5. Overfitting and Classification

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Summary

- Scoring classifiers
- Cross validation
- Logistic regression: model selection and regularization

Scoring classifiers

Scoring binary classifiers

- For regression, sum of squared distance to the line was useful:

$$E(\theta|\mathcal{X}) = \sum_{t=1}^{n} [y^t - g(x^t|\theta)]^2$$

- With Logistic Regression the function to minimize is:

$$E(\widetilde{w}) = -\sum_{n=1}^{N} [t_n \ln g_n + (1 - t_n) \ln(1 - g_n)]$$

$$g_n = \frac{1}{1 + e^{-(\vec{w}^T \vec{x_n} + w_0)}}$$

- (Regression to the probability of belonging to C_1)

Scoring binary classifiers

- How good is the hypothesis?
- The logistic loss or cross entropy function

$$L(\widetilde{w}) = \frac{1}{N}\sum_{n=1}^{N} H(p_n, q_n) = -\frac{1}{N}\sum [t_n \ln g_n + (1 - t_n)\ln(1 - g_n)]$$

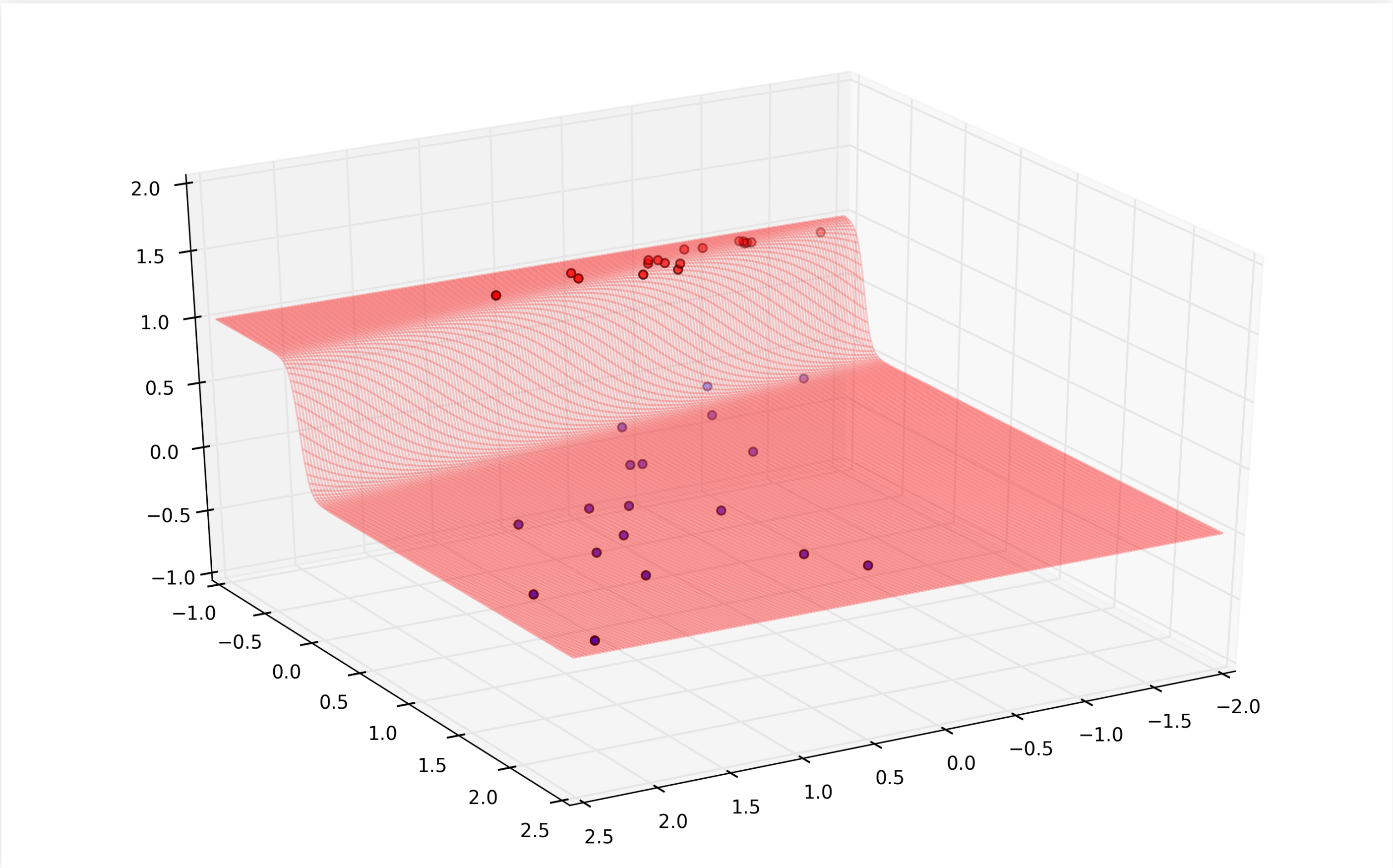
- Brier score: average quadratic error between the predicted probability and the class.

$$E(\widetilde{w}) = \frac{1}{N}\sum_{n=1}^{N}[t_n - g_n]^2$$

- Note: this is not a quadratic error to the discriminant but to the predicted probability.

Scoring binary classifiers

- Brier score: error between g_n and t_n



Scoring binary classifiers

- Confusion matrix:

	Example Class	
Prediction	**Class 1**	**Class 0**
Class 1	True Positive	False Positive
Class 0	False Negative	True Negative

Scoring binary classifiers

$$accuracy = \frac{true\ positives + true\ negatives}{N}$$

$$precision = \frac{true\ positives}{true\ positives + false\ positives}$$

$$recall = \frac{true\ positives}{true\ positives + false\ negatives}$$

Scoring binary classifiers

- F1 Score: harmonic mean of precision and recall

$$F_1 = 2 \times \frac{precision \times recall}{precision + recall}$$

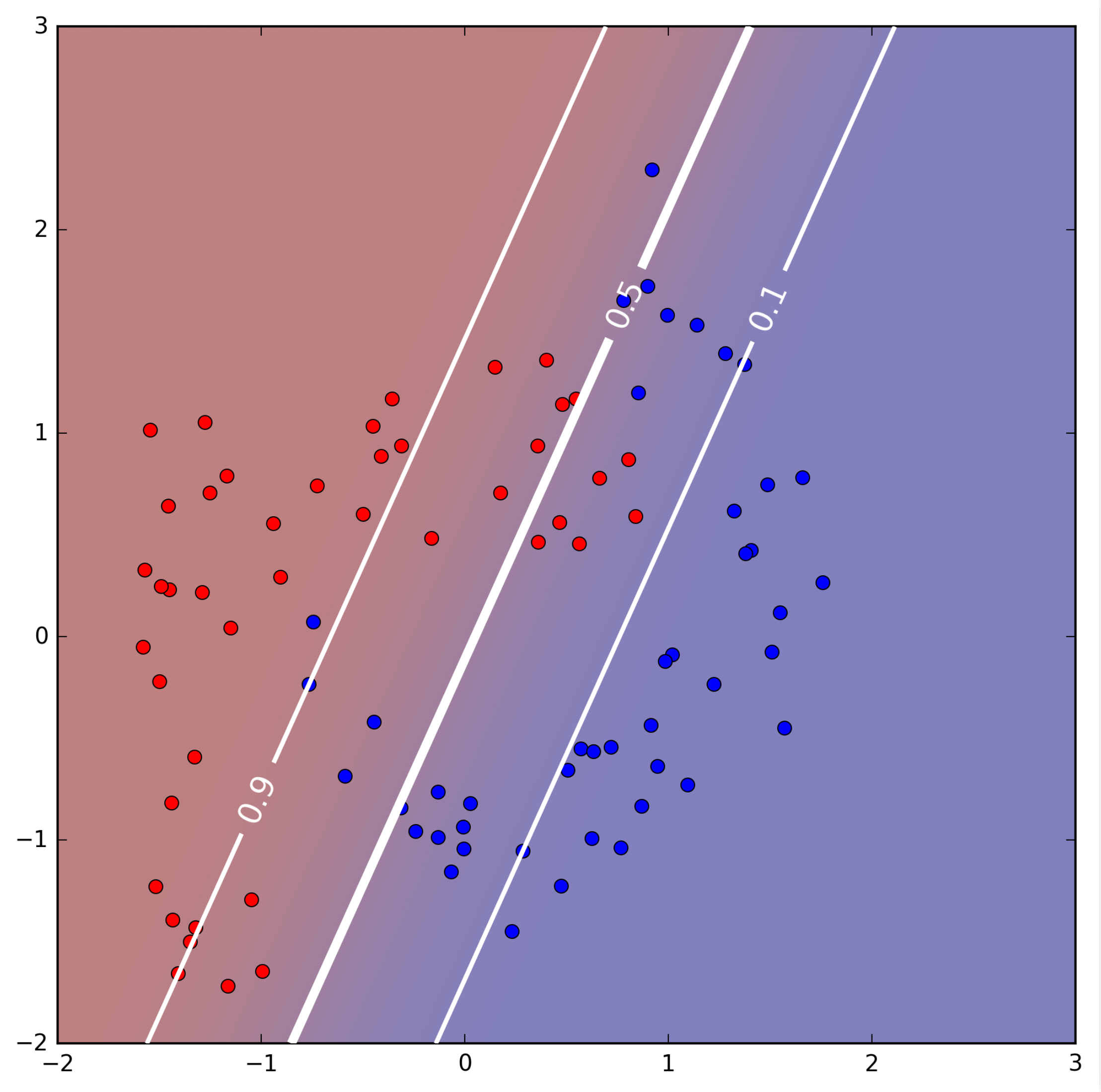
$$F_1 = \frac{2 \times true\ positives}{2 \times true\ pos. + false\ pos. + false\ neg.}$$

Scoring classifiers

Binary Classifiers

Tipically, consider $g_n \geq 0.5$ for predicting Class 1

More generally, consider $g_n \geq \alpha,\ \alpha \in [0, 1]$



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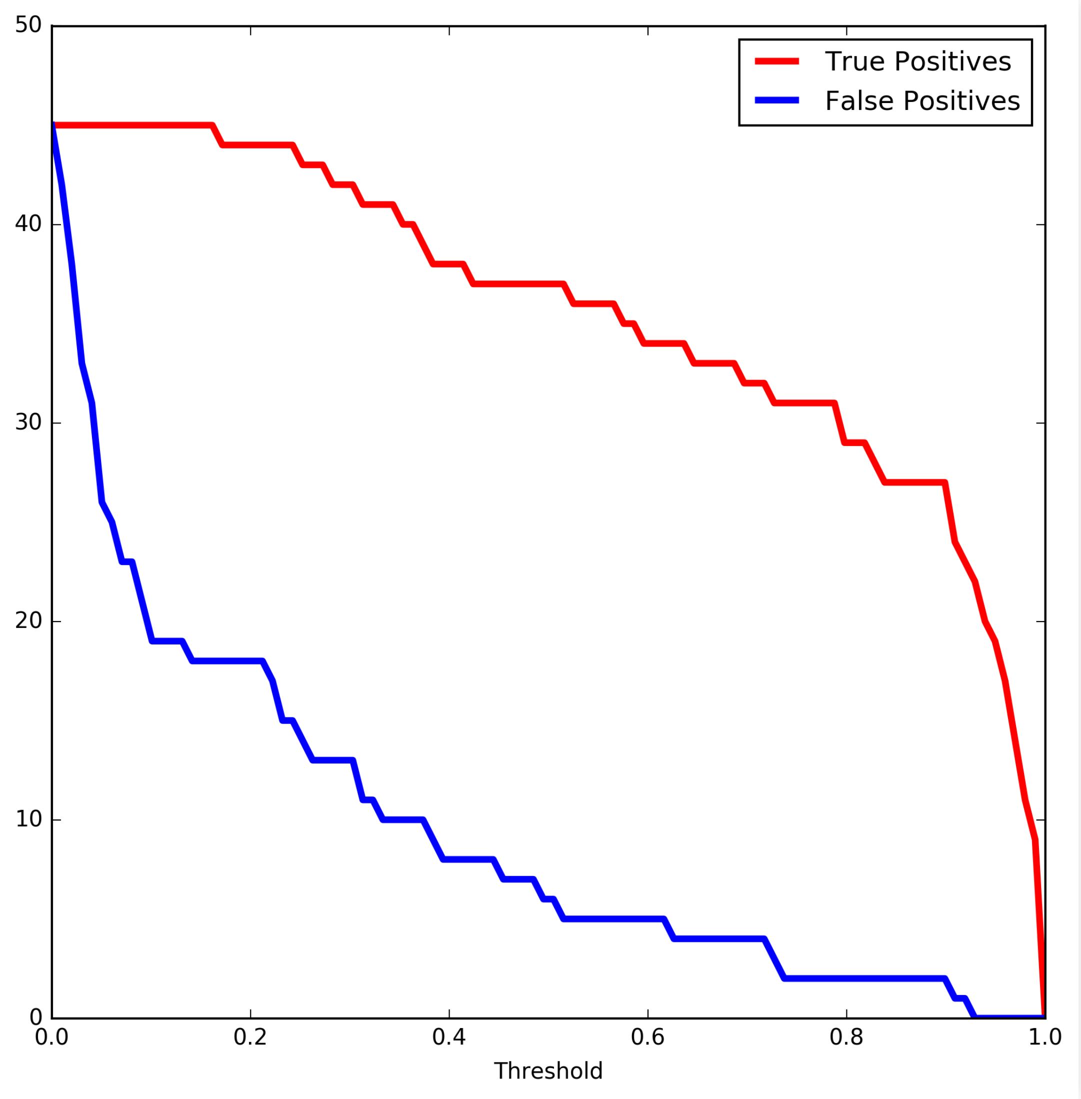
Scoring classifiers

