Multiclass, Bias and Variance

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Bias and Variance

Summary

- Multiclass classification
- Bias: deviation from expected value
- Variance: scattering of predictions
- Computing Bias and Variance with bootstrapping
- Relation to underfitting and overfitting

Multiclass Classification

Multiclass Classification

Some clasifiers naturally handle multiple classes

- k-NN: output majority class from k neighbours.
- Naïve Bayes: output class with greatest joint probability

$$C^{NaïveBayes} = \underset{k \in \{0,1,\ldots,K\}}{\operatorname{argmax}} \ln p(C_k) + \sum_{j=1}^{N} \ln p(x_j | C_k)$$

Multiclass Classification

Example:

- Iris dataset, https://archive.ics.uci.edu/ml/datasets/Iris

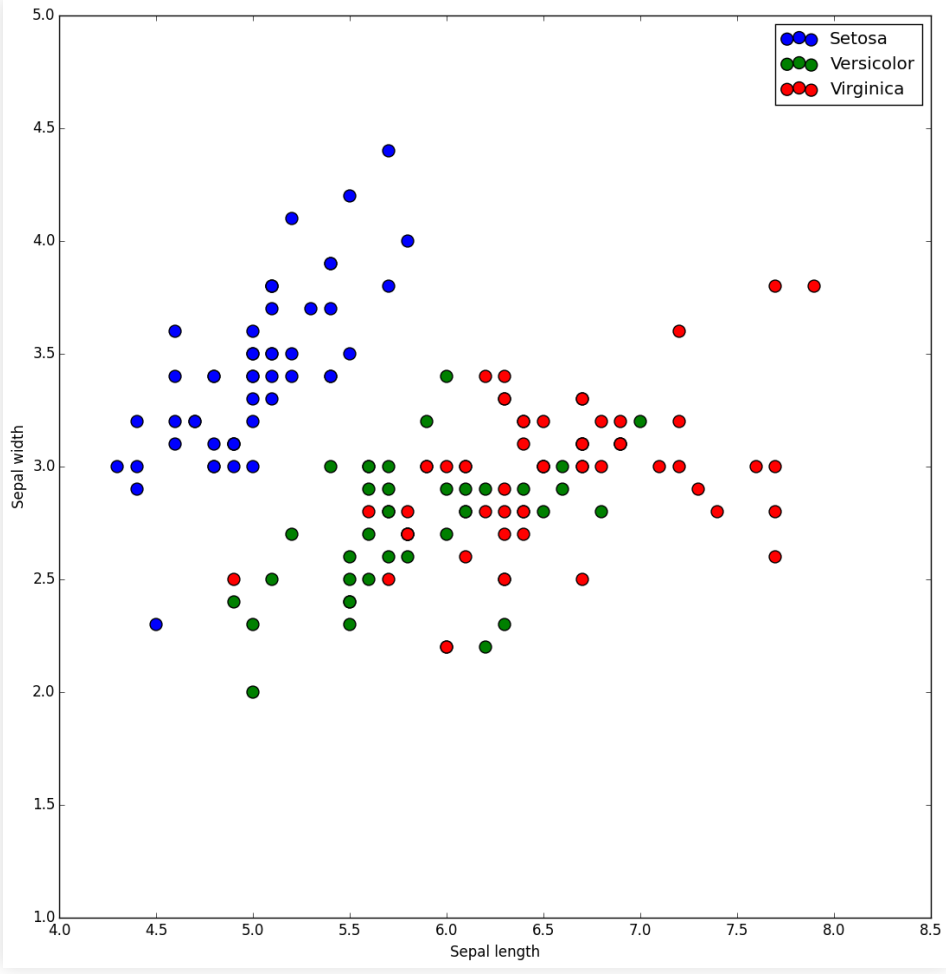
CC BY-SA: Gordon, Robertson3 classes:

- 3 Classes
  - Setosa
  - Versicolor
  - Virginica
- 4 Attributes:
  - Sepal length
  - Sepal width
  - Petal length
  - Petal width

Iris dataset

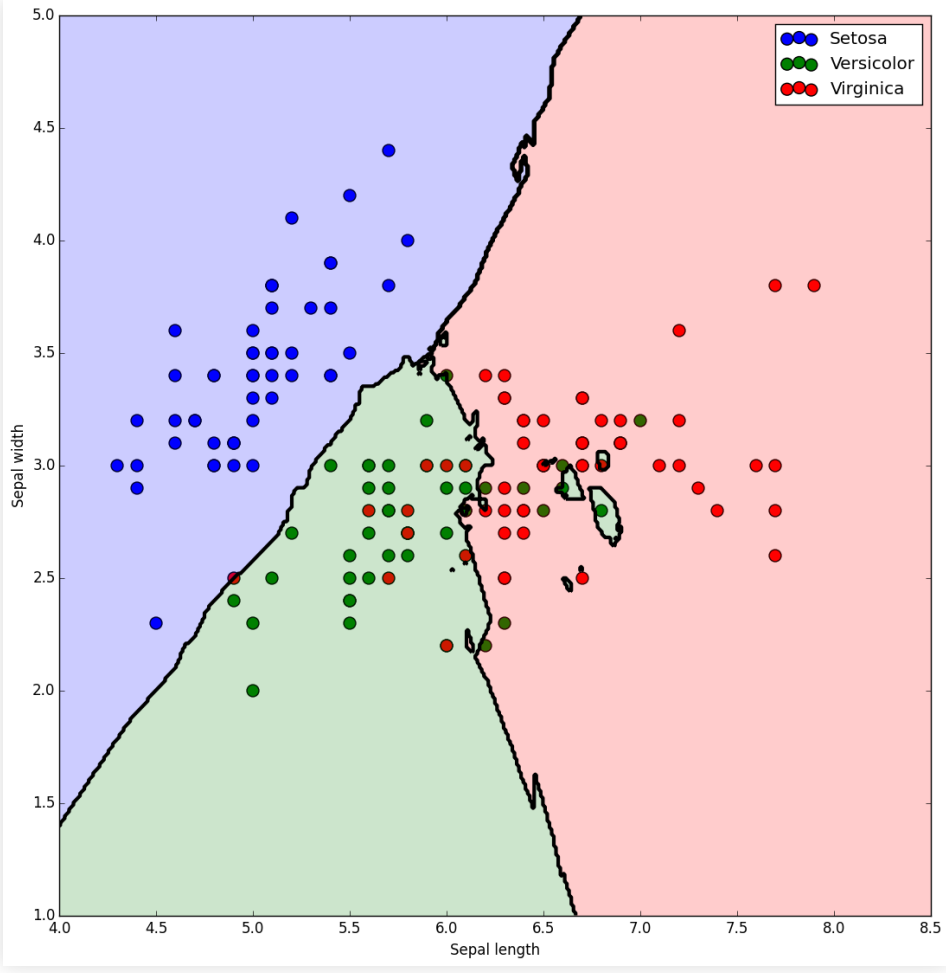
Multiclass Classification

- Example: Iris dataset



Multiclass Classification

k-NN classification (k = 15)



Multiclass Classification

Linear disciminant classifiers need some adaptation

$$\vec{w}^T \vec{x} + w_0 = 0$$

- (Logistic Regression, SVM, MLP...)

Generic solutions for binary classifiers:

- One versus the rest: K-1
- One versus one: K(K-1)/2
- One versus the rest: K, max

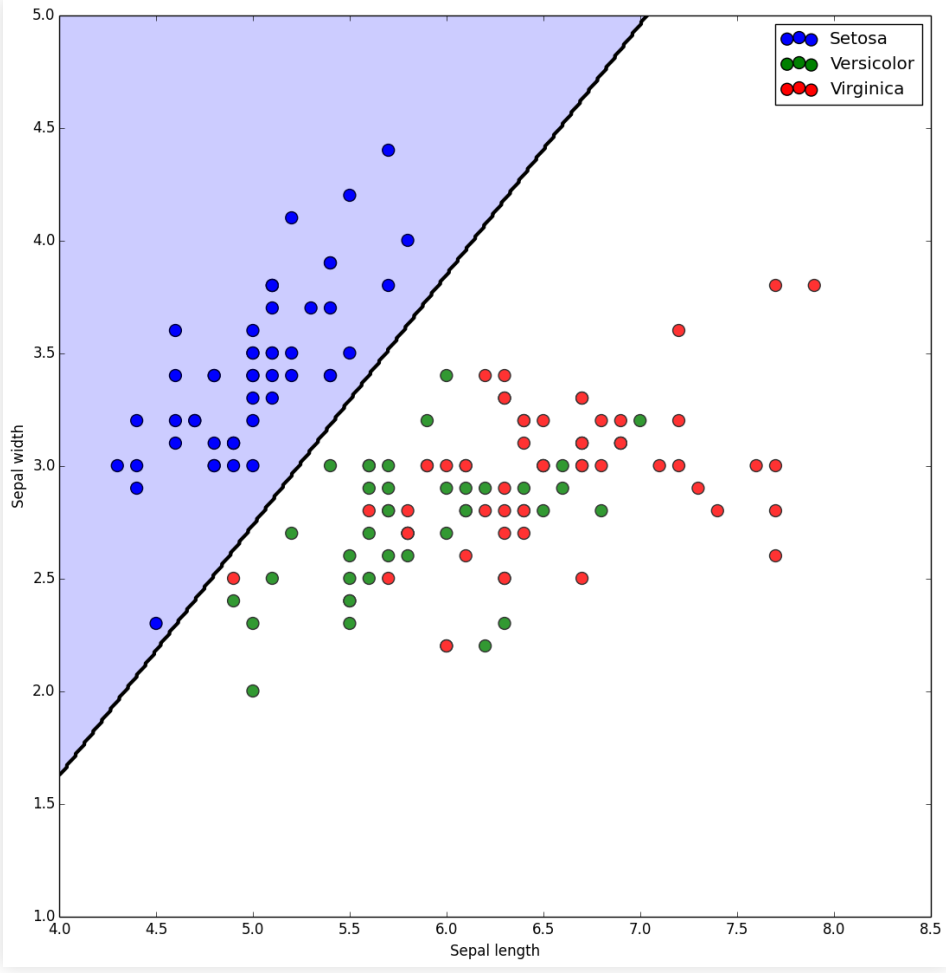
Multiclass Classification

Multiclass: one vs the rest (K-1)

- Create K-1 classifiers
- For each k in {1 ... K-1}, set class k as 1 and others as 0
- Assign class {1 ... K-1} according to which classifier returns 1, or class K if none.

