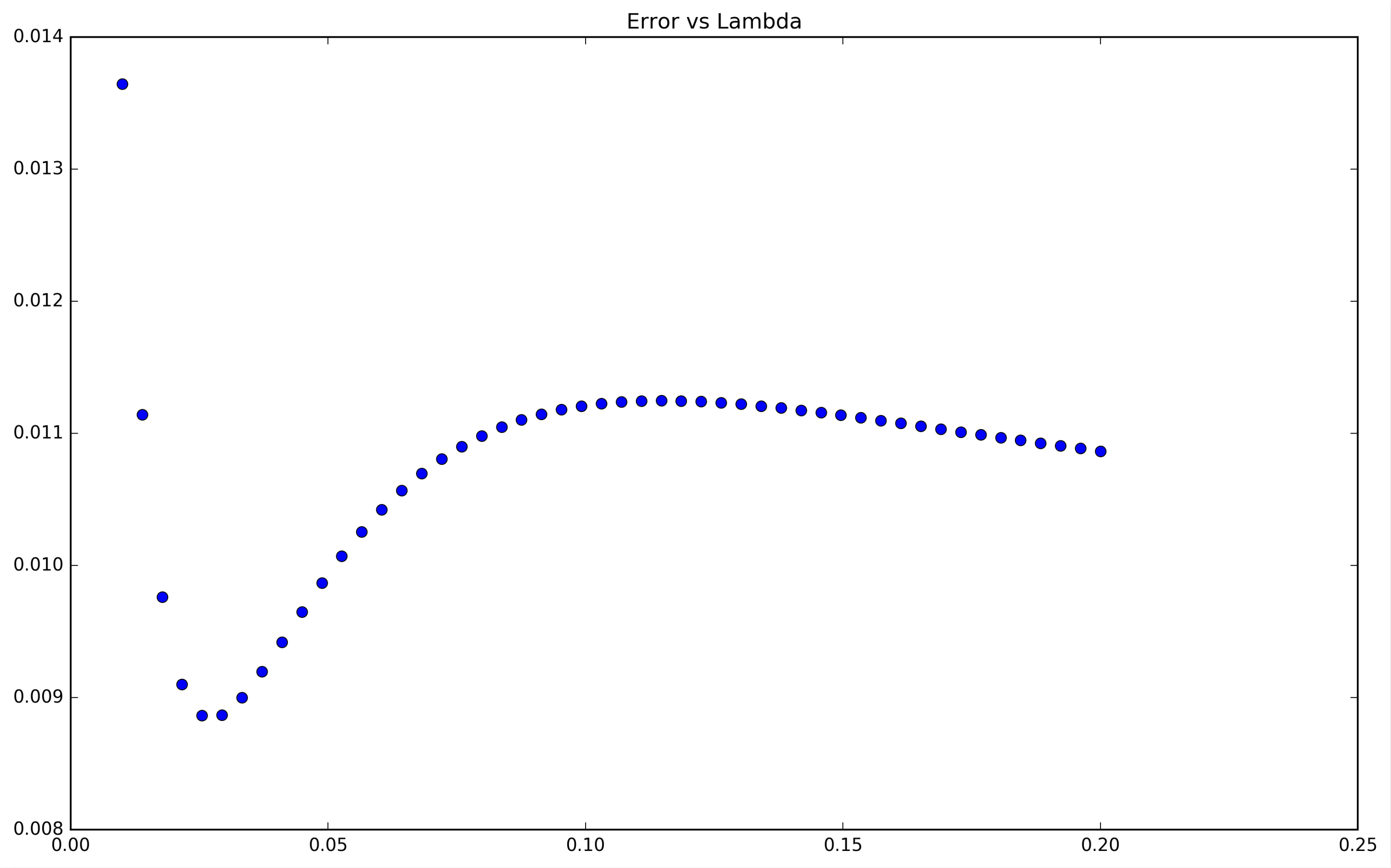
- Finding the best λ

```
from sklearn.linear_model import Ridge

lambs = np.linspace(0.01,0.2)
best_err = 100000
for lamb in lambs:
    solver = Ridge(alpha = lamb, solver='cholesky',tol=0.00001)
    solver.fit(train[:,:-1],train[:,-1])
    ys = solver.predict(valid[:,:-1])
    valid_err = np.mean((ys-valid[:,-1])**2)
    if valid_err<best_err:
        best_err = valid_err
        best_solver = solver
```