Binary Classifiers

Tipically, consider $g_n \geq 0.5$ for predicting Class 1

More generally, consider $g_n \geq \alpha,\ \alpha \in [0, 1]$

As α changes, the number of false and true positives also changes



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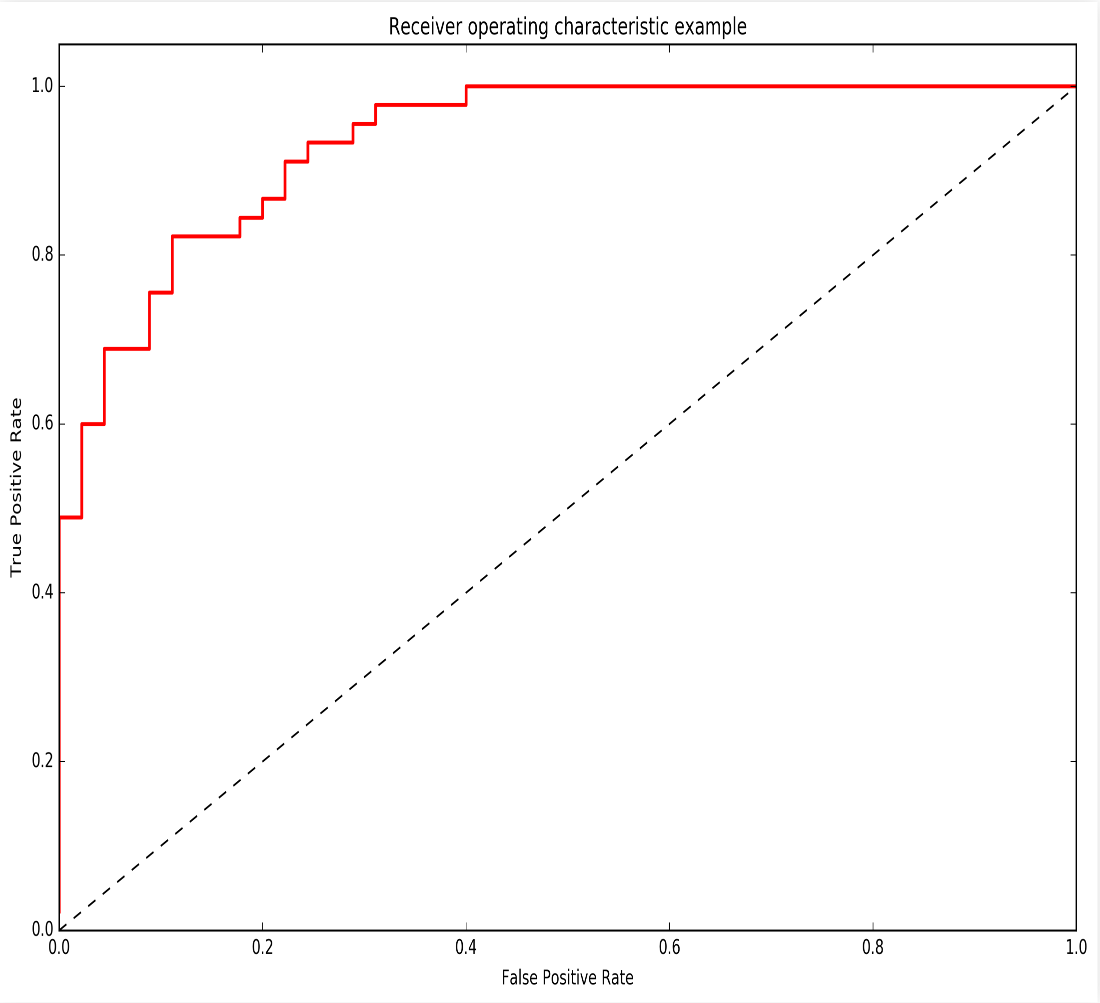
Receiver Operating Characteristic

Plot true pos. vs false pos. for different α

We can use area under the ROC curve as a possible score for binary classifier.



Scoring classifiers

Scoring binary classifiers

- Logistic Regression: Loss function, Brier score
- Precision, Recall, Accuracy
- Confusion Matrix
- Receiver Operating Characteristic curve

- Classifiers in Scikit Learn include a score method
  - Returns accuracy, the fraction of correctly classified examples

```
from sklearn.linear_model import LogisticRegression

reg = LogisticRegression()
reg.fit(X_r,Y_r)
test_error = 1-reg.score(X_t,Y_t)
```

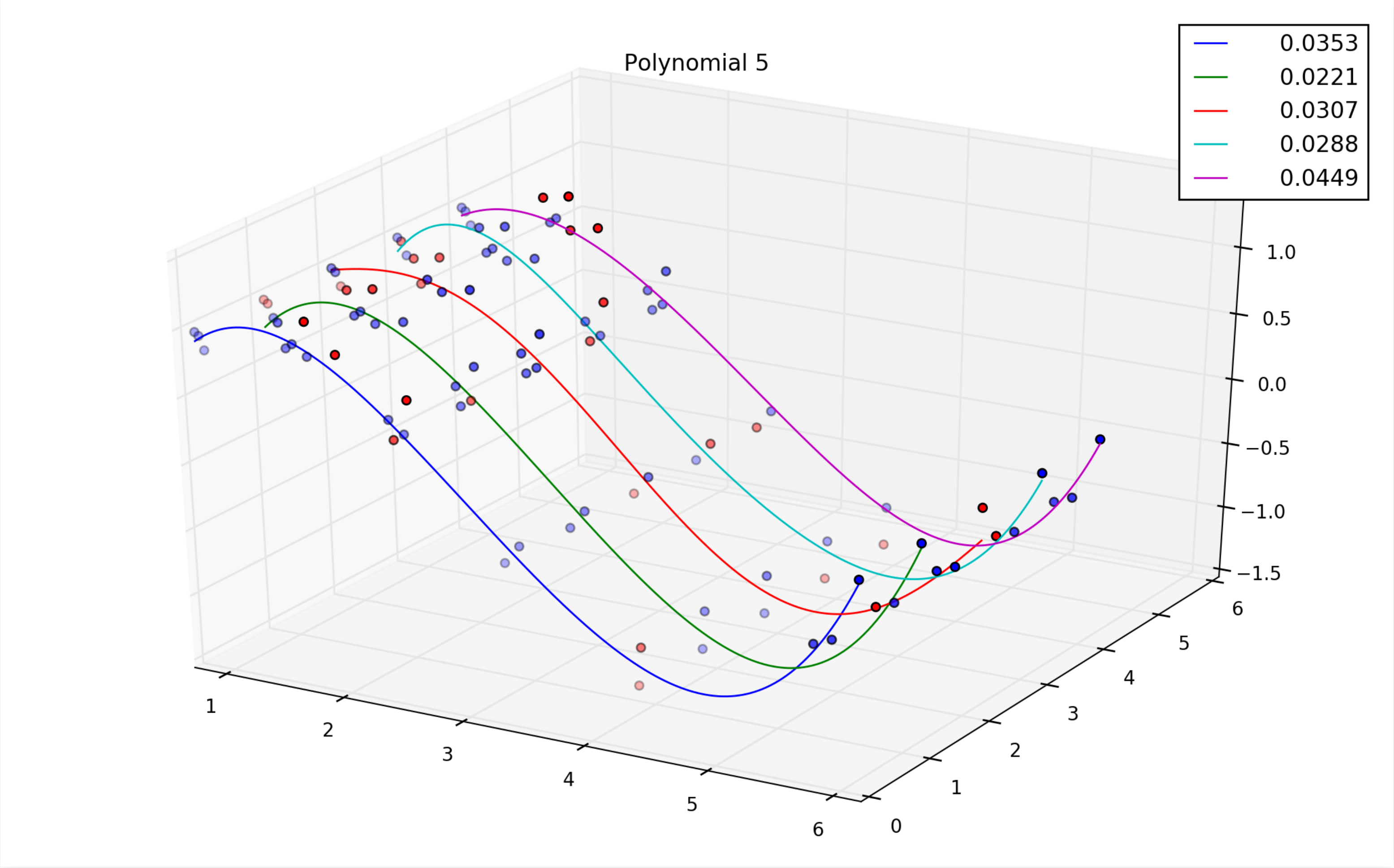
Cross-Validation

Train, Validate, Test

- Previously, we saw:
  - Minimize $\boxed{\text{Training Error}}$ to generate hypothesis
  - Measure $\boxed{\text{Validation Error}}$ on hypothesis to select
  - Measure $\boxed{\text{Test Error}}$ to estimate $\boxed{\text{True Error}}$
- Problem: select model based on one estimate (one hypothesis)

Cross-Validation

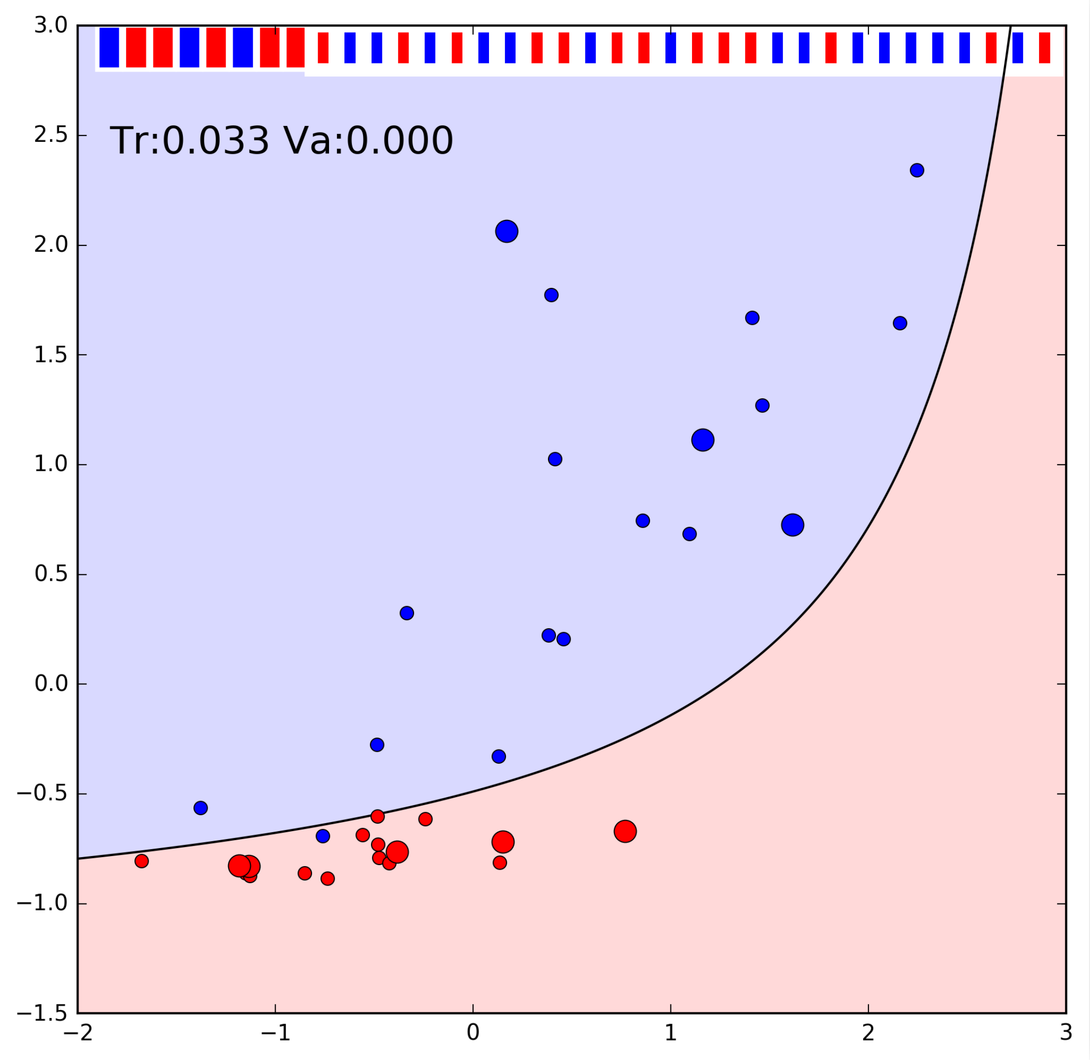
- Each train and validation split is one sample