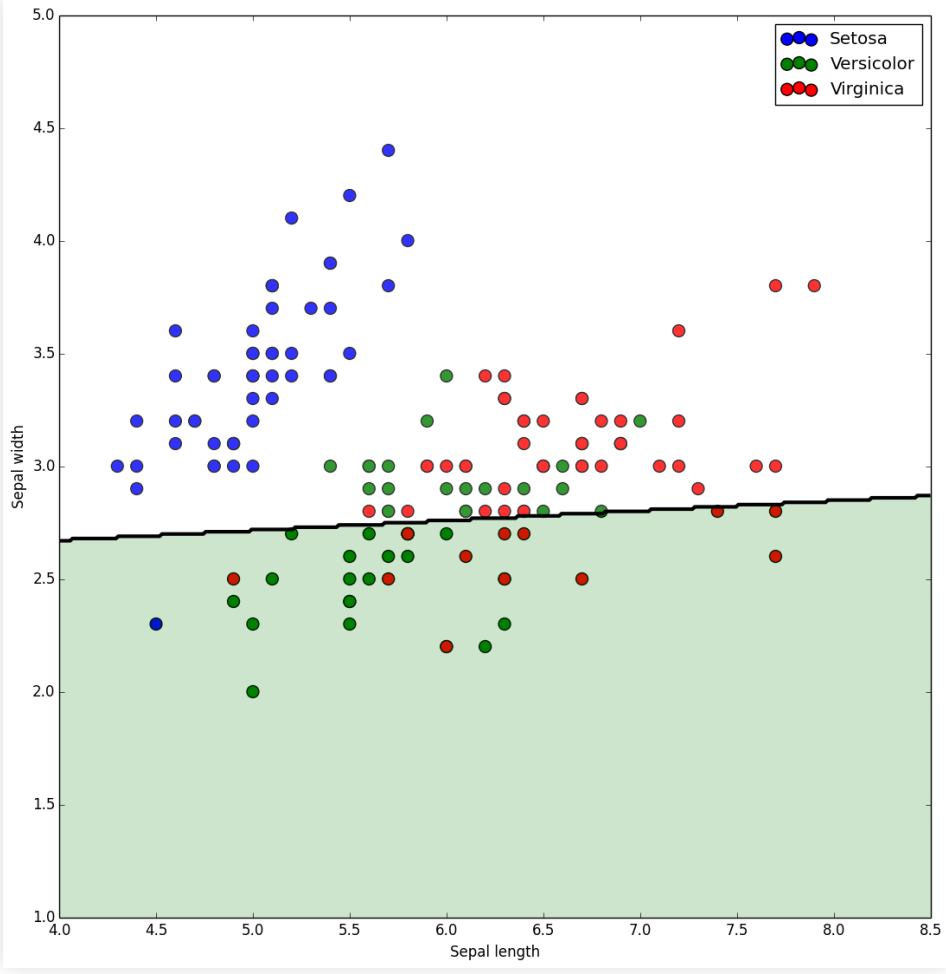
Multiclass Classification

- One vs the rest (K-1), Classifier for Setosa



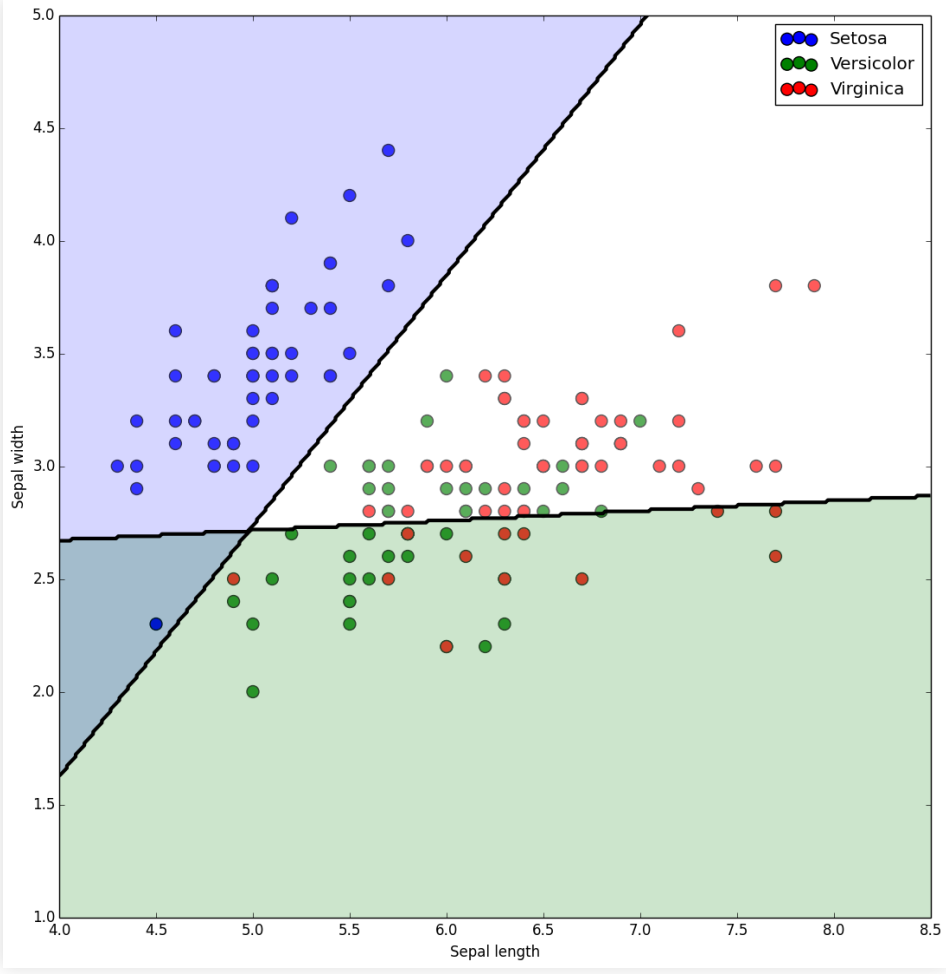
Multiclass Classification

- One vs the rest (K-1), Classifier for Versicolor



Multiclass Classification

- One vs the rest (K-1), Final classifier (ambiguous areas)



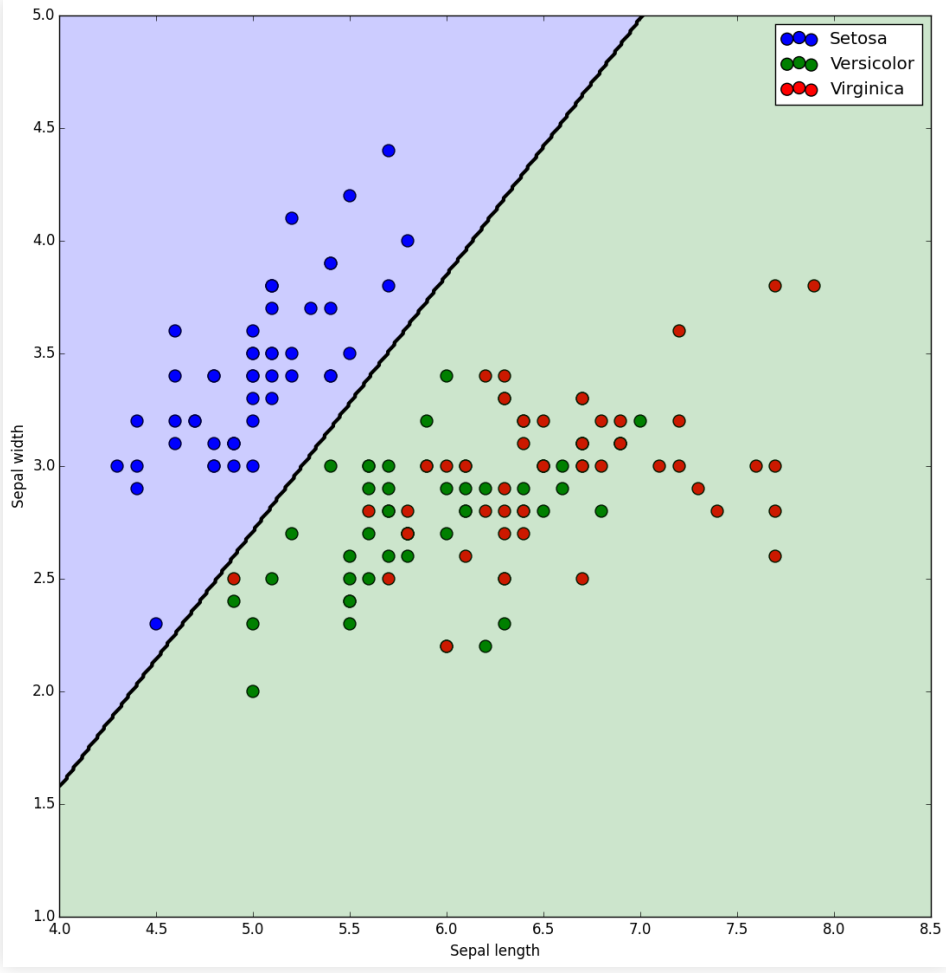
Multiclass Classification

Multiclass: one vs one K(K-1)/2

- Build classifiers for all pairs.