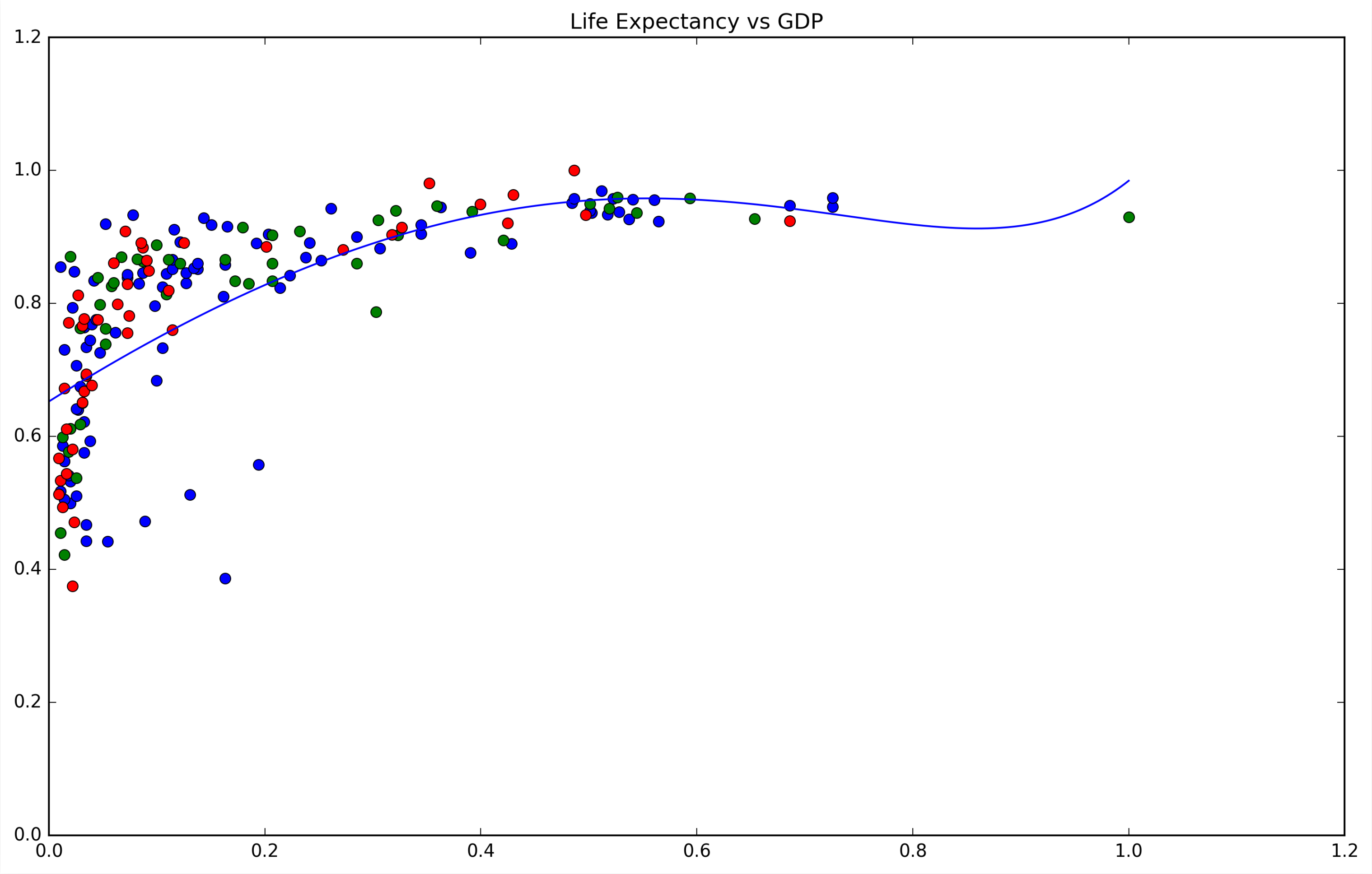
Example

- Best λ from validation error



Example

- Final result, degree 10 with regularization



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Summary

Summary

- Error measures and estimates
  - Training error, measured on training set
  - Used to adjust parameters, so is biased estimate of true error
  - Validation error, measured outside training set
  - Used to choose model or hyperparameter, so becomes biased estimate of true error
  - Test error, measured outside training set
  - Never used to choose anything
  - Is unbiased estimate of true error
- Error estimates are stochastic
- Model selection and Regularization

Overfitting

Further reading

- Bishop, Section 3.1
- Alpaydin, Sections 2.6-2.8
- Scikit-learn:http://scikit-learn.org/stable/modules/linear_model.html