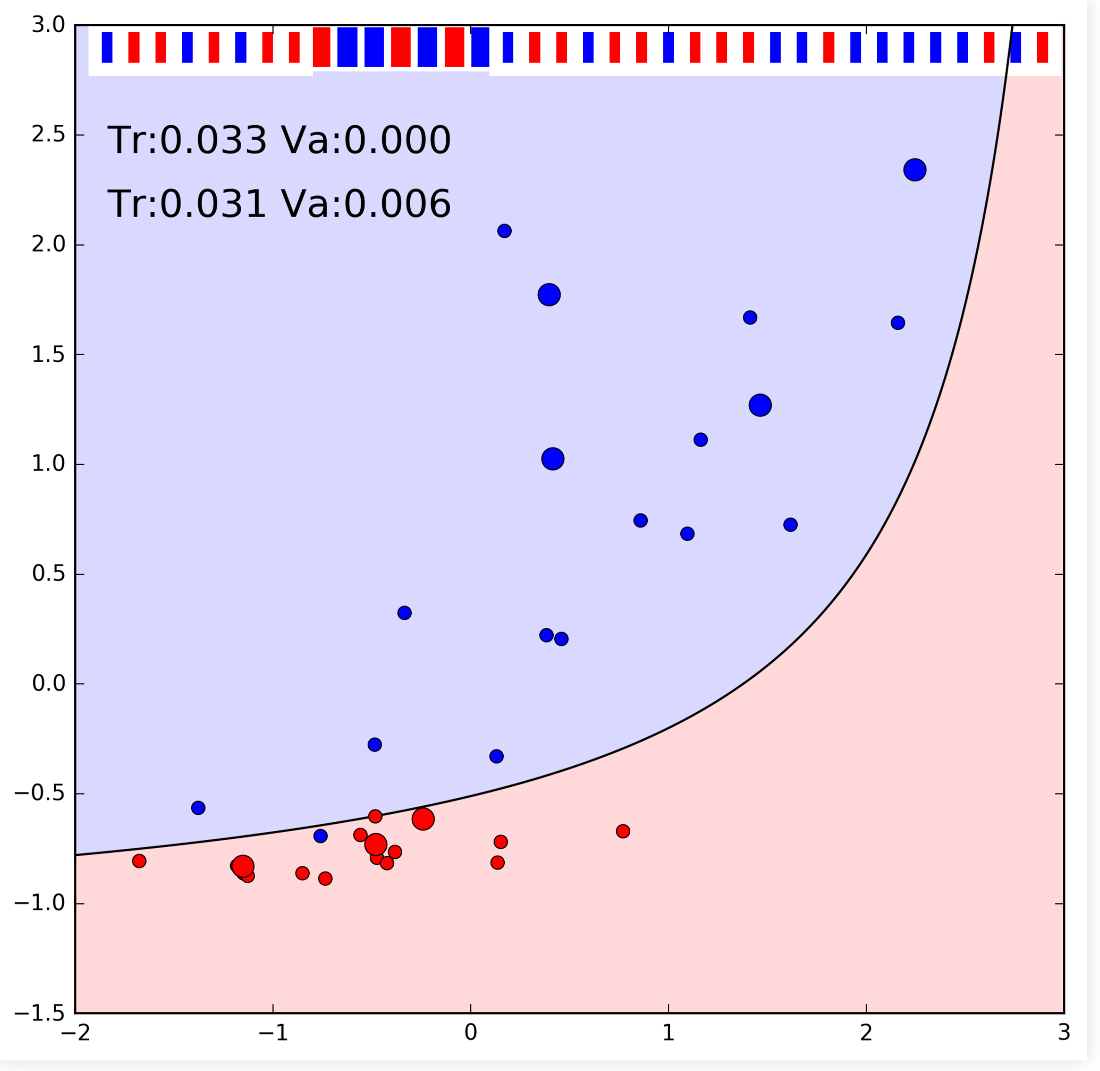
Average hypotheses from the same class (model)

- Split data into Training Set and Test Set
  - The Test Set is for an unbiased estimate of the true error of the final hypothesis
- Validate with average of K hypotheses
  - Split Training Set into K folds
  - Average K validations: each fold after training on the other K-1 folds