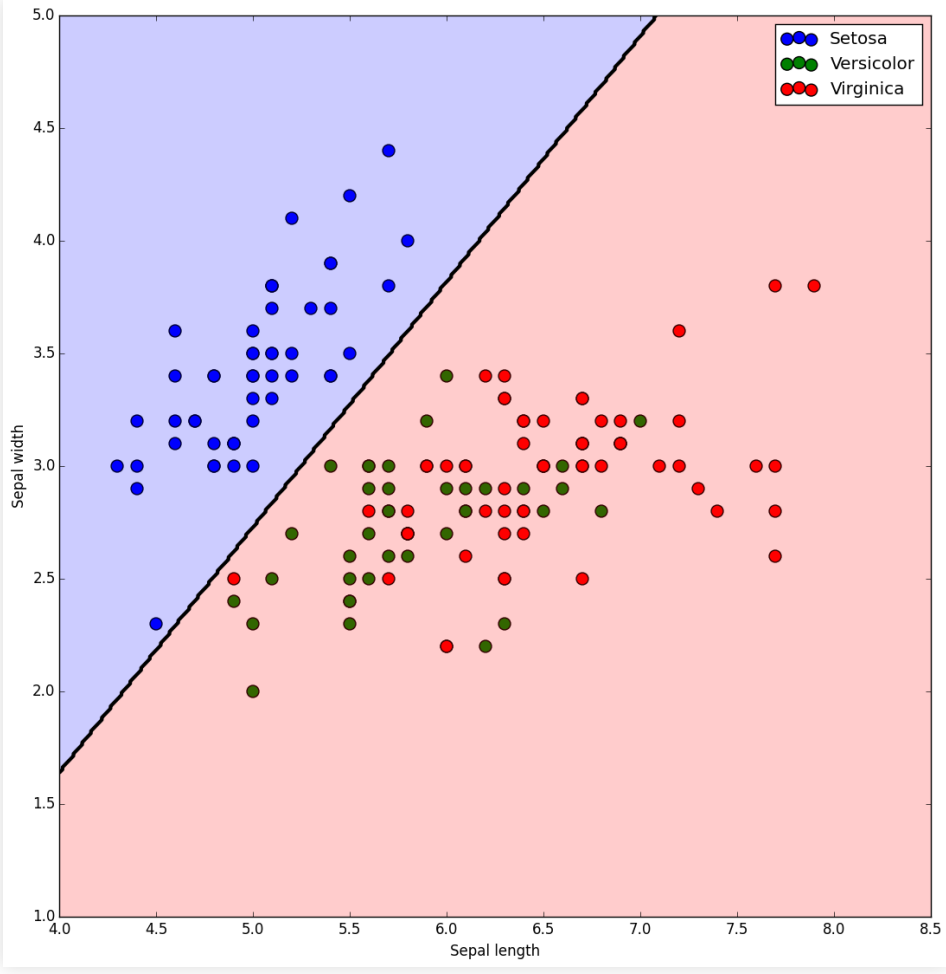
Multiclass Classification

- One vs one K(K-1)/2, Setosa vs Versicolor



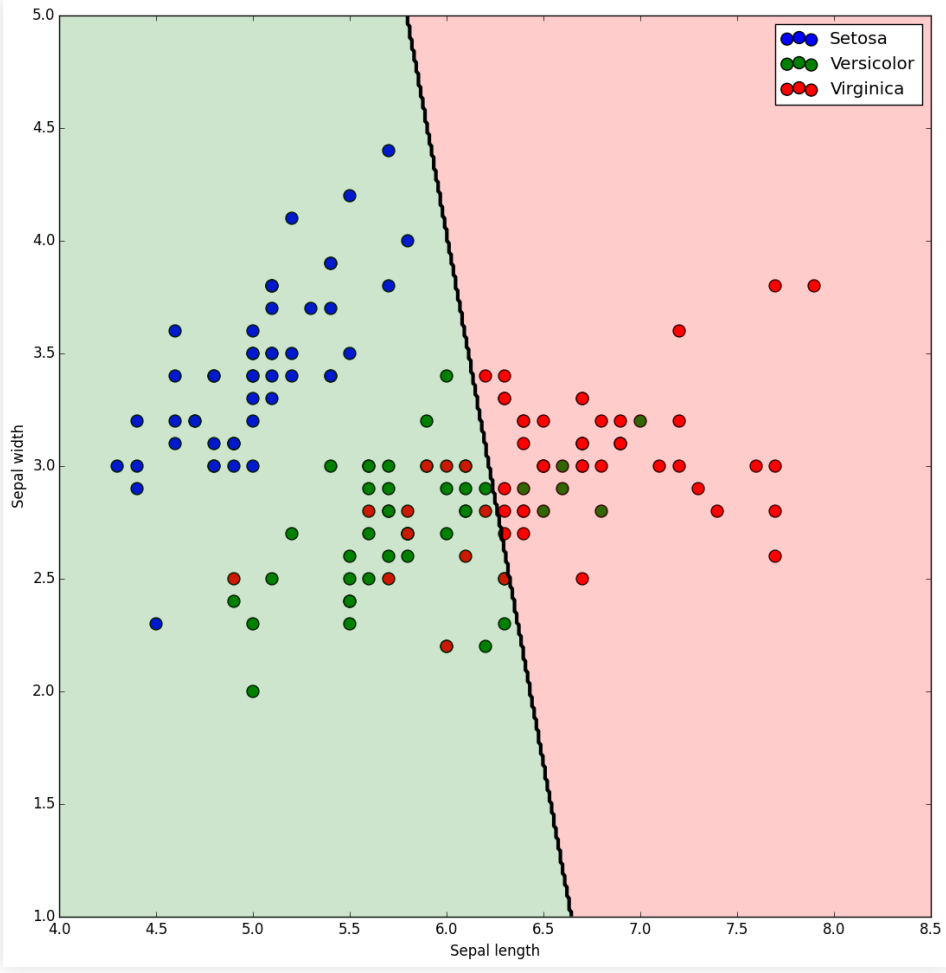
Multiclass Classification

- One vs one K(K-1)/2, Setosa vs Virginica



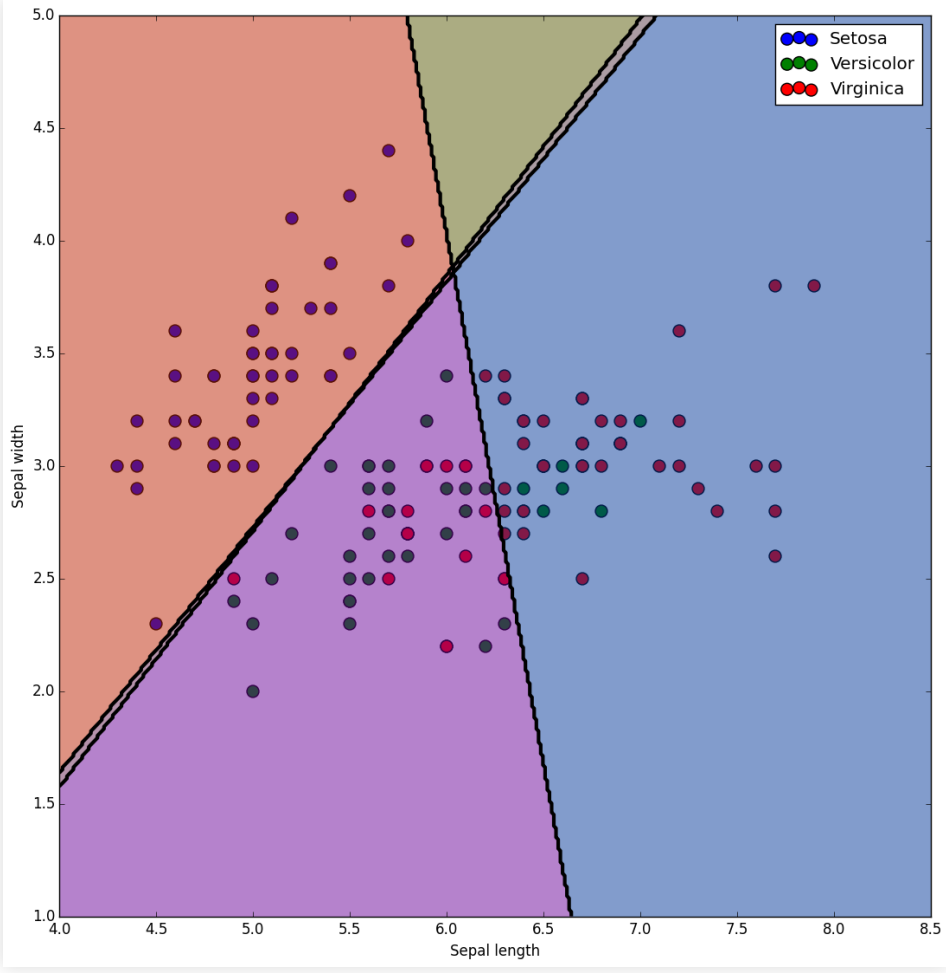
Multiclass Classification

- One vs one K(K-1)/2, Versicolor vs Virginica



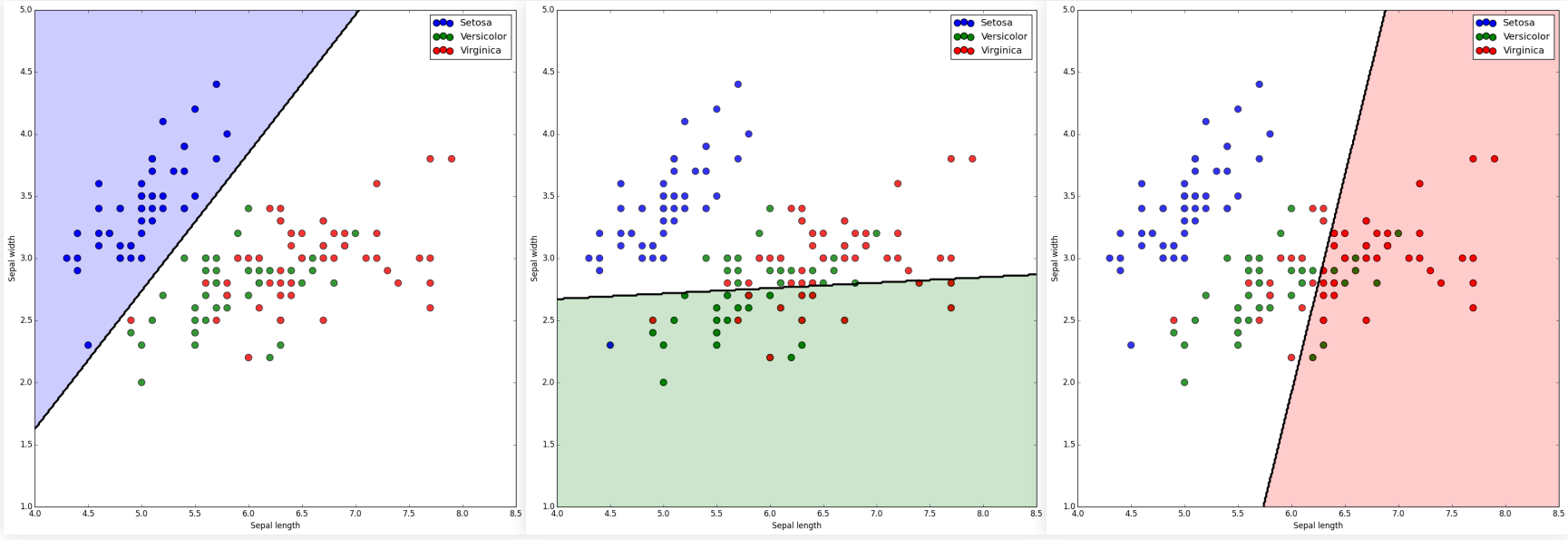
Multiclass Classification

- One vs one K(K-1)/2, Final: also ambiguous areas



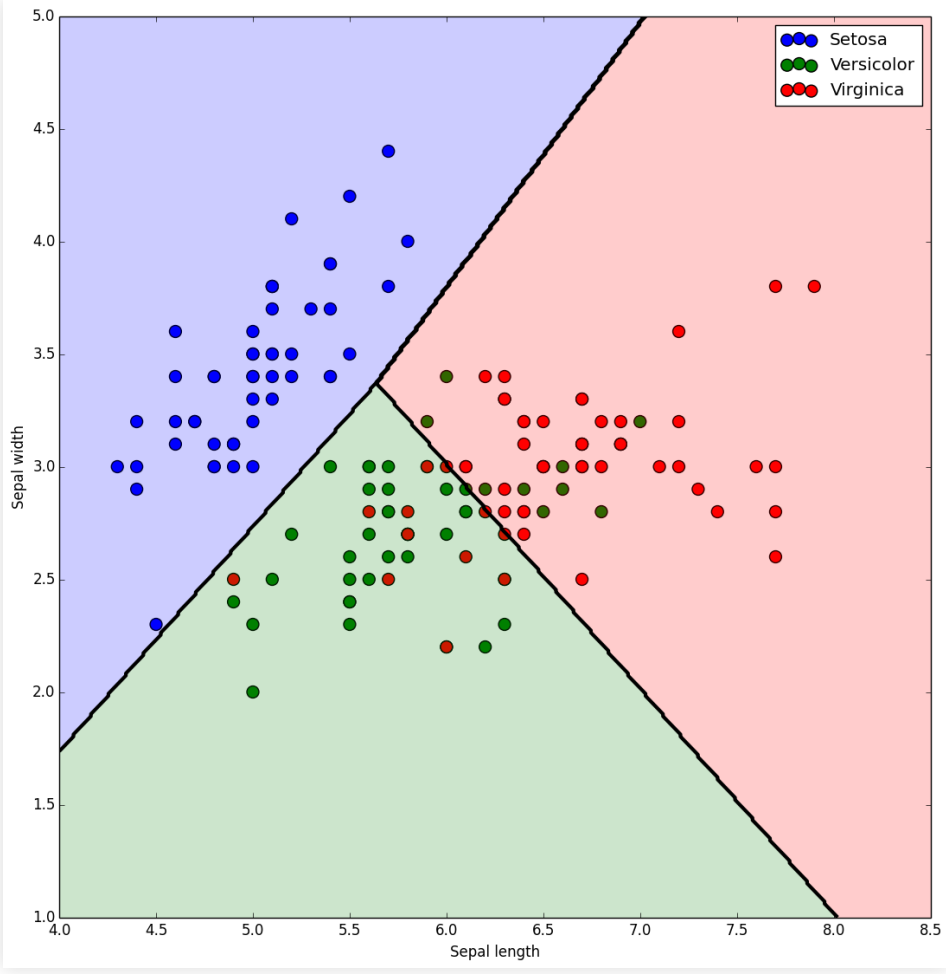
Multiclass: one vs rest K (or one vs all)

- Better: K OvR classifiers



Multiclass Classification

- One vs rest: Classify using max of decision function



Multiclass Classification

Pros of multiclass classification with one vs rest:

- Classify using max of decision function
- Helps avoid ambiguous classifications (depending on decision function)

Cons of multiclass classification with one vs rest:

- Classifiers may be unbalanced (more negative than positive)
- The confidence values of the decision function may not be directly comparable

Logistic Regression

- Extend cross-entropy error function:

$$p(T|w_1,\ldots,w_K) = \prod_{n=1}^{N}\prod_{k=1}^{K} p(C_k|\phi_n)^{t_{nk}} = \prod_{n=1}^{N}\prod_{k=1}^{K} y_{nk}^{t_{nk}}$$

$$E(w_1,\ldots,w_K) = -\sum_{n=1}^{N}\sum_{k=1}^{K} t_{nk}\ln y_{nk}$$

- Where $t_n k$ is 1 if the point is in class k, 0 otherwise

```
from sklearn.linear_model import LogisticRegression
#One versus rest, max
logreg = LogisticRegression(C=1e5,multi_class='ovr')
logreg.fit(X, Y)

#Cross entropy
logreg = LogisticRegression(C=1e5,multi_class='multinomial')
logreg.fit(X, Y)
```

Multilayer Perceptron

- For 2 classes, need only one output neuron
  - Sigmoid, probability of belonging to C_1
- For K classes, use K output neurons with softmax function:
  - (extension of sigmoid)

$$\sigma : \mathbb{R}^K \rightarrow [0,1]^K \qquad \sigma(\vec{x})_j = \frac{e^{x_j}}{\sum_{k=1}^{K} e^{x_k}}$$

- Softmax returns a vector where $\sigma_j \in [0,1]$ and $\sum_{k=1}^{K} \sigma_k = 1$
- Represents probability of example belonging to each class C_j

Multiclass Classification

General solution: One vs Rest

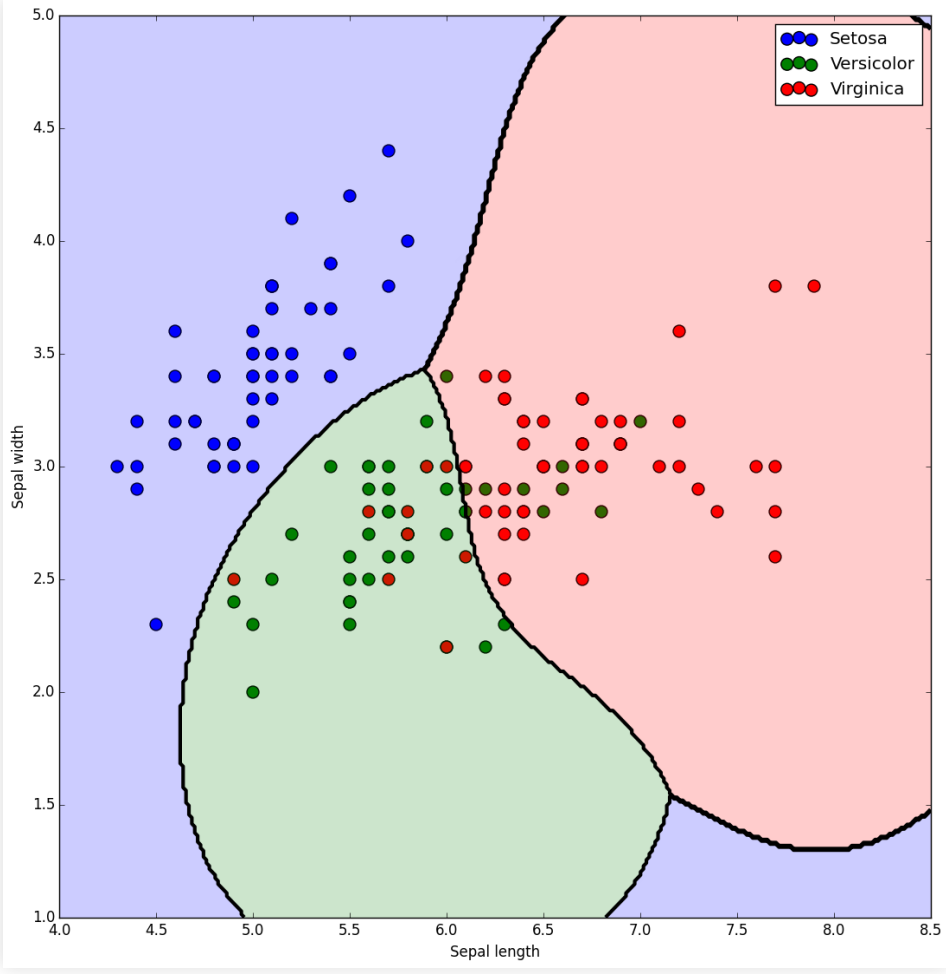
`OneVsRestClassifier`

- Fits one classifier per class, calling `fit()`
- Predicts from maximum of `decision_function()`

```
ovr = OneVsRestClassifier( SVC(kernel='rbf', gamma=0.7, C=10) )
ovr.fit(X, Y)
ovr.predict(test_set)
```

Multiclass Classification

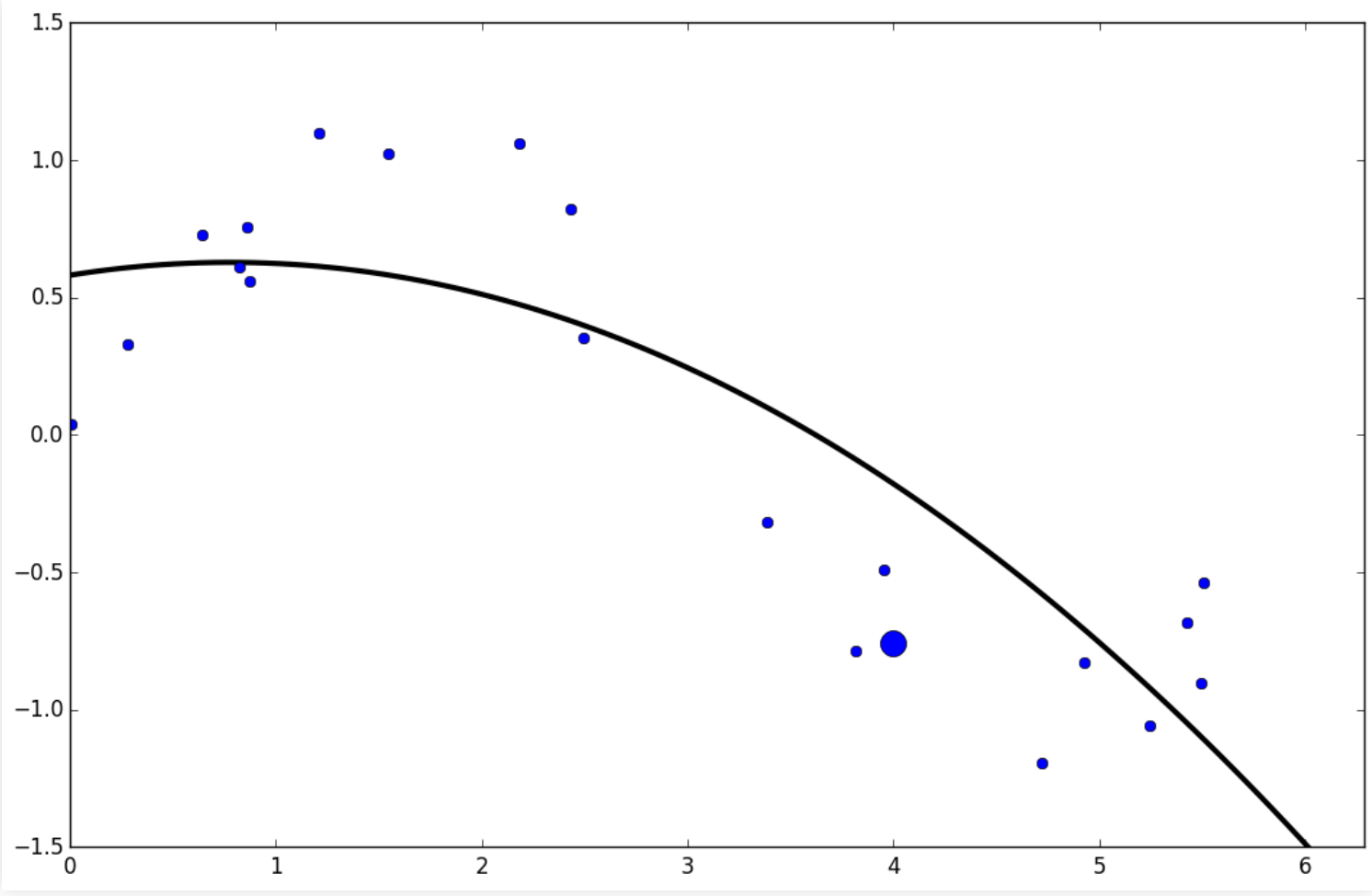
- `OneVsRestClassifier`: automate OvR, max. decision