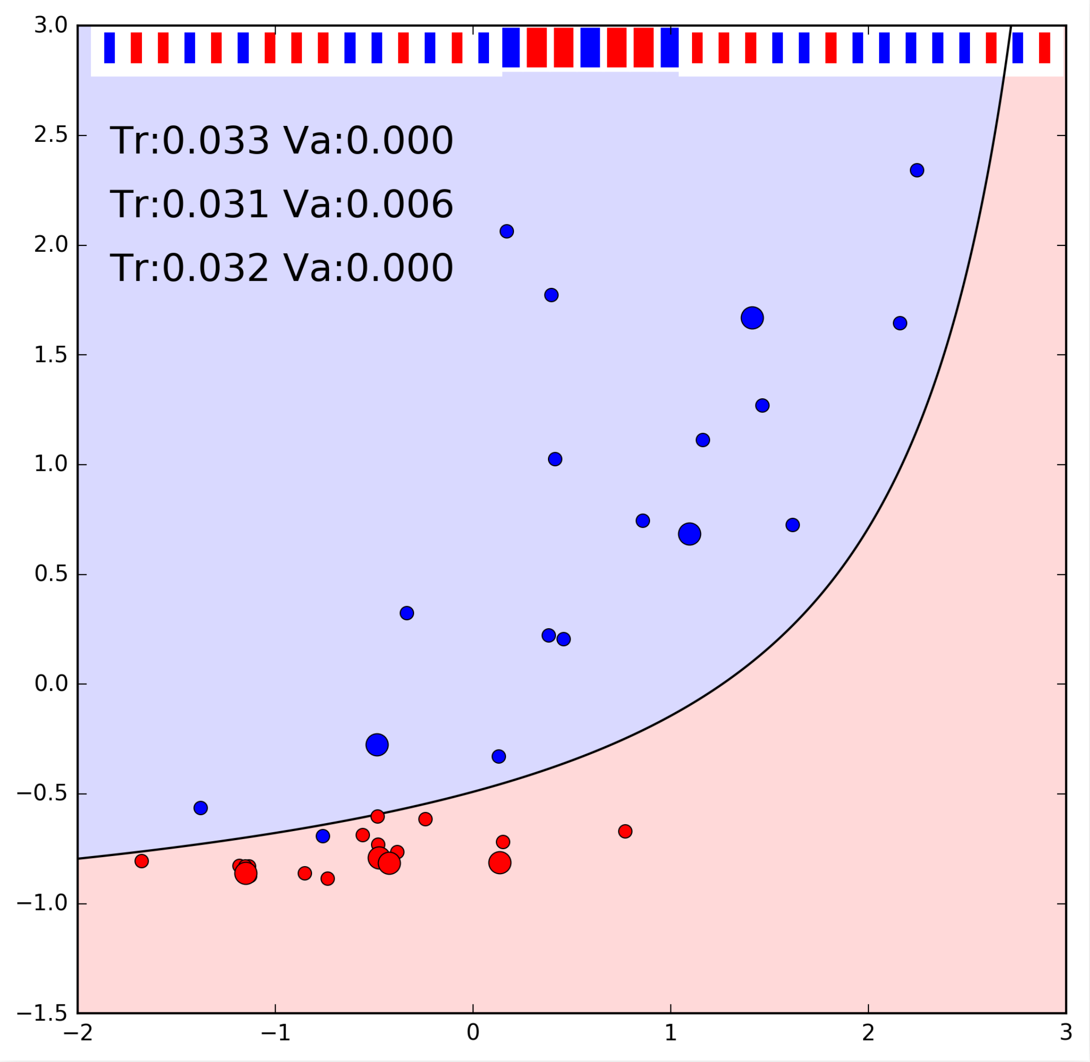
Cross-Validation



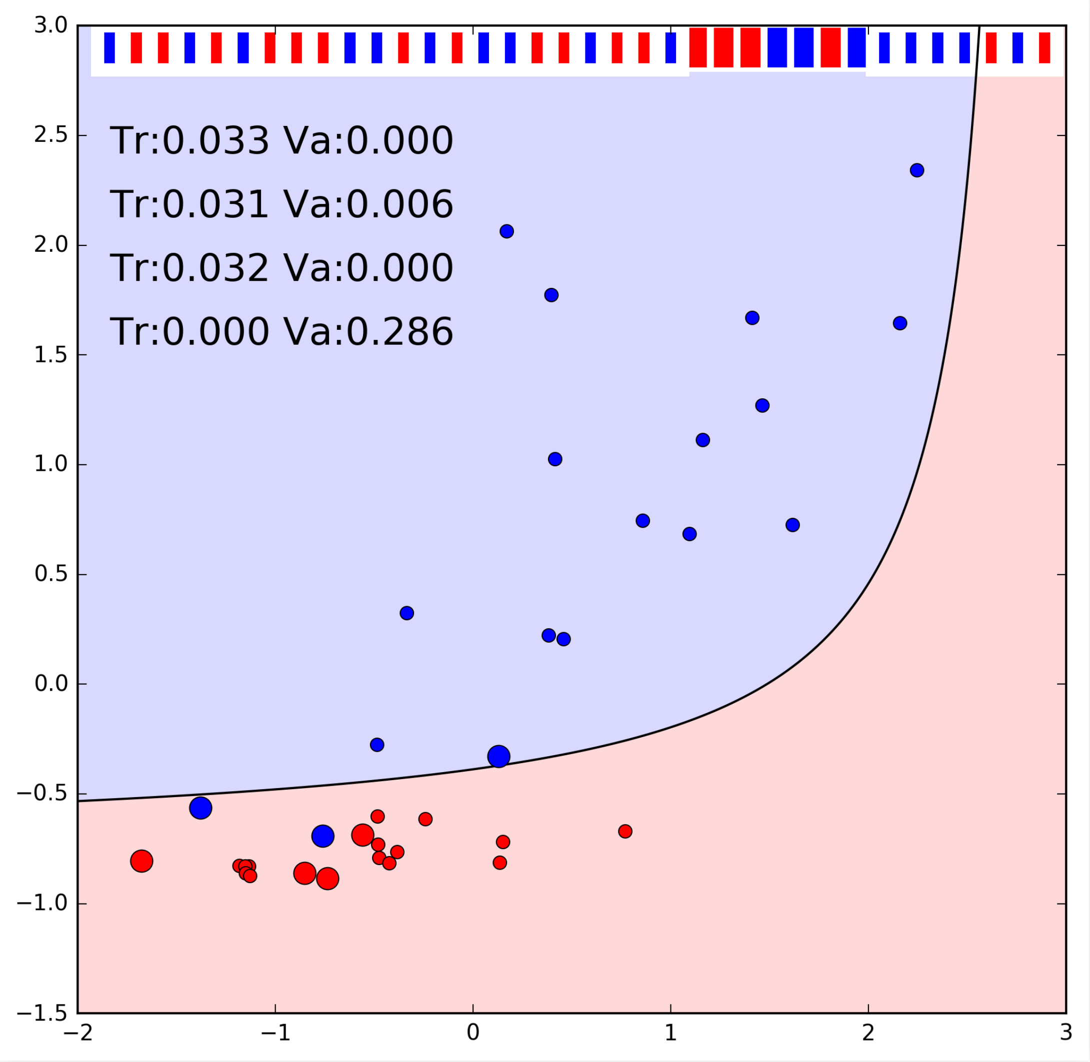
Cross-Validation



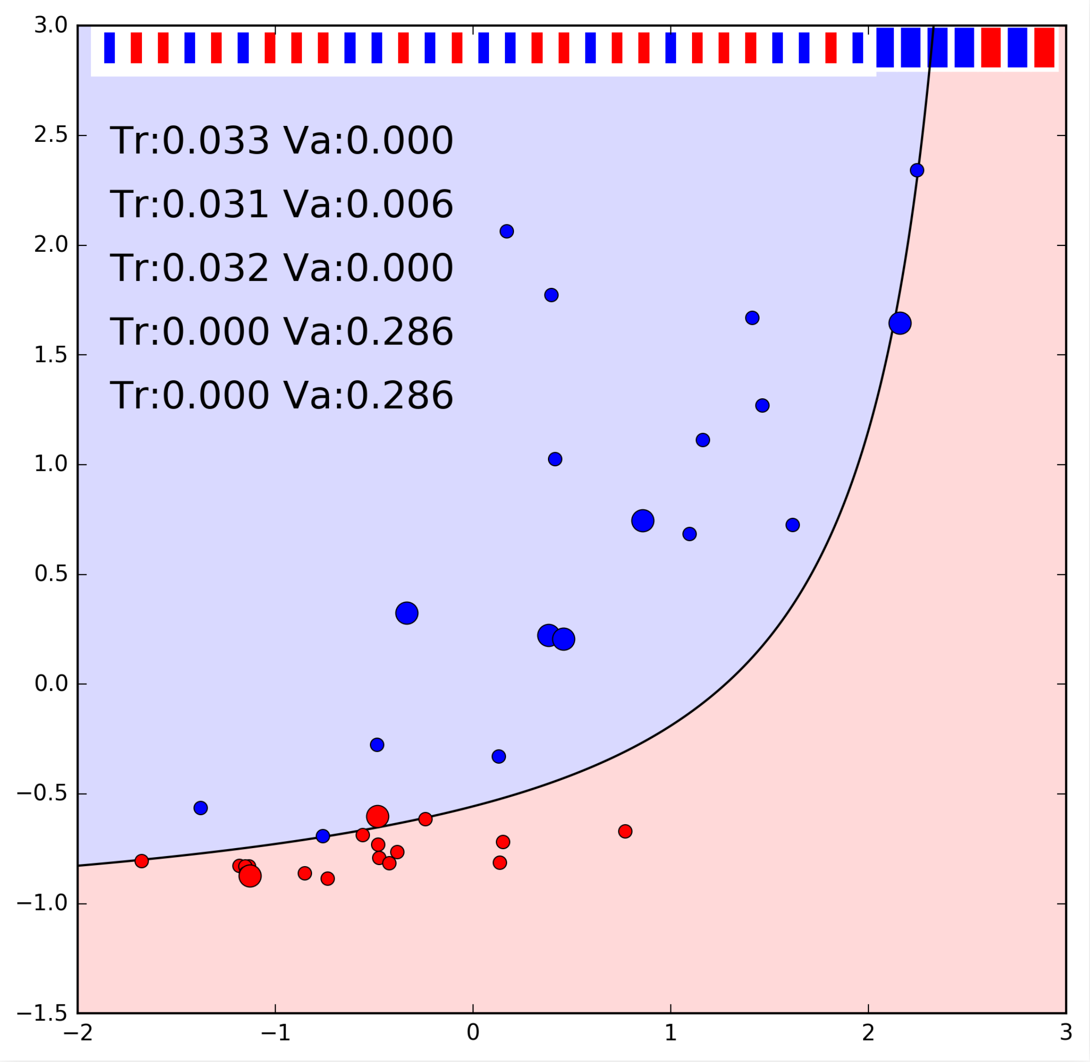
Cross-Validation



Cross-Validation



Cross-Validation



Train+Validation vs Cross-Validation

- With training and validation we estimate the true error of an hypothesis
  - We then use these estimates to select the best hipothesis from different models
- With cross-validation we average the estimated true error of several hypotheses
  - This gives us a better estimate of the true error for that model, on average, on this kind of data
  - But does not give an estimate of the true error of any specific hypothesis

K-fold Cross-Validation

- Split points into K folds
  - With N folds: leave-one-out cross-validation.

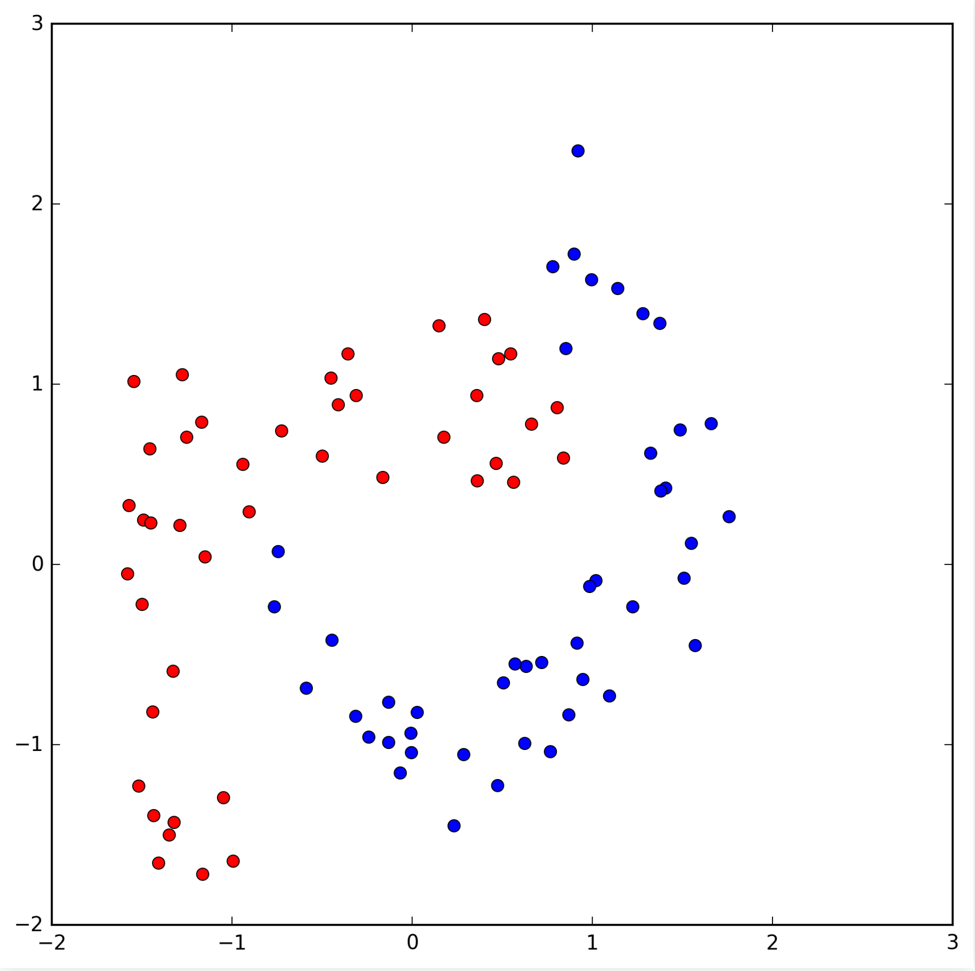
Cross-Validation and Testing

- Possible problem: class imbalance.
- Unless large data set, class proportions may change in folds or training and test.
  - Use Stratified sampling: random sampling that preserves proportions.

Example

Example

- Find the best model for classifying these data:



Example

Load, shuffle, standardize features:

```
import numpy as np
from sklearn.utils import shuffle

mat = np.loadtxt('dataset_90.txt',delimiter=',')
data = shuffle(mat)
Ys = data[:,0]
Xs = data[:,1:]
means = np.mean(Xs,axis=0)
stdevs = np.std(Xs,axis=0)
Xs = (Xs-means)/stdevs
```

Example

We want to select the best model expanding the data:

$$\{x_1, x_2\}$$
$$\{x_1, x_2, x_1 \times x_2\}$$
$$\{x_1, x_2, x_1 \times x_2, x_1^2\}$$
$$\ldots$$

```
def poly_16features(X):
    """Expand data polynomially
    """
    X_exp = np.zeros((X.shape[0],X.shape[1]+14))
    X_exp[:,:2] = X
    X_exp[:,2] = X[:,0]*X[:,1]
    X_exp[:,3] = X[:,0]**2
    X_exp[:,4] = X[:,1]**2
    X_exp[:,5] = X[:,0]**3
    X_exp[:,6] = X[:,1]**3
    X_exp[:,7] = X[:,0]**2*X[:,1]
    X_exp[:,8] = X[:,1]**2*X[:,0]
    #... rest of the expansion here
    return X_exp
```

Example

Expand and split (stratified):

```
from sklearn.model_selection import train_test_split

Xs=poly_16features(Xs)
X_r,X_t,Y_r,Y_t = train_test_split(Xs, Ys, test_size=0.33, stratify = Ys)
```

Generate the fold indexes with KFold (example)

```
from sklearn.model_selection import KFold

x = [0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]
kf = KFold(n_splits=4)
for train, valid in kf.split(x):
    print (train, valid)
```

```
[ 3  4  5  6  7  8  9 10 11] [0 1 2]
[ 0  1  2  6  7  8  9 10 11] [3 4 5]
[ 0  1  2  3  4  5  9 10 11] [6 7 8]
[ 0  1  2  3  4  5  6  7  8] [9 10 11]
```

Example

Stratified k-folds:

- Tries to keep the same distribution of classes in each fold

```
from sklearn.model_selection import StratifiedKFold
ys = [1,1,0,1,0,1,0,1,0,1,1,1]
kf = StratifiedKFold(n_splits=4)
for train,valid in kf.split(ys,ys):
    print(train,valid)
```

```
[ 3  4  5  6  7  8  9 10 11] [0 1 2]
[ 0  1  2  6  7  8  9 10 11] [3 4 5]
[ 0  1  2  3  4  5  8 10 11] [6 7 9]
[ 0  1  2  3  4  5  6  7  9] [8 10 11]
```

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Example

- Compute train and validation Brier error: (assumes classes 0,1)

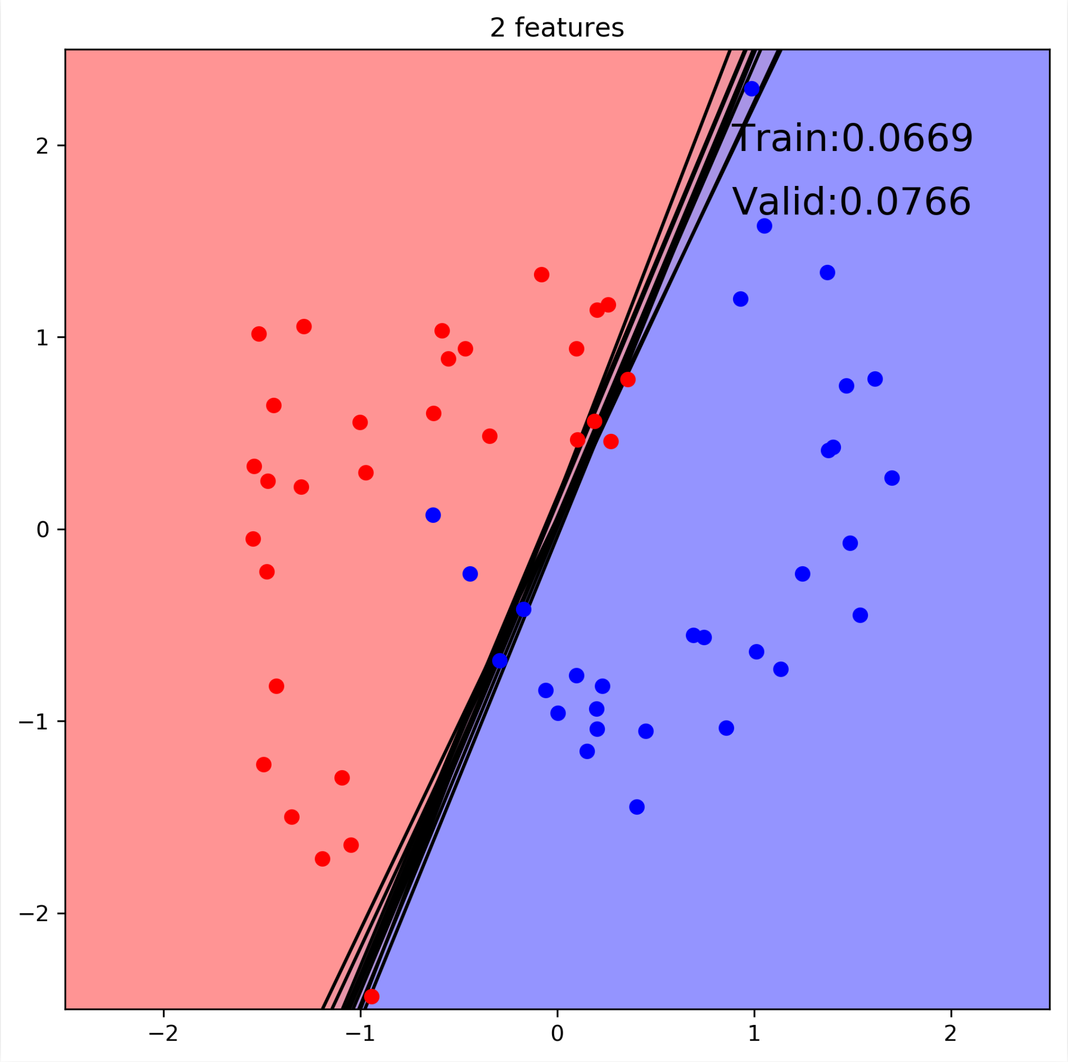
```
from sklearn.linear_model import LogisticRegression

def calc_fold(feats, X,Y, train_ix,valid_ix,C=1e12):
    """return error for train and validation sets"""
    reg = LogisticRegression(C=C, tol=1e-10)
    reg.fit(X[train_ix,:feats],Y[train_ix])
    prob = reg.predict_proba(X[:,:feats])[:,1]
    squares = (prob-Y)**2
    return np.mean(squares[train_ix]),np.mean(squares[valid_ix])
```