Bias

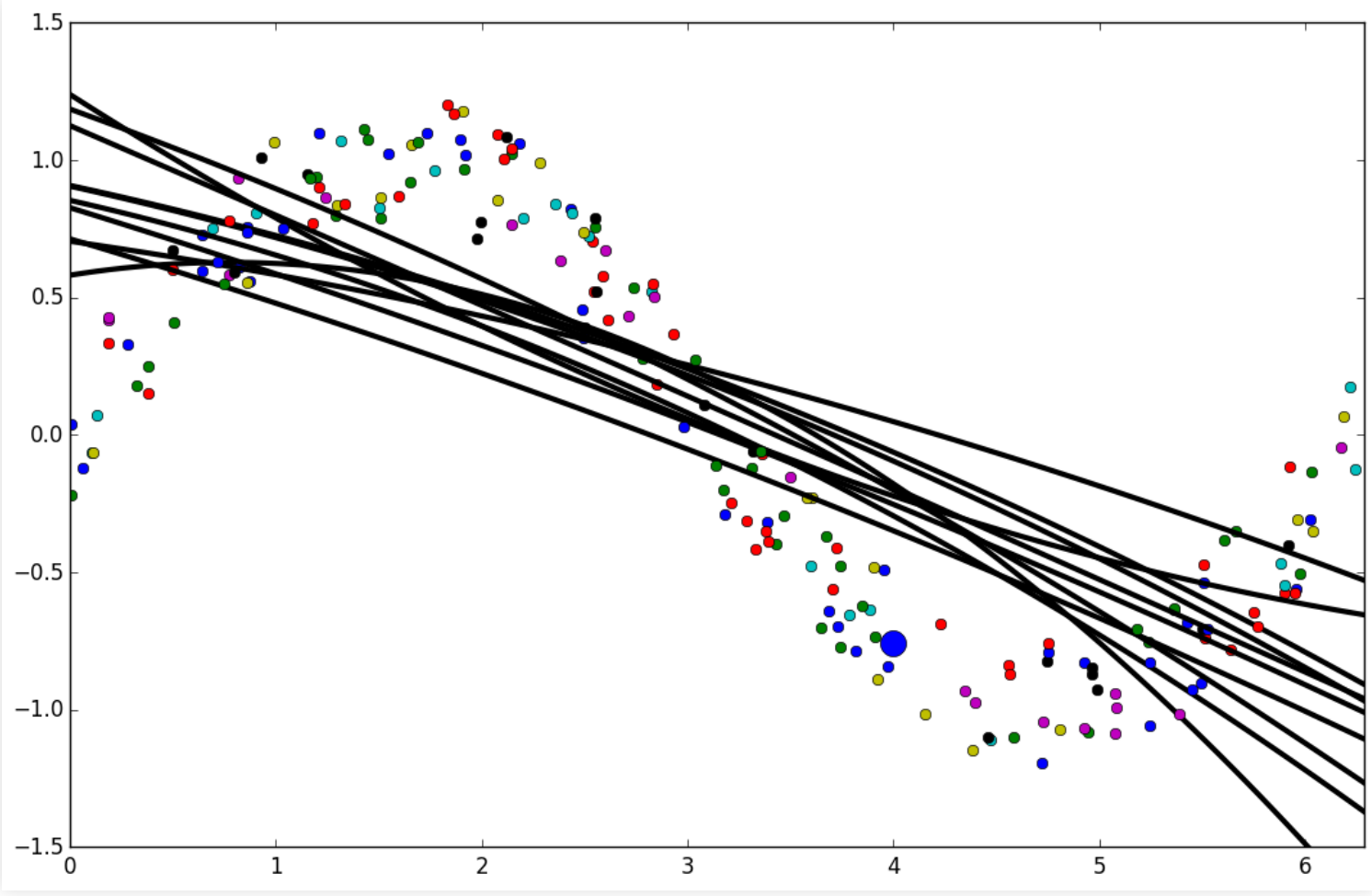
Bias

- Suppose the model cannot fit the data



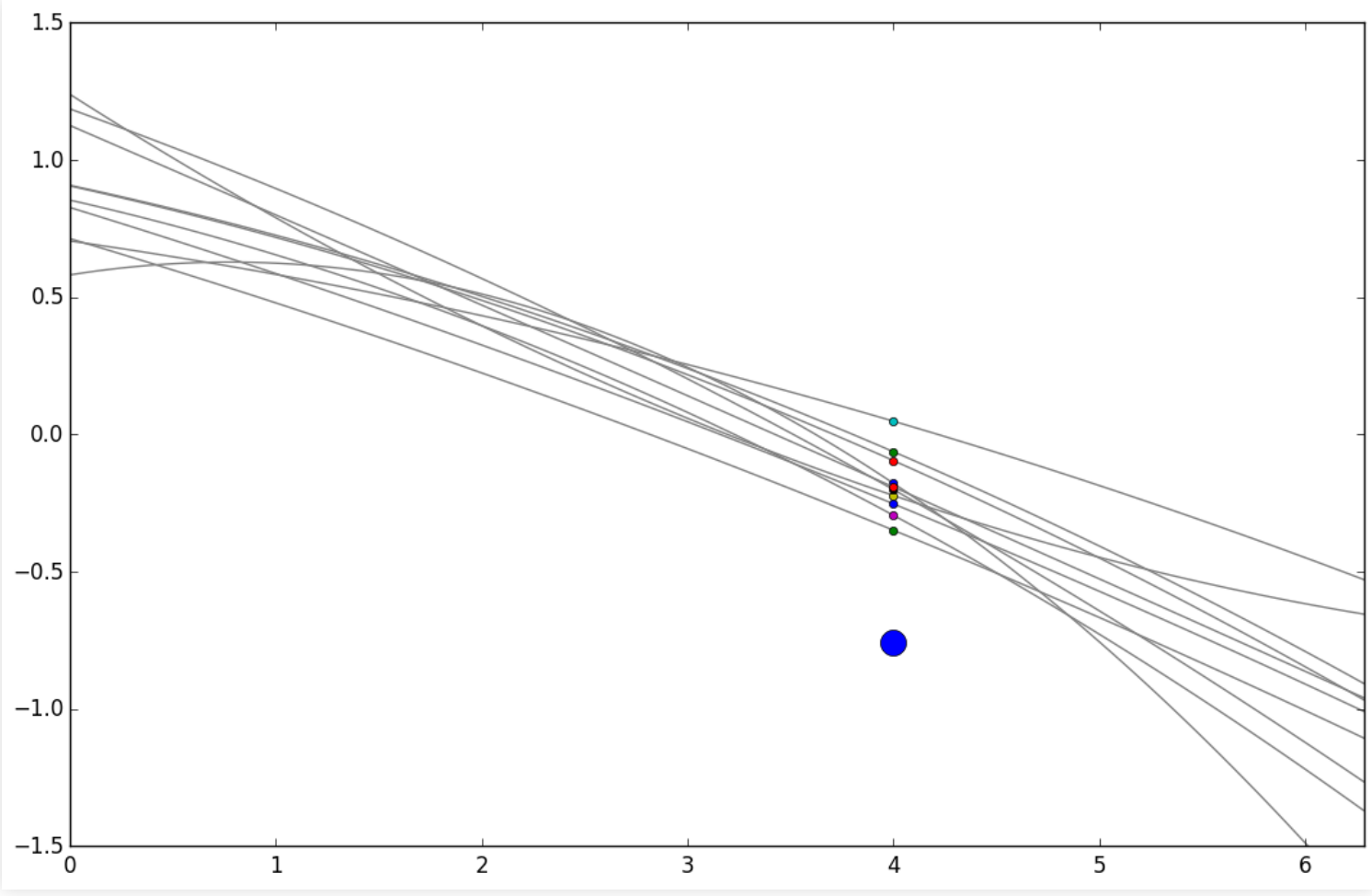
Bias

- When we average over different samples...



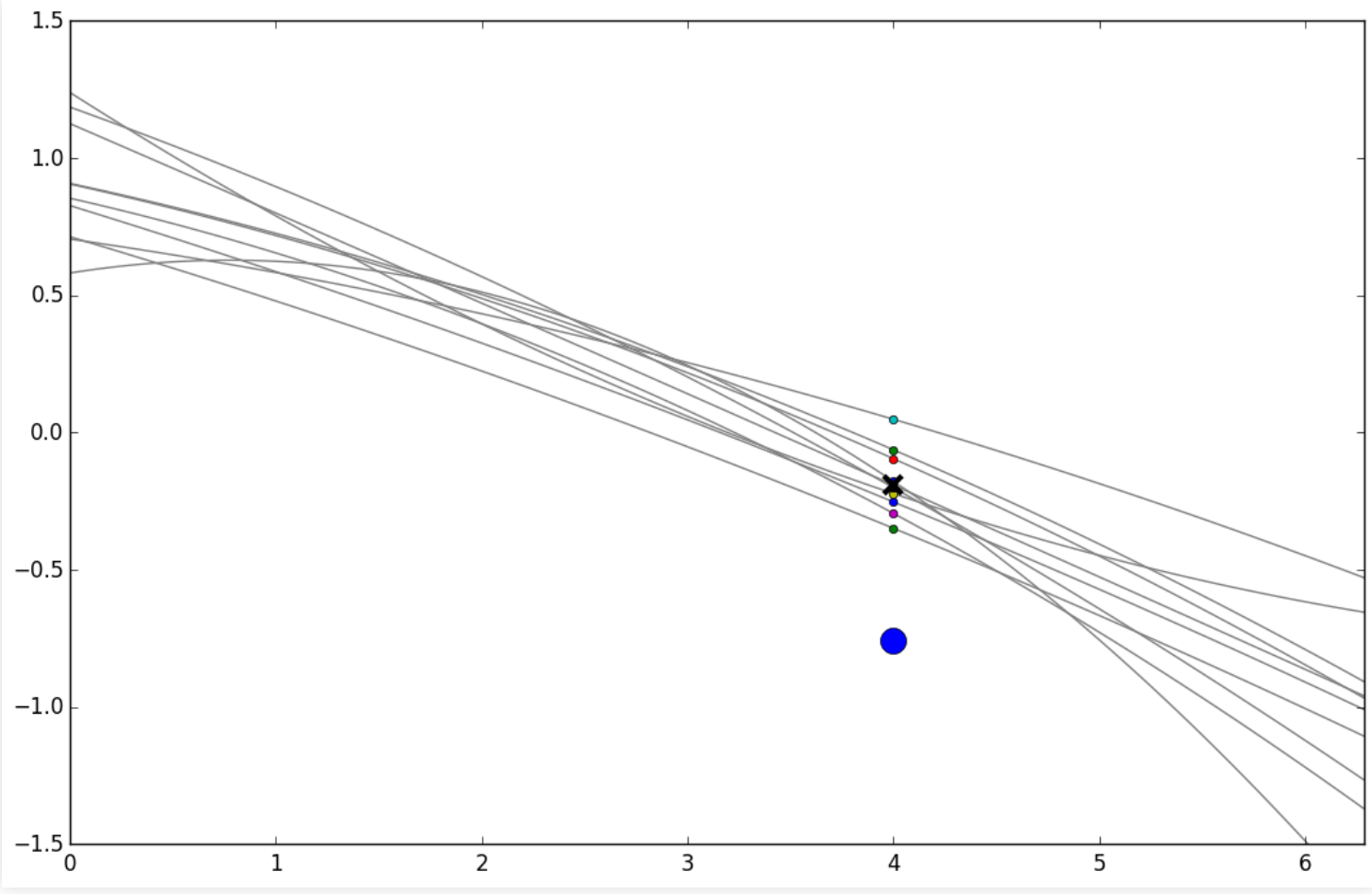
Bias

- ...there is a large bias in the prediction



Bias

- Bias: deviation of the average estimate from the target value



Bias

- Bias: deviation of the average estimate from the target value
- The bias for example n is the squared error between the true value for n and the average of the predictions for n, over all hypotheses trained on different samples:

$$bias_n = (\bar{y}(x_n) - t_n)^2$$

- The bias for the model is the average bias for all examples:

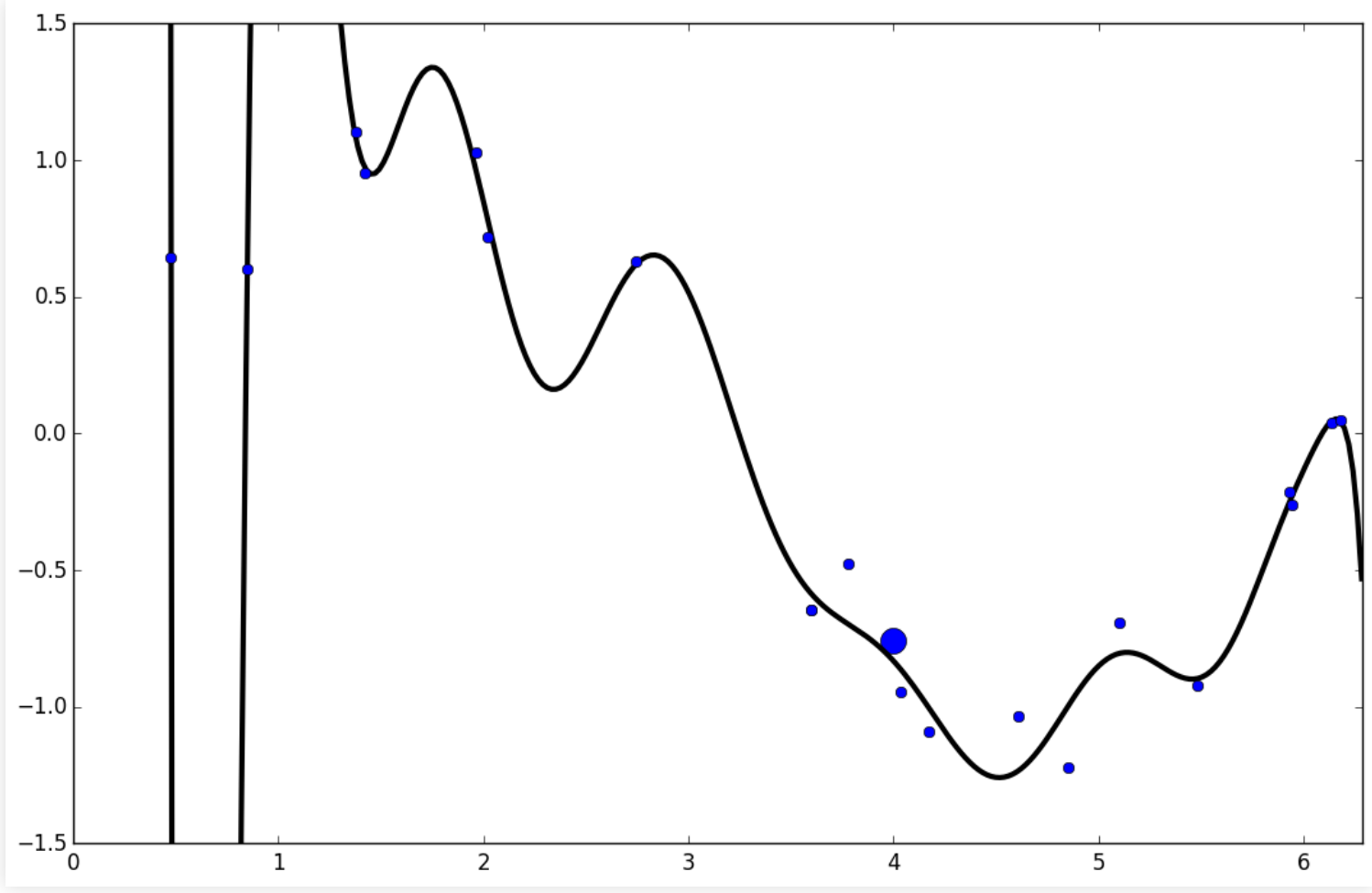
$$bias = \frac{1}{N} \sum_{n=1}^{N} (\bar{y}(x_n) - t_n)^2$$

- Note: the bias is often written as $bias^2$, but this is just to denote the squared error.

Variance

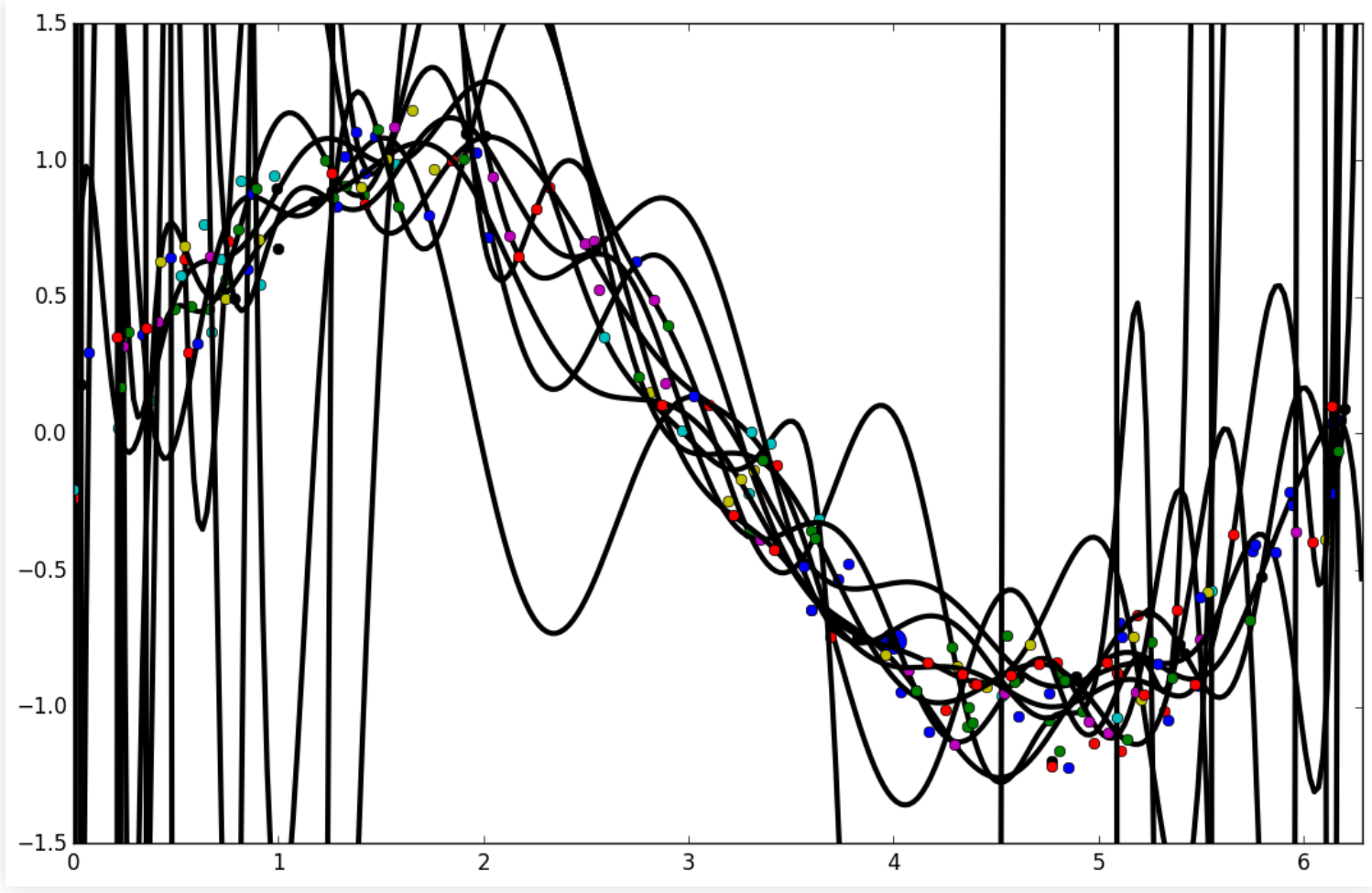
Variance

- If the model is overfitting, it adjusts the training data too much



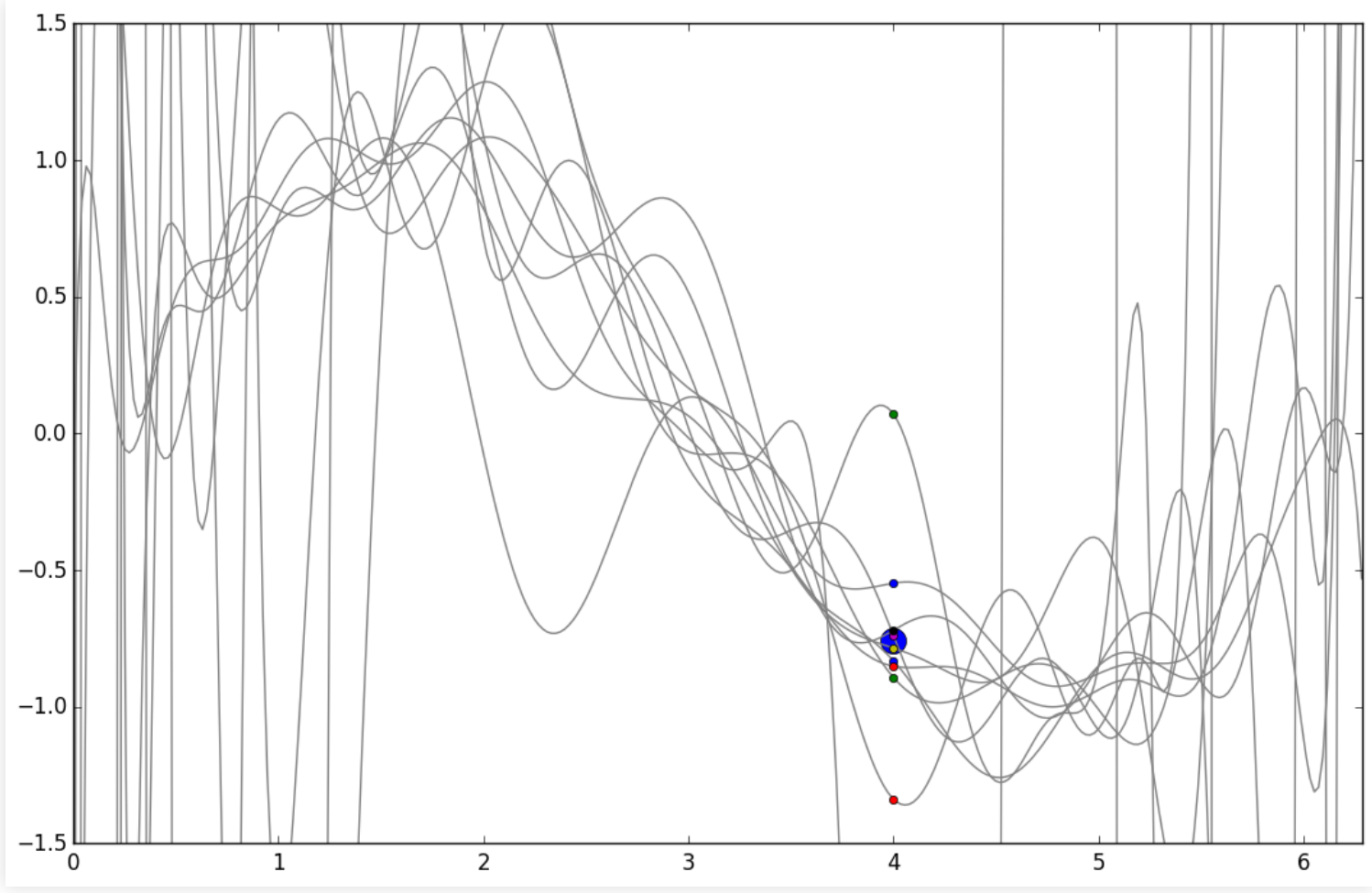
Variance

- Hypothesis varies over different training sets



Variance

- Variance: dispersion of predictions around their average



Variance

- Variance: dispersion of predictions around their average
- Variance of predictions for point n, over all hypotheses:

$$var_n = \frac{1}{M} \sum_{m=1}^{M} (\bar{y}(x_n) - y_m(x_n))^2$$

- (Average square dist. to average)

- Variance for the model is the average over all points

$$var = \frac{1}{NM} \sum_{n=1}^{N} \sum_{m=1}^{M} (\bar{y}(x_n) - y_m(x_n))^2$$

Bias and Variance

Bias: squared deviation from true value

$$bias = \frac{1}{N}\sum_{n=1}^{N}(\bar{y}(x_n) - t_n)^2$$

Variance: squared deviation from mean prediction

$$var = \frac{1}{NM}\sum_{n=1}^{N}\sum_{m=1}^{M}(\bar{y}(x_n) - y_m(x_n))^2$$

- Note: Bias and Variance depend on what the model does on average and not on any single hypothesis

Bias-variance decomposition

Bias-variance decomposition

- If we have a squared loss function, then the expected error is:

$$E\left((y-t)^2\right) = (E(y)-E(t))^2 + E\left((y-E(y))^2\right) + E\left((t-E(t))^2\right)$$

$$bias + var + noise$$

Bias-variance decomposition

- How to compute: average over different training sets, evaluate outside training set.
- But we have only one training set
- We need a resampling method

Bias-variance decomposition

Bootstrapping

- From the training set, sample at random with replacement
- Generate M replicas of N points each
- Measure over the replicas

We also want an error estimate

- To get unbiased estimates of the errors, we need to measure it outside the training set.
- We can use a test (or validation) set

Bias-variance decomposition

Bootstrapping

```
def bootstrap(samples,data):
    train_sets = np.zeros((samples,data.shape[0],data.shape[1]))
    for sample in range(samples):
        ix = np.random.randint(data.shape[0],size=data.shape[0])
        train_sets[sample,:] = data[ix,:]
    return train_sets
```