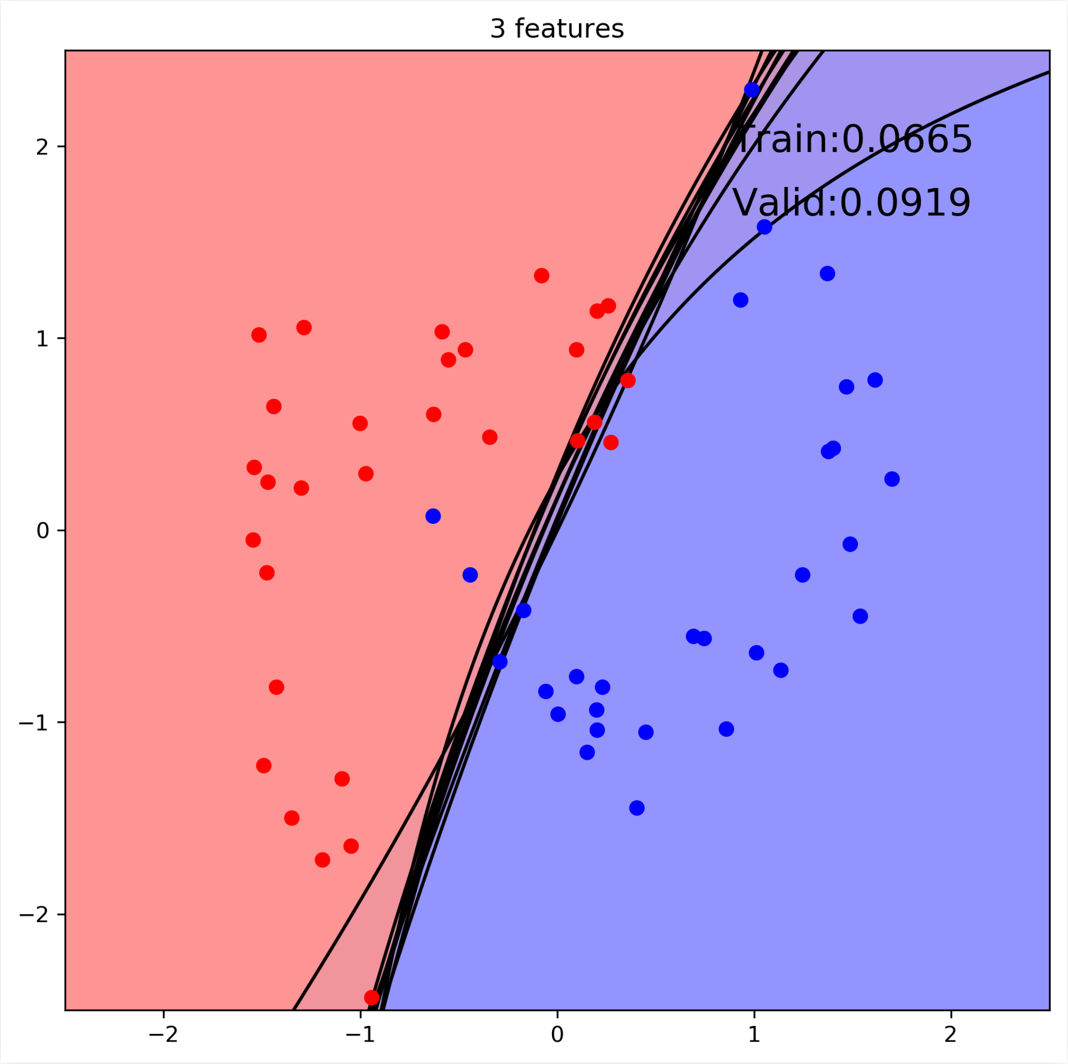
- Generate folds and loop

```
folds = 10
kf = StratifiedKFold(n_splits=folds)
for feats in range(2,16):
    tr_err = va_err = 0
    for tr_ix,va_ix in kf.split(Y_r,Y_r):
        r,v = calc_fold(feats,X_r,Y_r,tr_ix,va_ix)
        tr_err += r
        va_err += v
    print(feats,':', tr_err/folds,va_err/folds)
```