- Training sets all have the same size, N, sampled with reposition

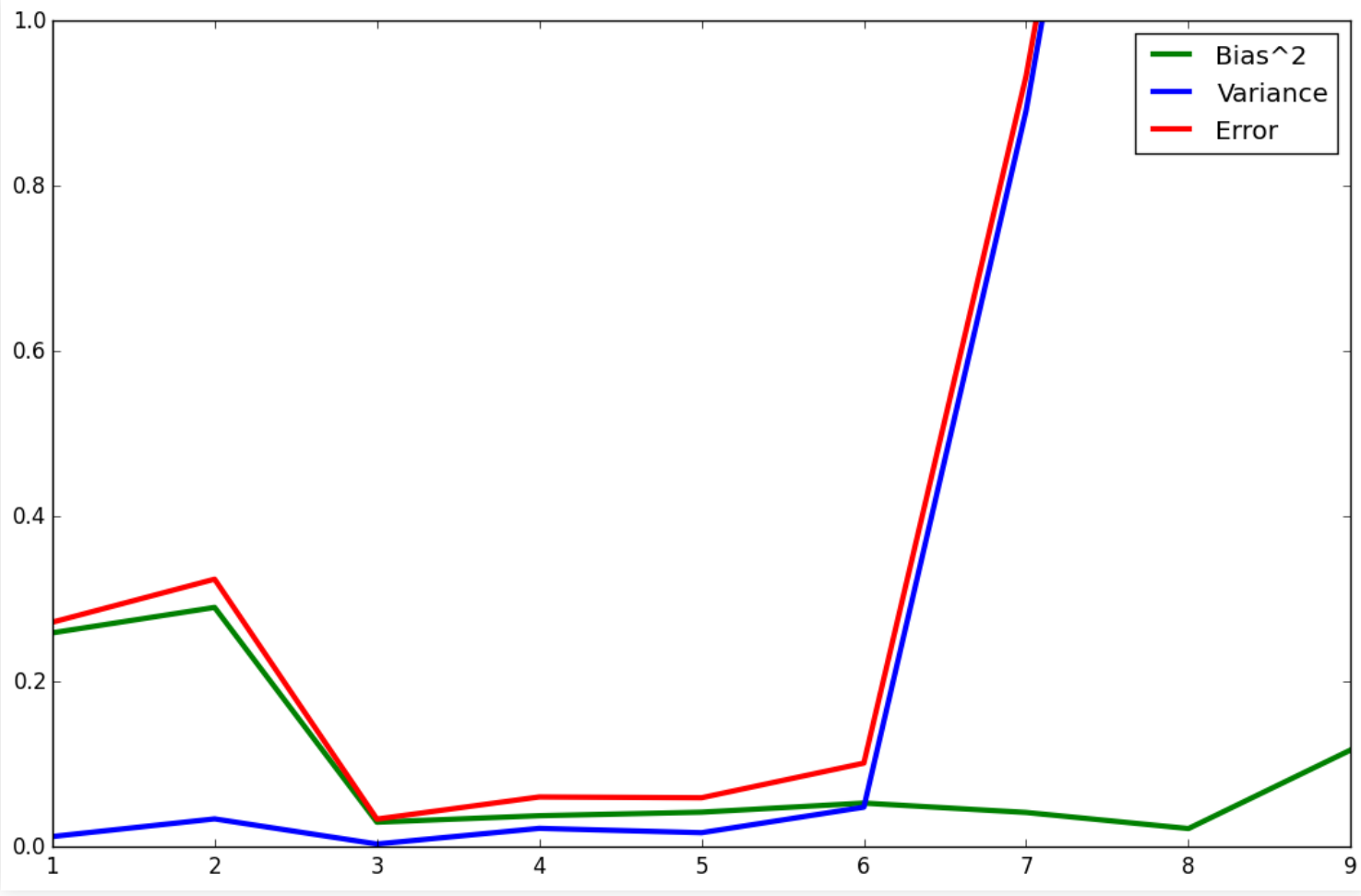
Bias-variance decomposition

Polynomial regression

```
def bv_poly(degree, train_sets, test_set):
    samples = train_sets.shape[0]
    predicts = np.zeros((samples,test_set.shape[0]))
    for ix in range(samples):
        coefs = np.polyfit(train_sets[ix,:,0],
                    train_sets[ix,:,1],degree)
        predicts[ix,:] = np.polyval(coefs,test_set[:,0])

    mean_preds = np.mean(predicts,axis=0)
    bias_per_point = (mean_preds-test_set[:,-1])**2
    bias = np.mean(bias_per_point)

    var_per_point = np.mean((predicts-mean_preds)**2,axis=0)
    var = np.mean(var_per_point)

    return bias,var
```

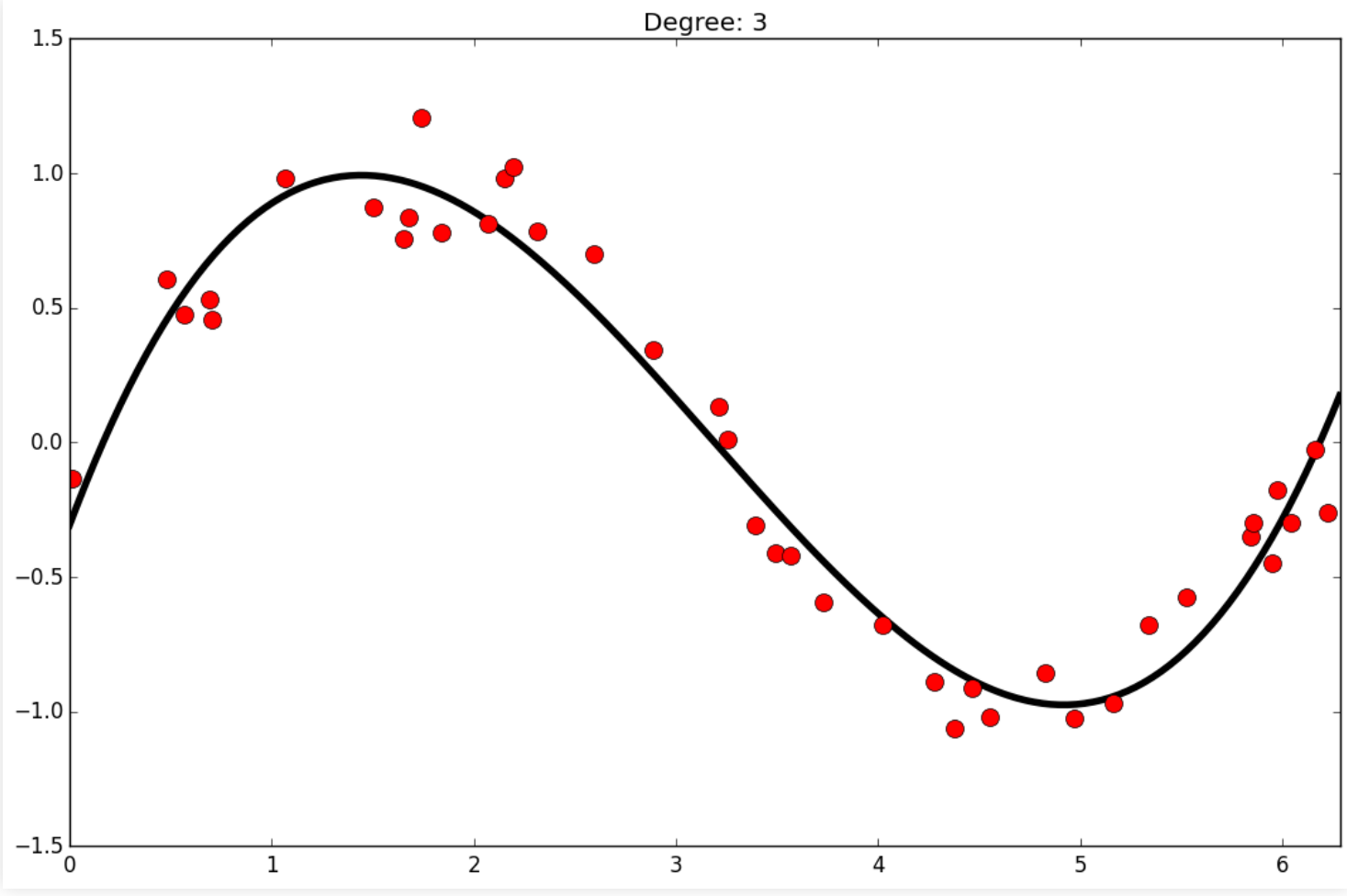
Bias-variance decomposition

- Bias-variance decomposition, polynomial regression



Bias-variance decomposition

- Lowest total error



Bias-variance decomposition

B-V with classifiers

- With a 0/1 loss function, the main prediction for point i is the mode
- Assuming there is no noise, the Bias for point i is:

$$bias_i = L(Mo(y_{i,m}), t_i) \qquad bias_i \in \{0, 1\}$$

- And the Variance is:

$$var_i = E\left(L(Mo(y_{i,m}), y_{i,m})\right)$$

- To compute total error, we must consider that:

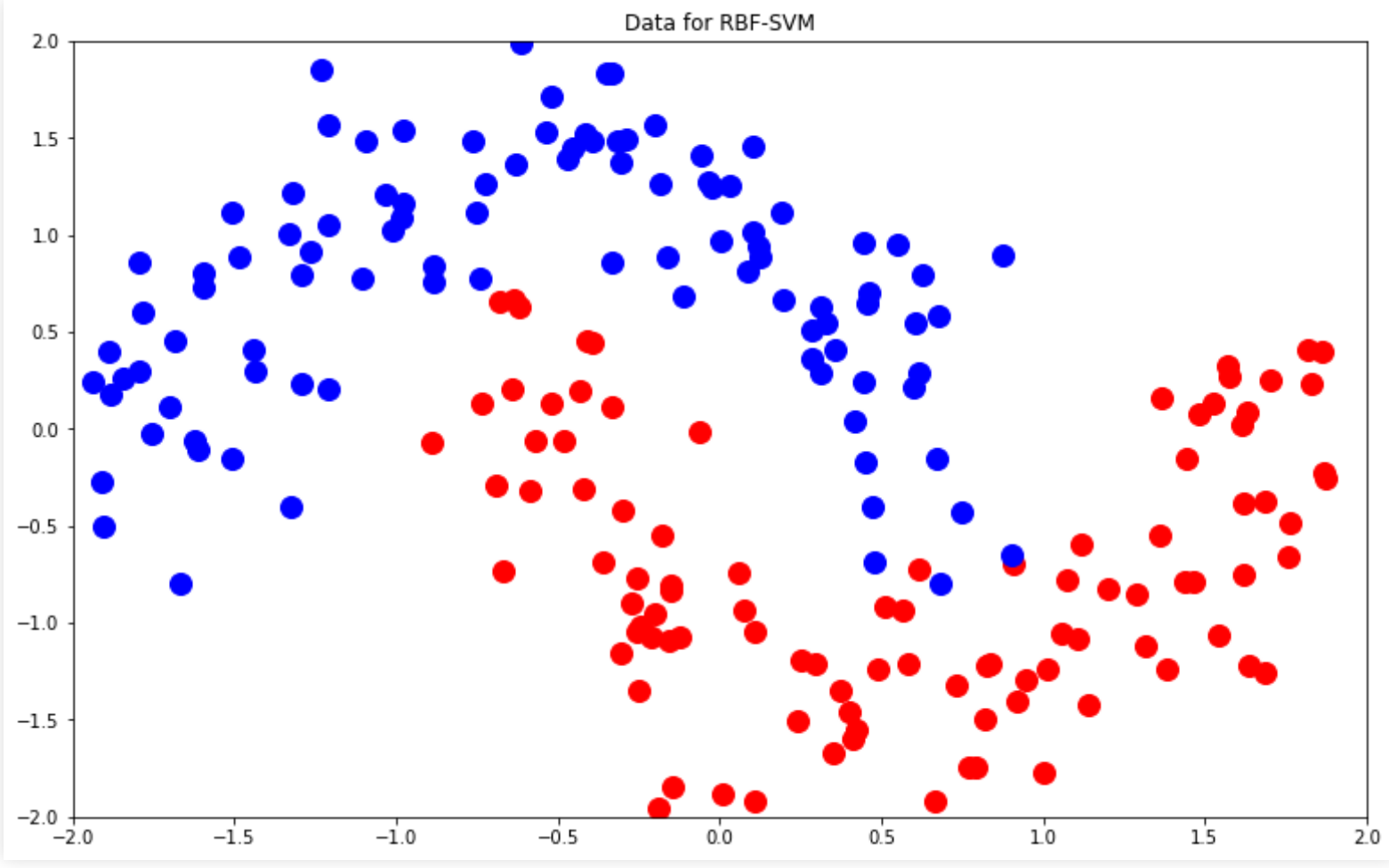
- If $bias_i = 0$, var_i increases error.
- If $bias_i = 1$, var_i decreases error.

- So for the error we must add or subtract the variances accordingly

$$E\left(L(t, y)\right) = E\left(B(i)\right) + E\left(V_{unb.}(i)\right) - E\left(V_{biased}(i)\right)$$

Bias-variance decomposition

KNN, Optimize neighbours

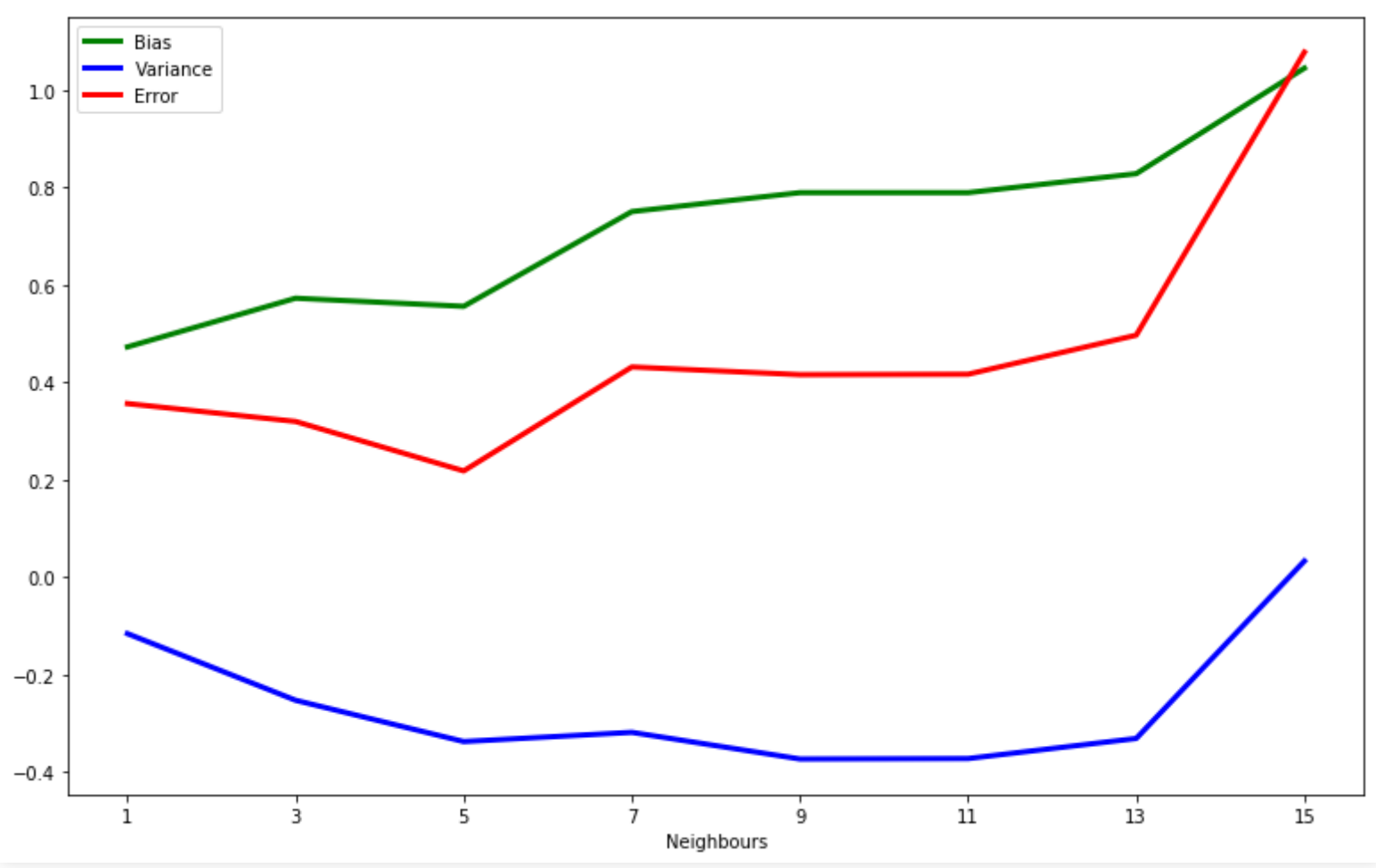


Bias-variance decomposition with KNN

```
def bv_knn(neighs, train_sets, test_set):
    samples = train_sets.shape[0]
    predicts = np.zeros((samples,test_set.shape[0]))
    for ix in range(samples):
        sv = KNeighborsClassifier(n_neighbors=neighs)
        sv.fit(train_sets[ix,:,:-1],train_sets[ix,:,-1])
        predicts[ix,:] = sv.predict(test_set[:,:-1])
    main_preds = np.round(np.mean(predicts,axis=0))
    bias_per_point = np.abs(test_set[:,-1]-main_preds)
    var_per_point = np.mean(np.abs(predicts-main_preds),axis=0)
    u_var = np.sum(var_per_point[bias_per_point == 0])/test_set.shape[0]
    b_var = np.sum(var_per_point[bias_per_point == 1])/test_set.shape[0]
    print(u_var,b_var)
    return bias,u_var-b_var
```

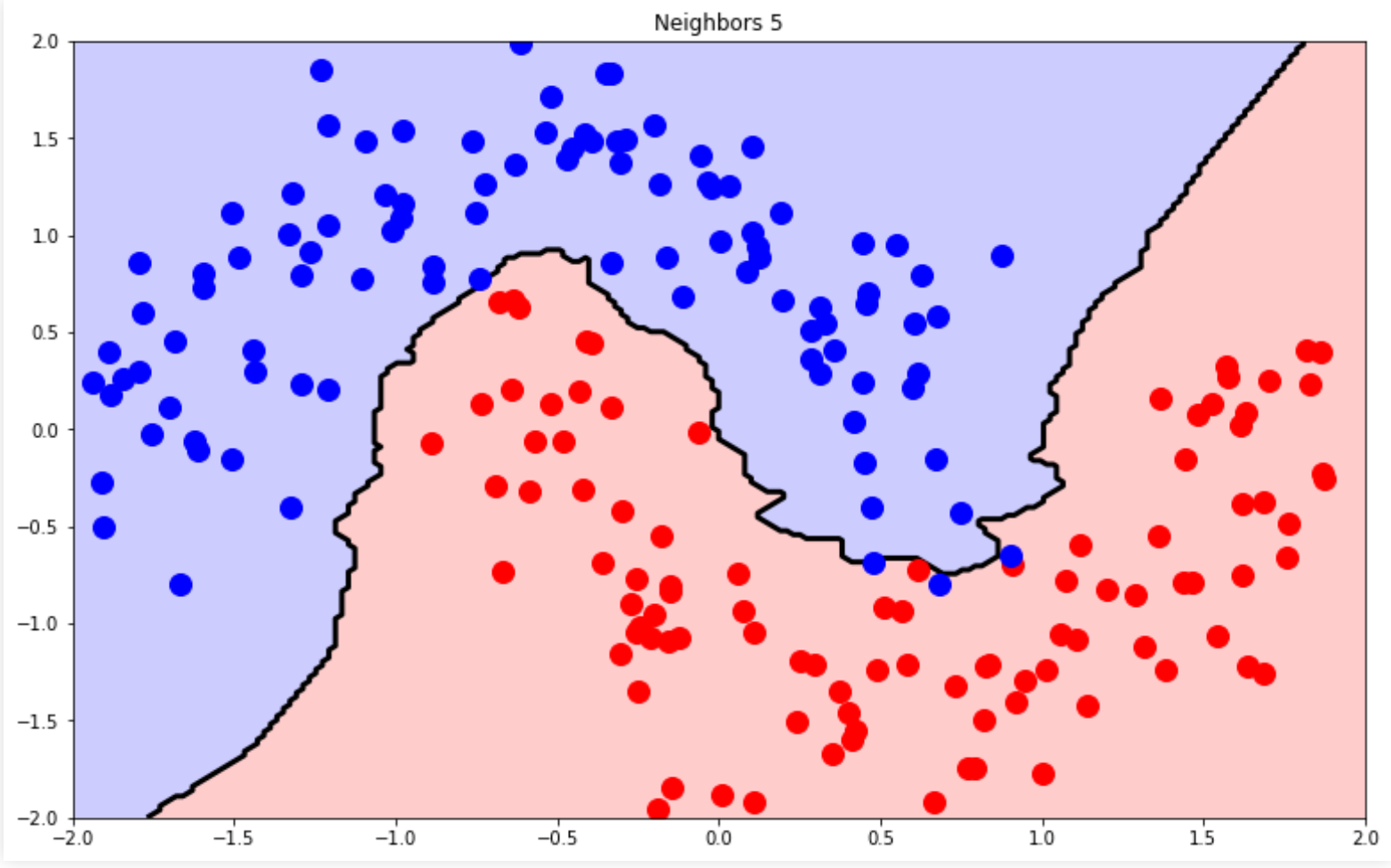
Bias-variance decomposition

- Bias-variance decomposition with KNN



Bias-variance decomposition

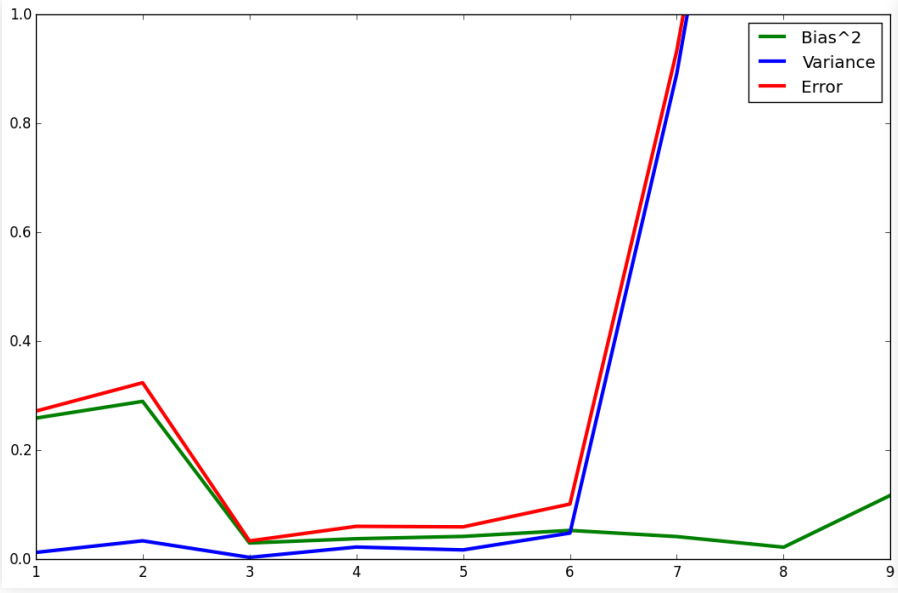
- Bias-variance KNN, lowest estimated error (apart from noise)

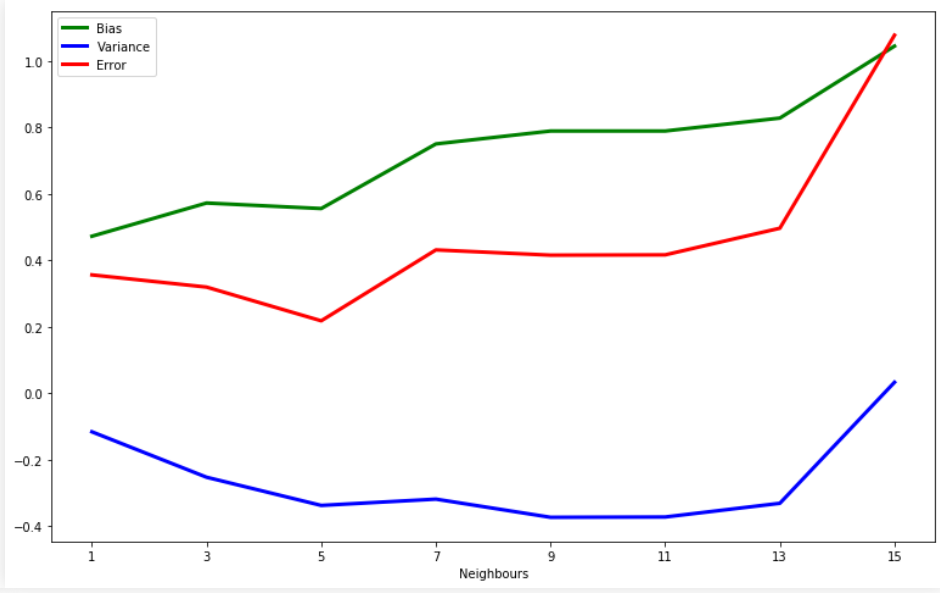


Bias-variance decomposition

Bias-variance tradeoff

- In general, reducing *bias* increases *variance* and vice-versa





- Note: Bias-Variance decomposition is useful for understanding the components of the error but, in practice, it is easier to use cross-validation and just consider the total error.

Summary

Bias-variance decomposition

Summary

- Bias: average deviation from true value
- Variance: dispersion around the average prediction

- Classification: variance increases or decreses error depending on bias

- Bias and variance related to underfitting and overfitting

Further reading

- Alpaydin, Section 4.3
- Bishop, Sections 4.1.2, 4.3.4, 7.1.3
- Optional:

- Domingos, Pedro. "A unified bias-variance decomposition." Proceedings of 17th International Conference on Machine Learning. Stanford CA Morgan Kaufmann. 2000.