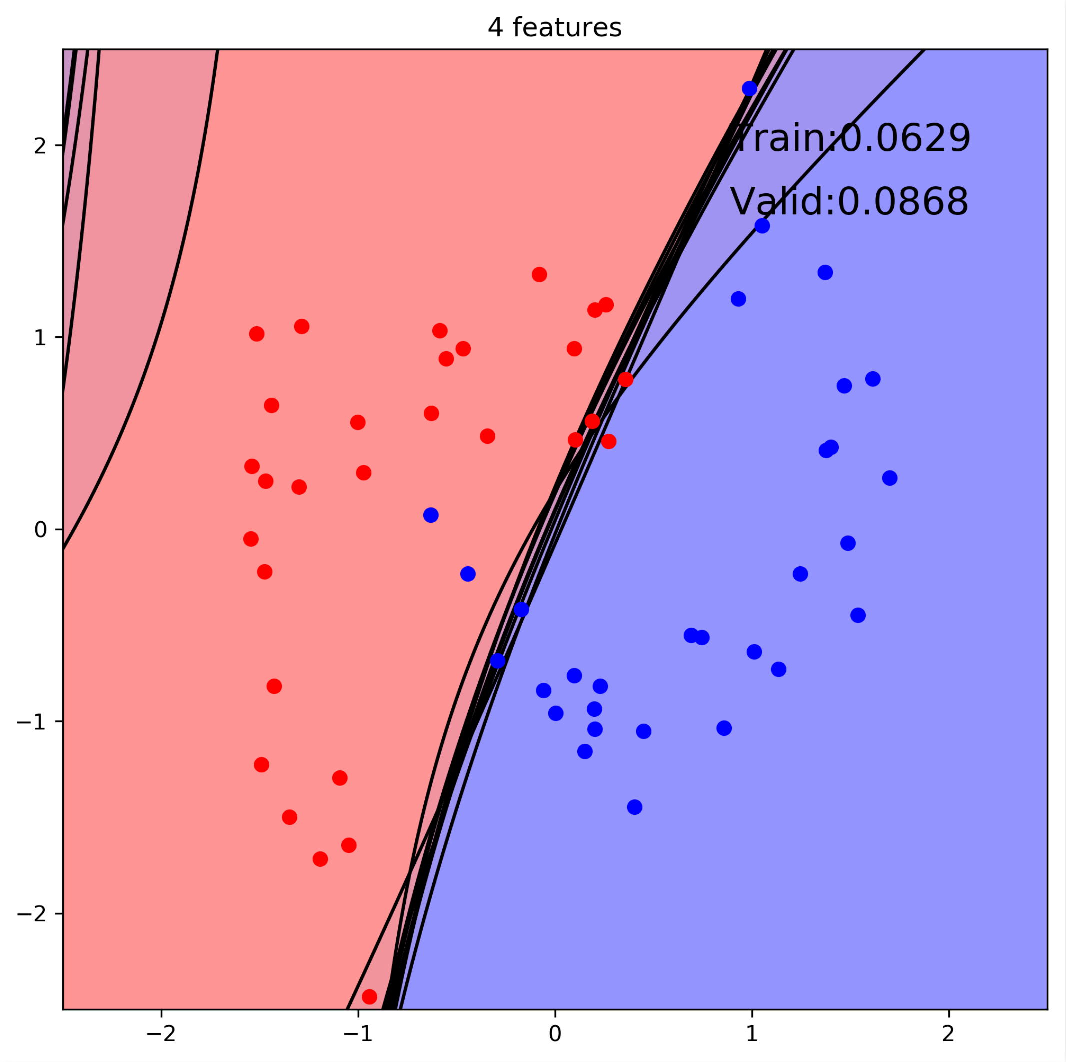
Example



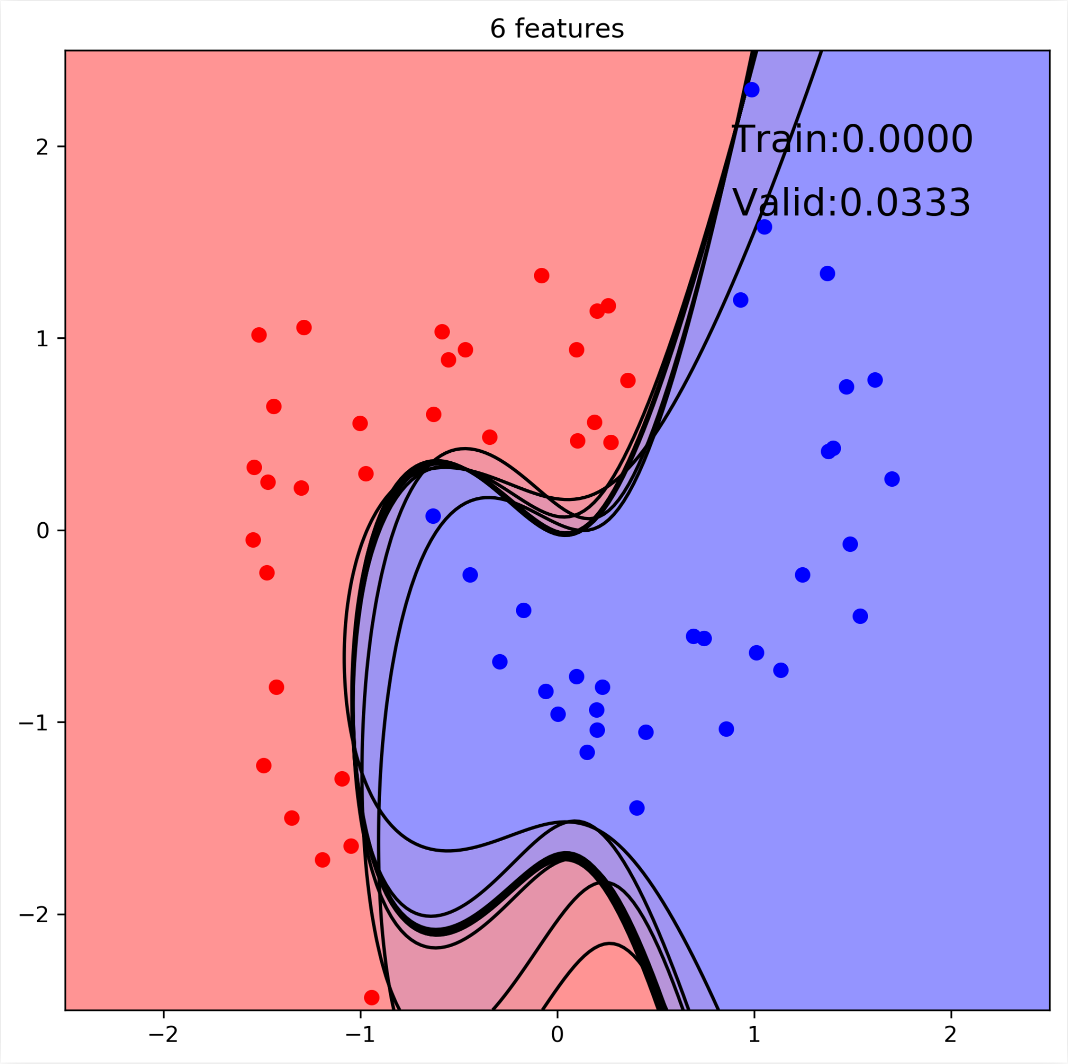
Example



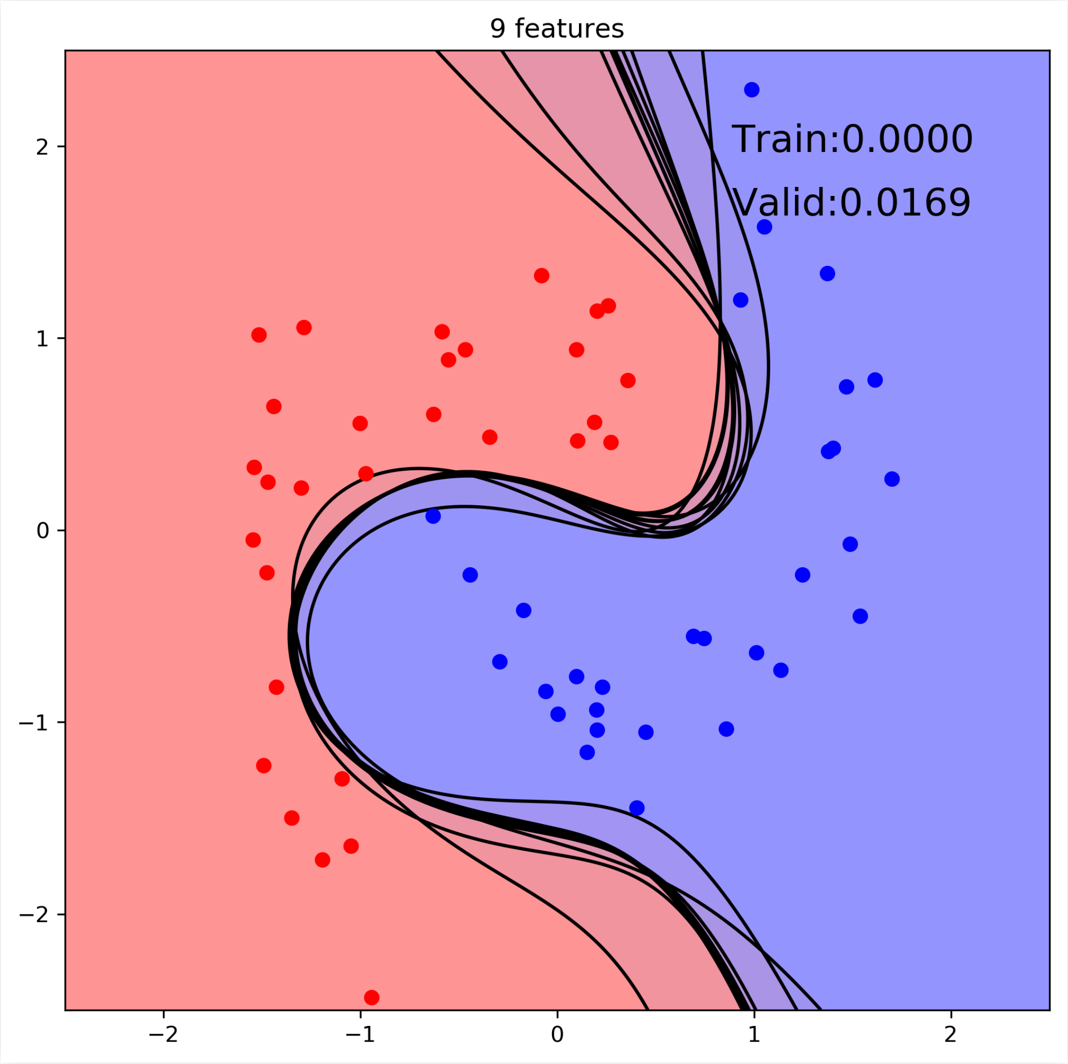
Example



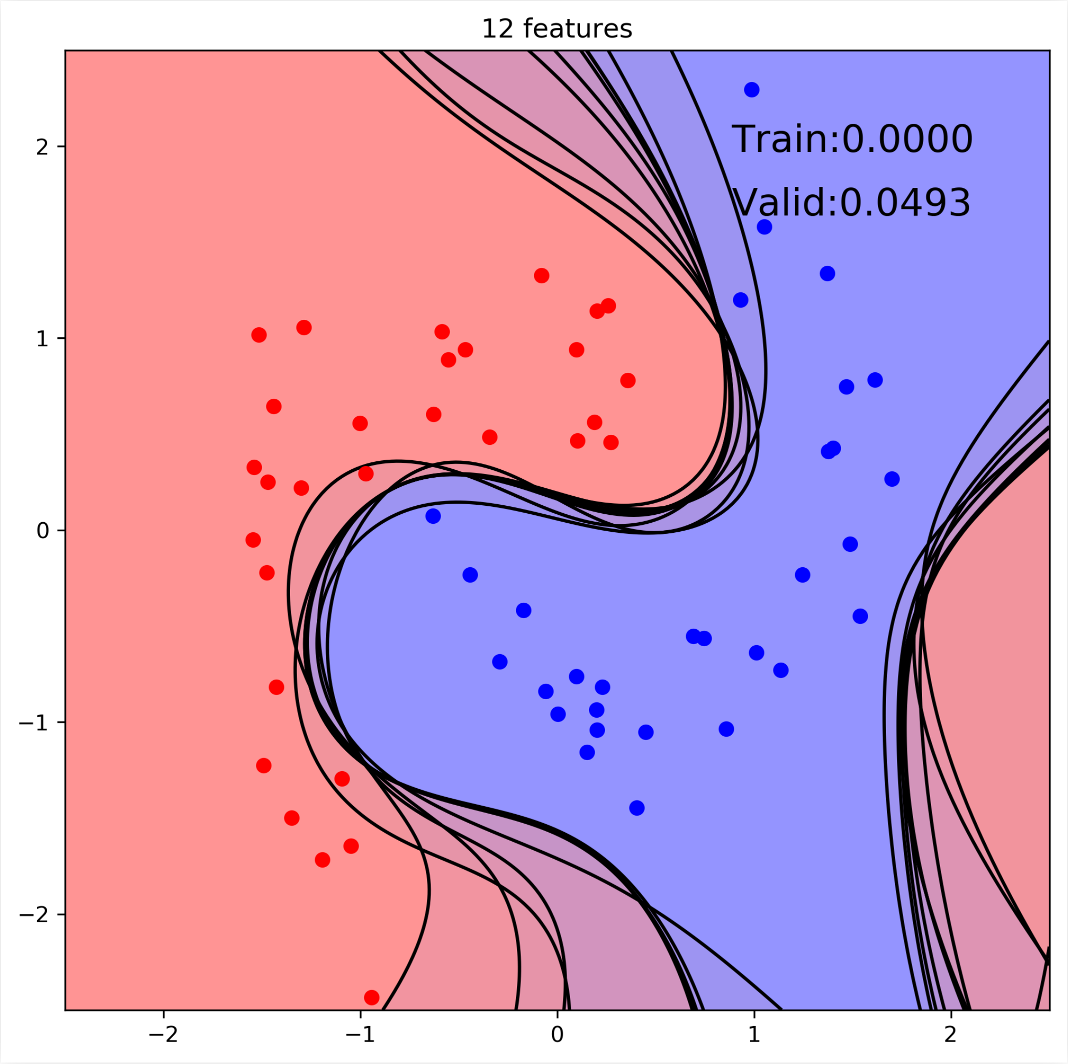
Example



Example

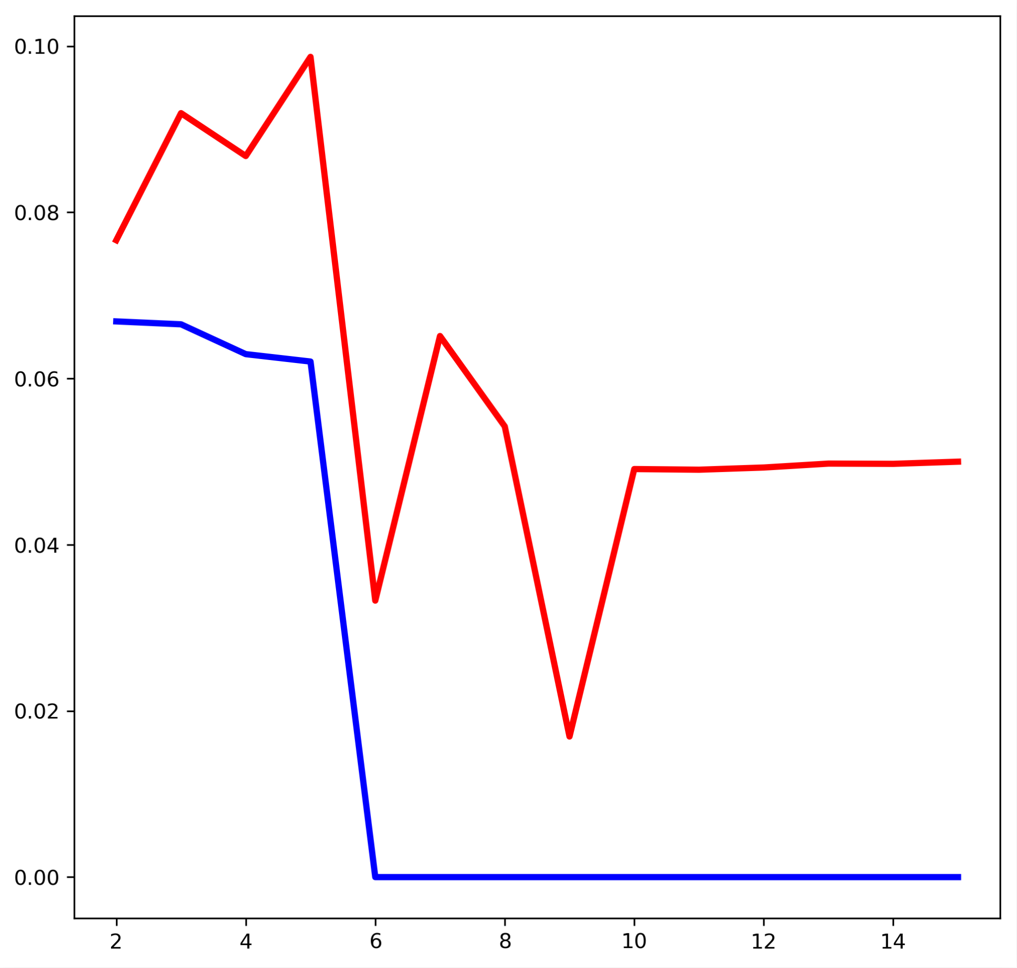


Example



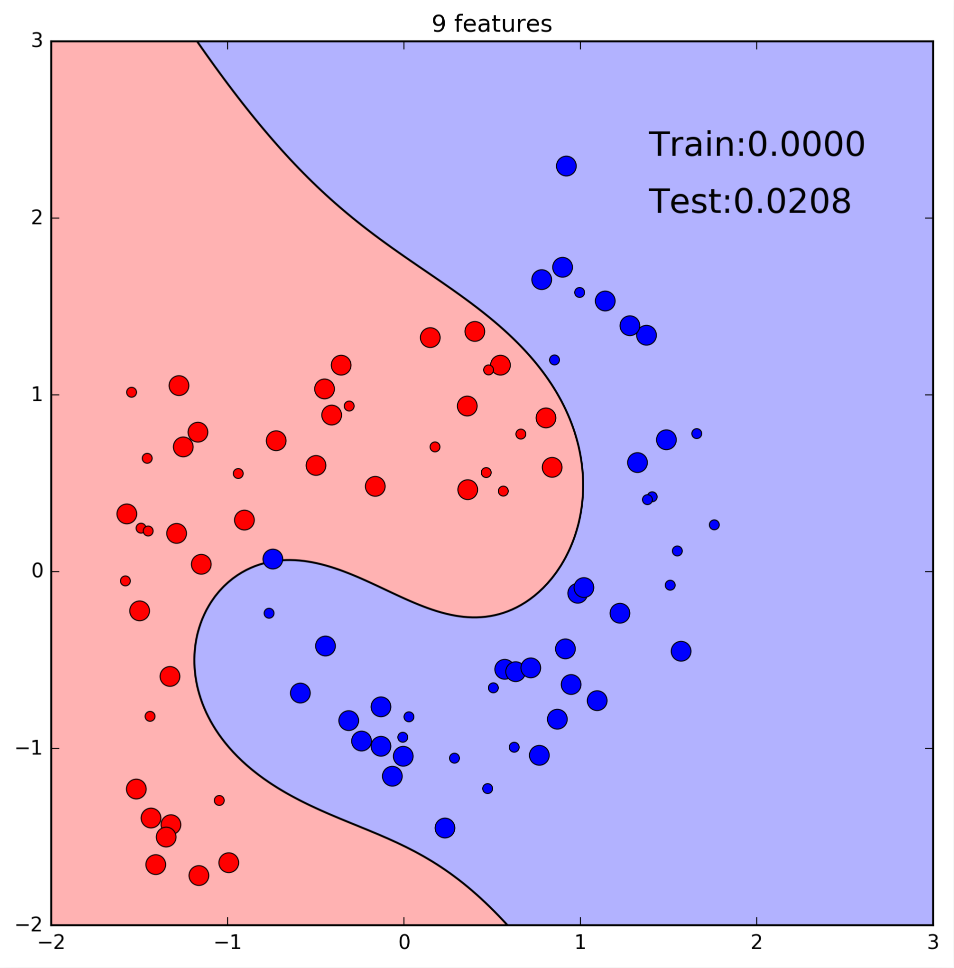
Example

- Cross-validation error (red), best model: 9 features



Example

- Retrain on whole training set, measure test error.



Example

Model selection with cross-validation

- Preprocess: shuffle; normalize or standardize
- Reserve a $\boxed{\text{test set}}$ (stratified?)
- Partition $\boxed{\text{training set}}$ into n folds (stratified?)
- $\boxed{\text{Cross validation}}$ to select the best model
- Train best model with all $\boxed{\text{training set}}$
- Estimate true error of final hypothesis on $\boxed{\text{test set}}$

- Why?
- Cross-validation error is unbiased and could be a good estimate of the true error
- But becomes biased by using it (and those examples) to select the best model

Regularization

Regularization

Logistic regression can be regularized

- For example, with L2 norm

$$\lambda \sum_{j=1}^{m} w_j^2$$

- LogisticRegression class offers a C parameter:

$$\frac{1}{C} \sum_{j=1}^{m} w_j^2$$

Regularization

Ridge regression is intuitive:

$$y = \theta_1 x^2 + \theta_2 x + \theta_3$$

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

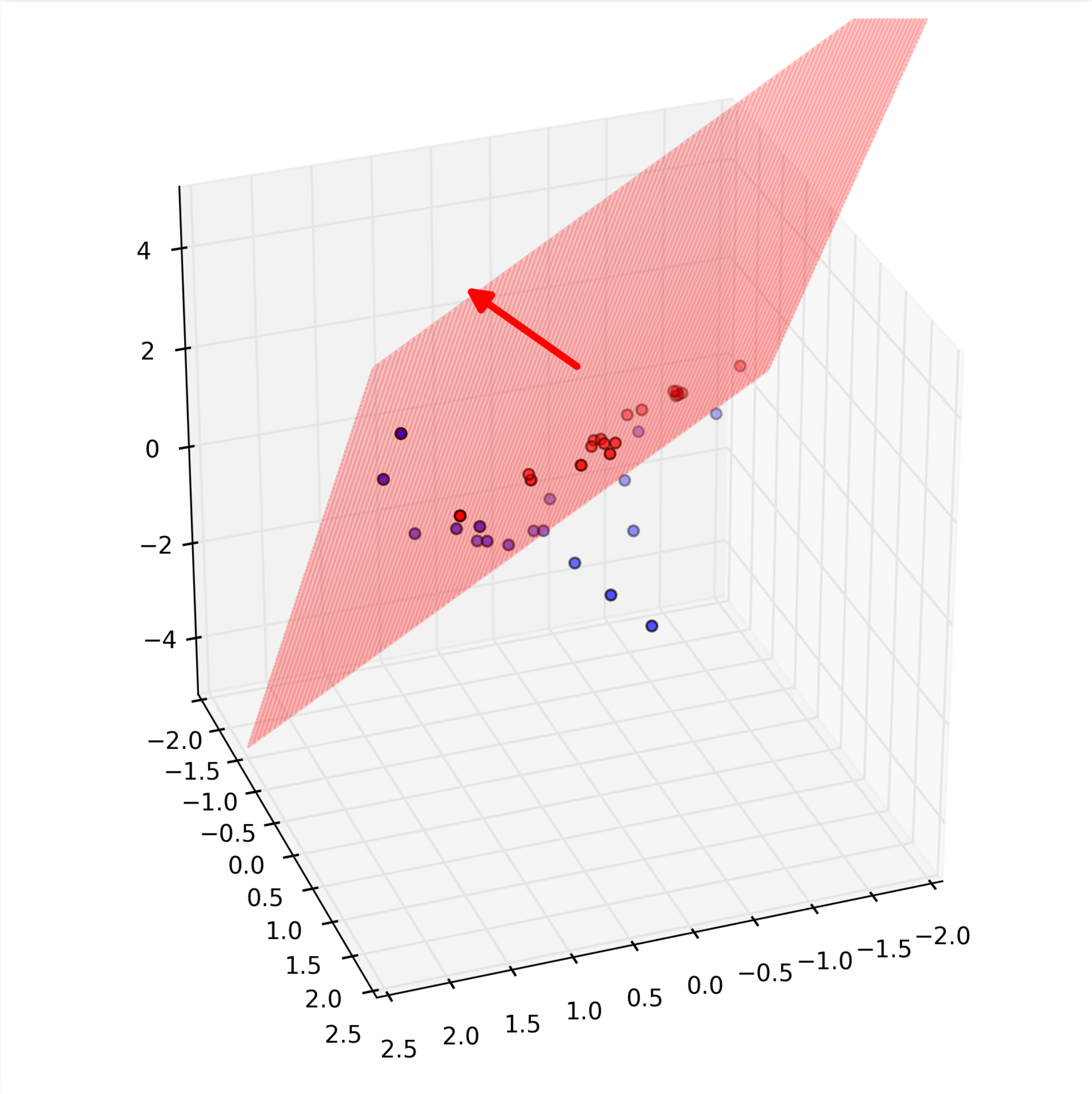
In logistic regression this seems less intuitive:

$$g(\vec{x}, \widetilde{w}) = \frac{1}{1 + e^{-\widetilde{w}^T \vec{x}}}$$

$$\frac{1}{C} \sum_{j=1}^{m} w_j^2$$

Regularization

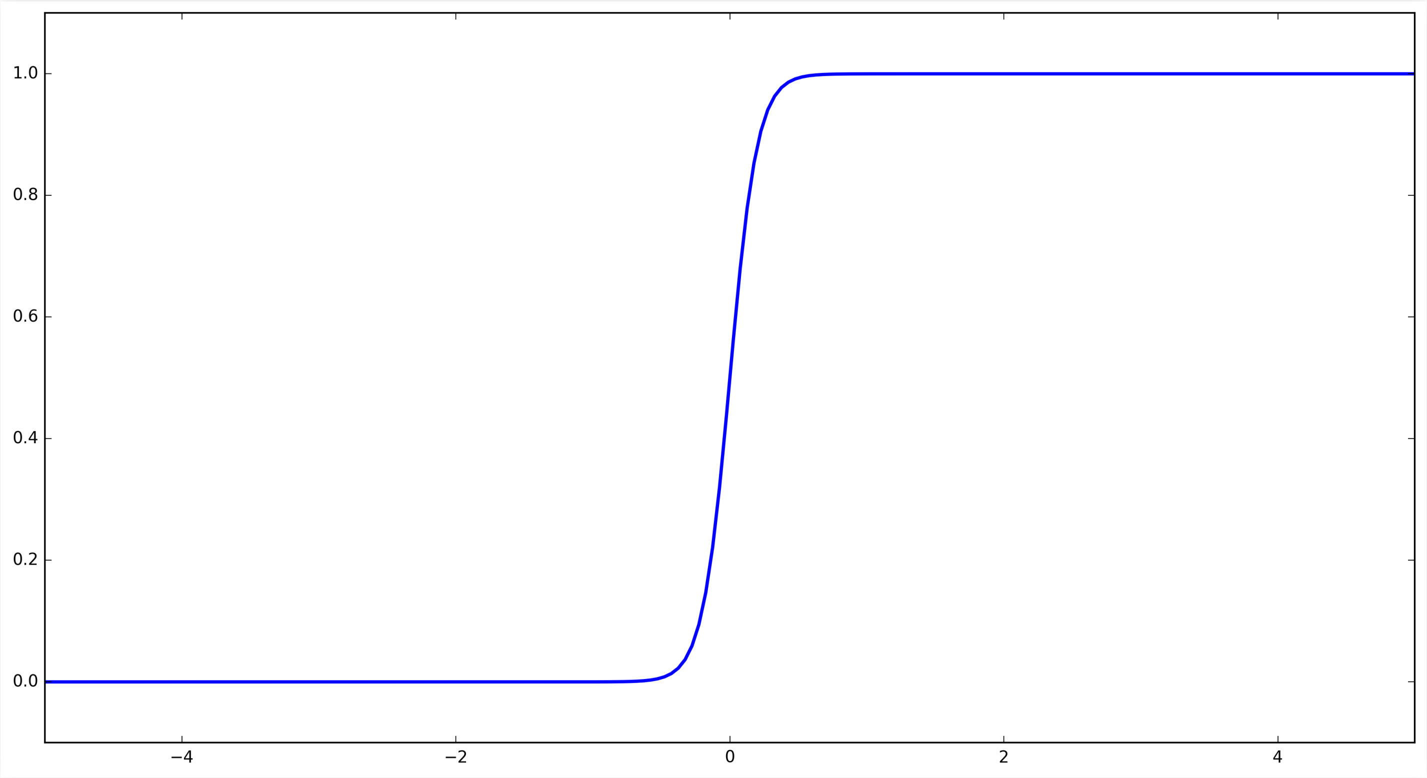
$$\tilde{w}^T \vec{x} = 0$$



Regularization

- Large $\widetilde{w}$, steep logistic function

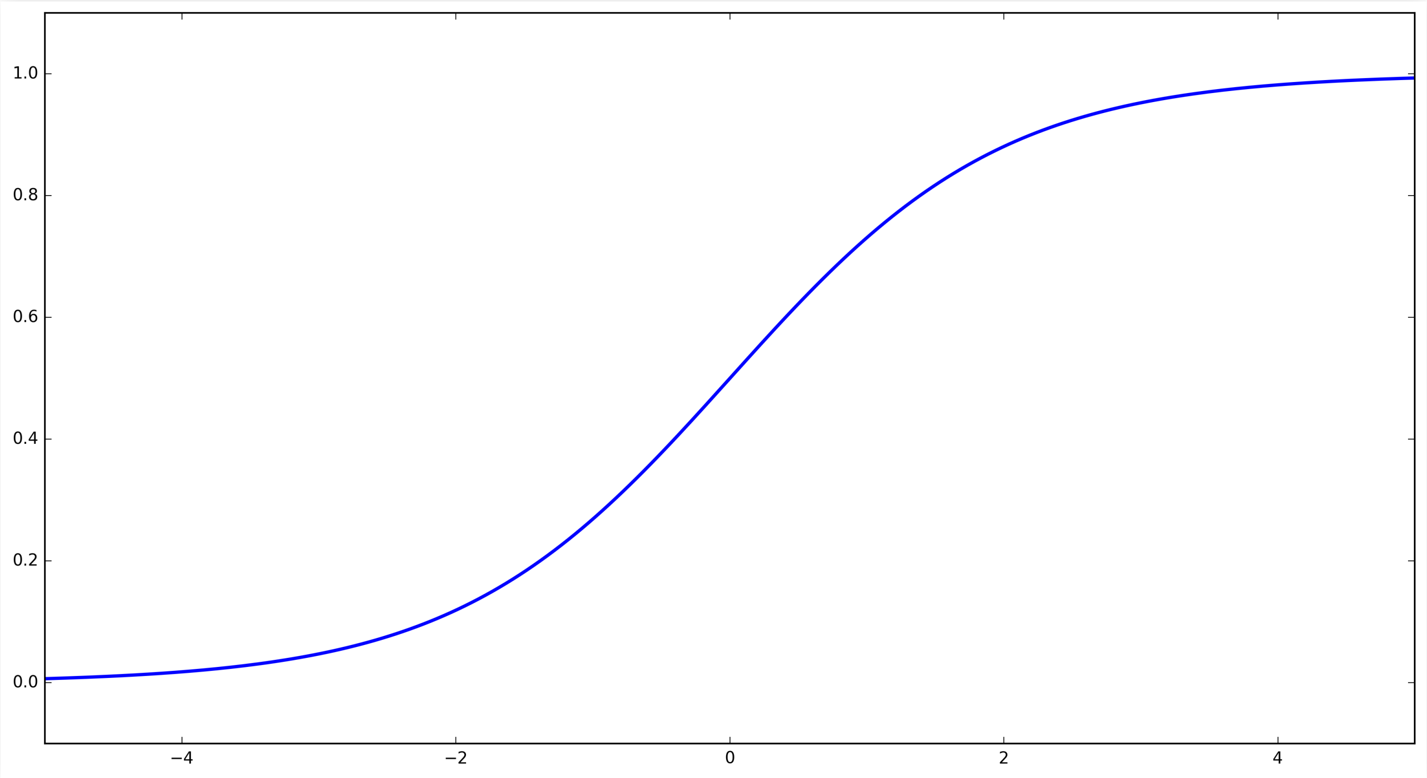
$$g(\vec{x}, \widetilde{w}) = \frac{1}{1 + e^{-\widetilde{w}^T \vec{x}}}$$



Regularization

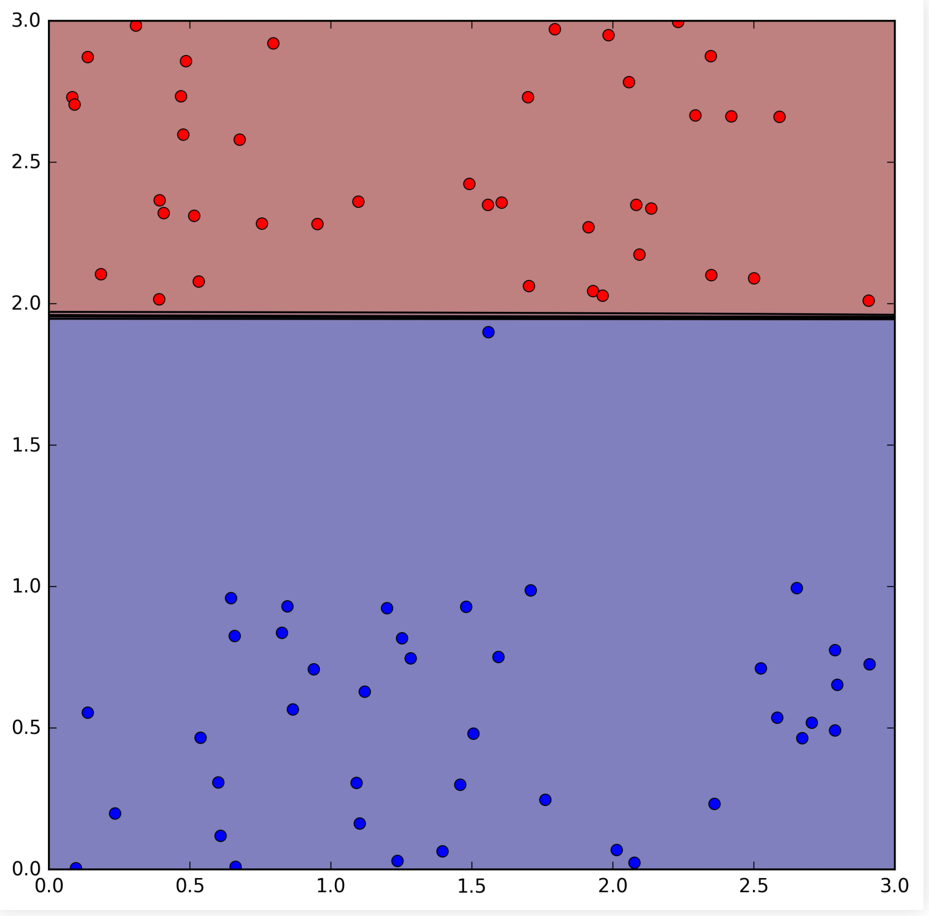
- A small $\widetilde{w}$ lowers the slope

$$g(\vec{x}, \widetilde{w}) = \frac{1}{1 + e^{-\widetilde{w}^T \vec{x}}}$$



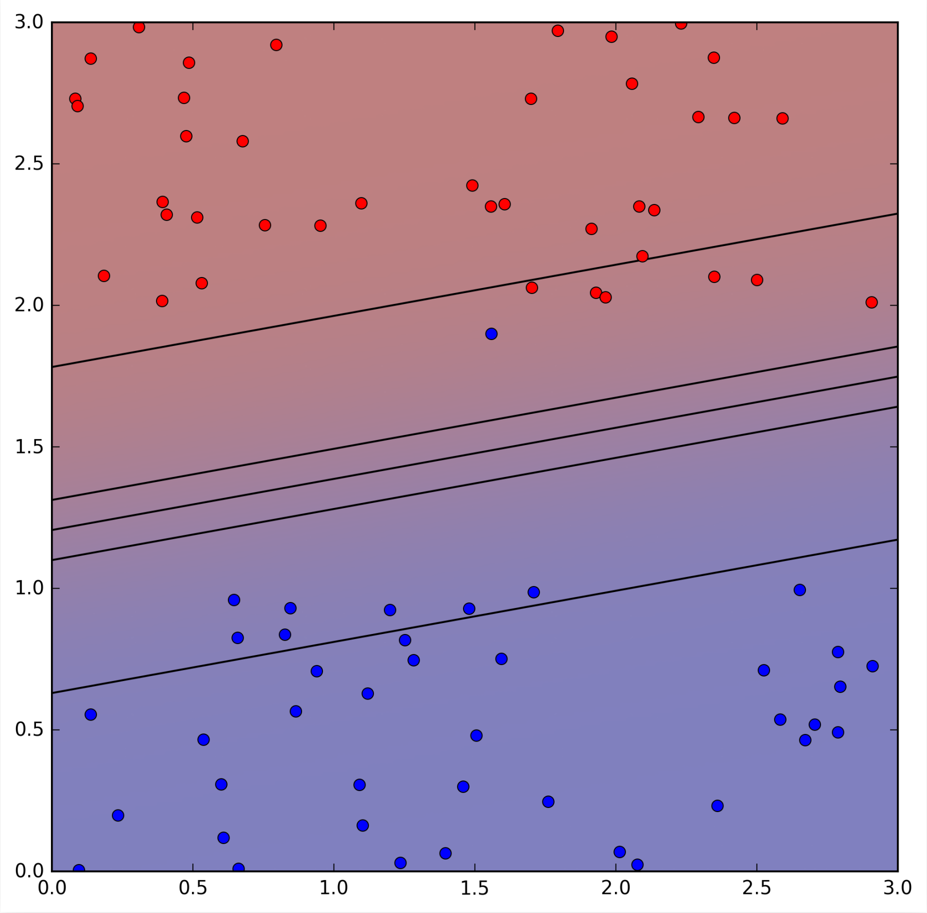
Regularization

- No regularization, overfitting



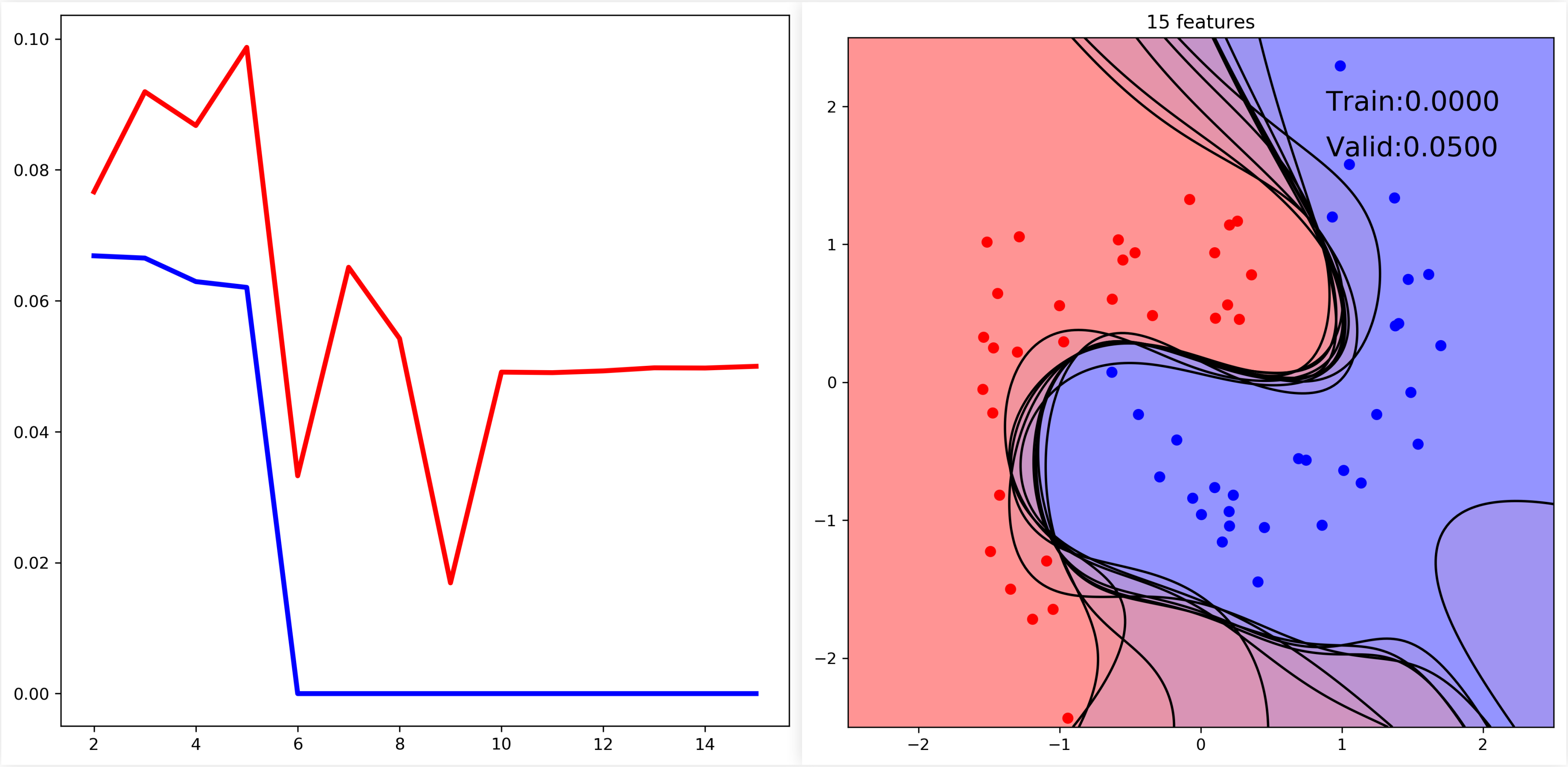
Regularization

- Regularization, large margins



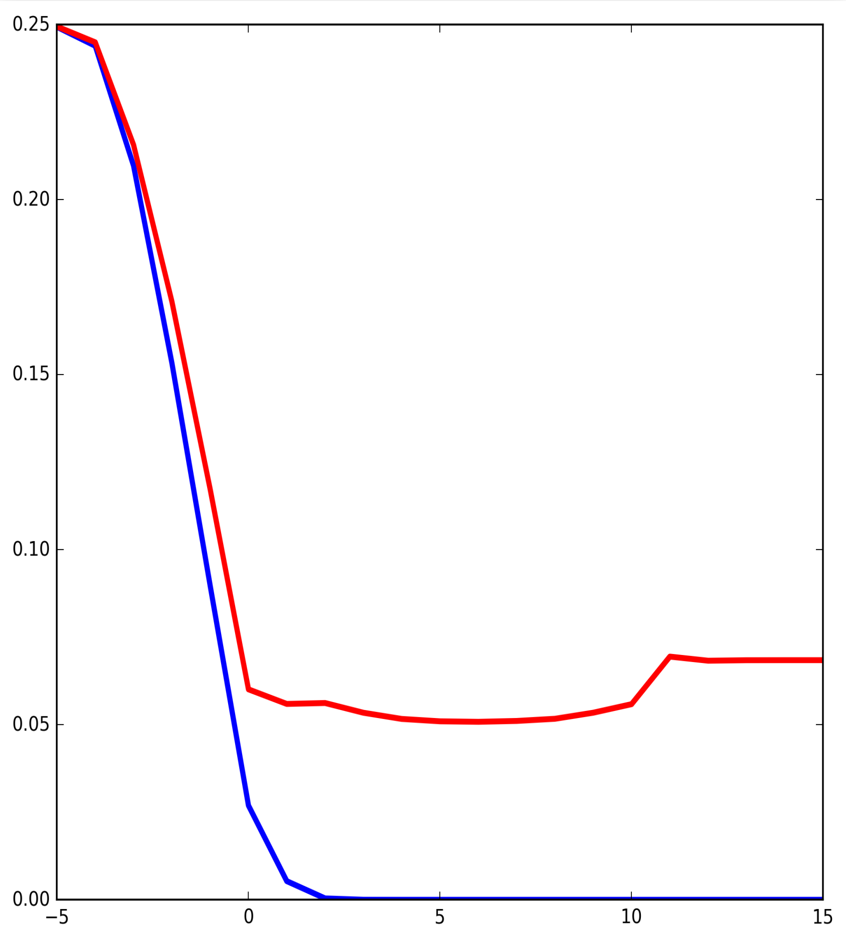
Regularization

- We'll use the 15 features model (overfitting)

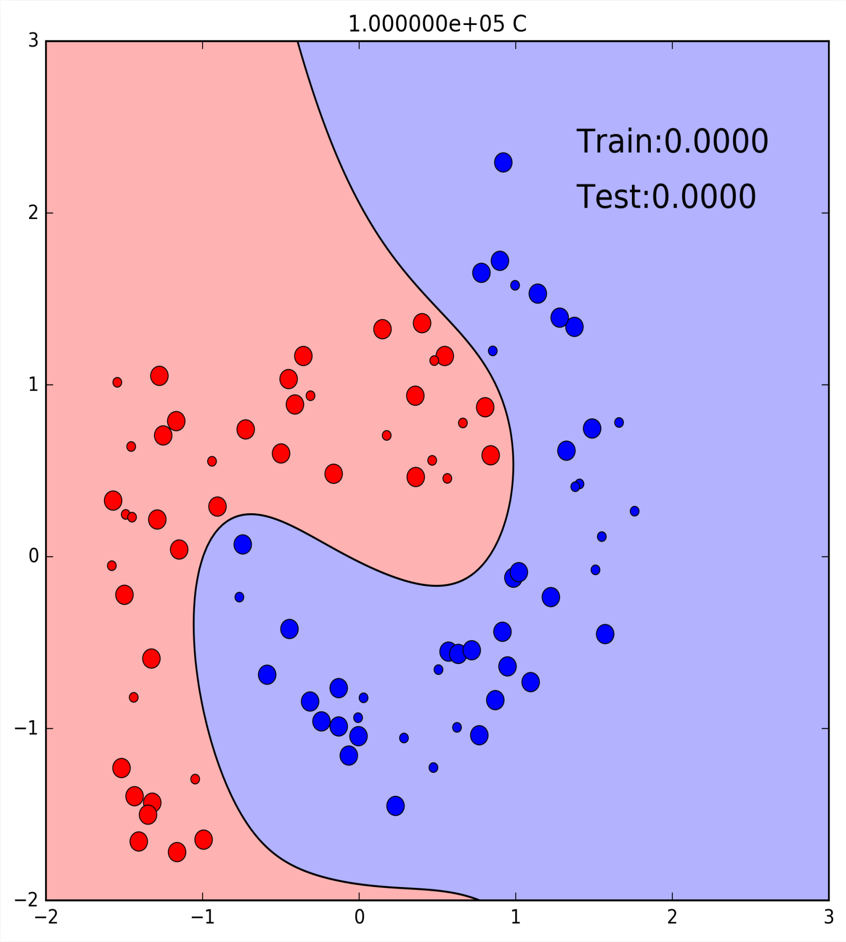


Regularization

Cross-val. error vs $log_{10}(C)$



15 features, $C = 10^5$



Note

Note on data expansion

- We are doing this manually to illustrate the idea
- In practice, we would use other classifiers (we'll see later)

Summary

Summary

- Scoring and evaluating classifiers
- Cross-validation and model selection
- Cross-validation and regularization
- Stratified sampling: train, folds, test

Further reading

- Alpaydin Section 2.7