Session 11:

Machine learning introduction

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Some coding advice

- *How do I extract an object from my function?* Print or return?
- Solving complex problems: One thing at a time

Machine learning in this course

ML: short for machine learning

- basic concepts of ML
    - overfitting, underfitting, model validation
    - model selection and hyperparameters
- linear ML models
    - regularization
    - getting hands dirty
- emphasize differences and synergies between ML and statistics
- brief intro of non-linear models (value of linear)

Agenda

1. Why machine learing
2. What is machine learning
3. Classification models
    A. the perceptron
    B. beyond the perceptron

Learning ML

- During lectures copy code for see what it does - ***listen*** to me. Write own notes.
- After lecture > understand code details
- Learn with your group - VERY IMPORTANT!

Math review

Vector: 1-d dimensional array of numbers

$$\boldsymbol{x} = [x_0, x_1, x_2, ..]$$

Matrix: 2-d dimensional array of numbers

$$\begin{aligned}\boldsymbol{X} = [&[x_{00}\ , x_{01}\ , x_{02}\ , ..],\\ &[x_{10}\ , x_{11}\ , x_{12}\ , ..],\\ &[x_{20}\ , x_{21}\ , x_{22}\ , ..],\\ &[...\ , ...\ , ...\ , ..]]\end{aligned}$$

Function fitting

What does (supervised) machine learning do?

Suppose we have some data y we want to model/predict from input x.

The aim is to find a function f such that the distance between actual values y and predicted values $f(x)$ are minimized.

What are some Examples?

- Linear form: $y = x\beta$.
- Logistic form: $y = g(x\beta)$

where $x^T\beta = \beta_0 + x_1\beta_1 + x_2\beta_2 + \ldots + x_n\beta_n$ (vector dot product)

Why machine learning

Value of modelling

Why are models useful?

Models are pursued with differens aims. Suppose we have a linear model, $y = x\beta + \epsilon$.

- Social science:
  - They teach us something about the world.
  - We want to estimate $\hat{\beta}$ and distribution
- Data science:
  - To make optimal future decisions and precise predictions, i.e. $\hat{y}$.

Model fragility (1)

What is a polynomial regression?

- Fitting a curve with an *n-dimenstional polynomial*
- Can fit any "regular" curve ~ Taylor Series Approximation.

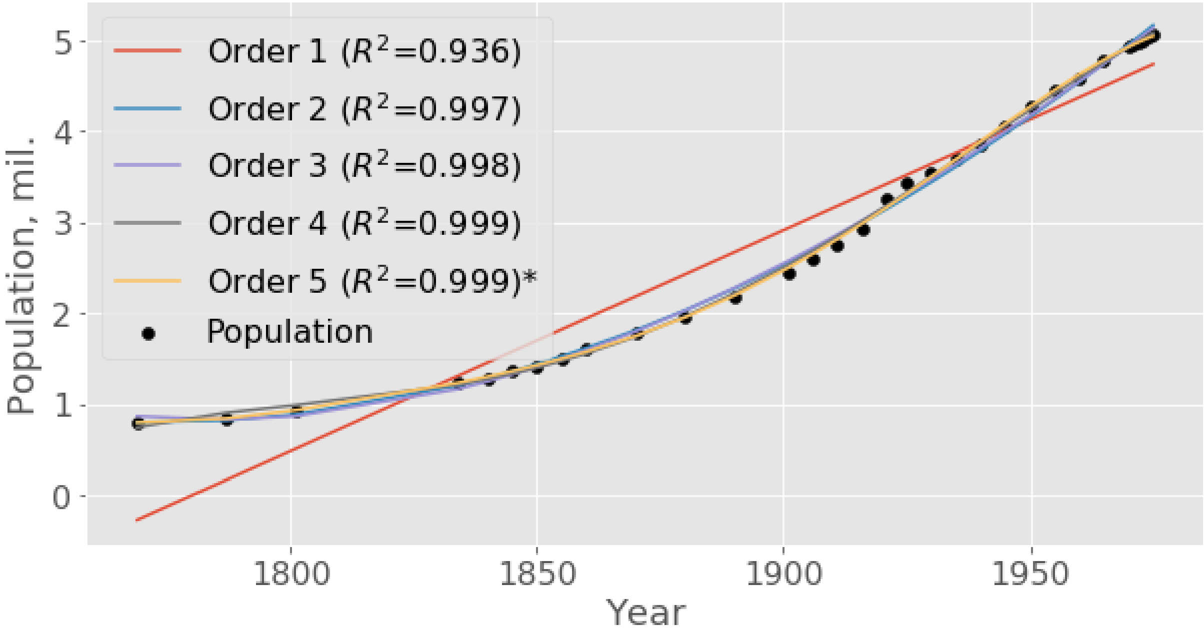
Model fragility (2)

Suppose we build models of the size of the Danish population, how do polynomial fits perform?

- We estimate model with data from 1769-1975.

In [25]:
```
f_pop1
```

Out[25]:

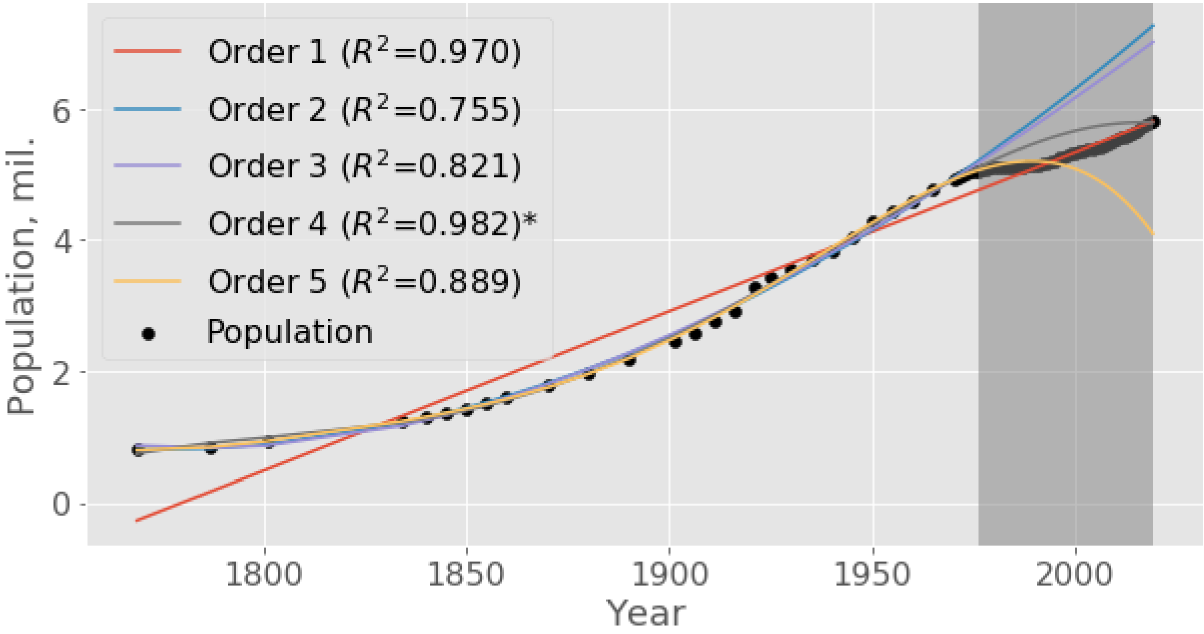


Model fragility (3)

Which model performs best when we extend the forecasting period from 1975 to now?

In [26]:
```
f_pop2
```

Out[26]:



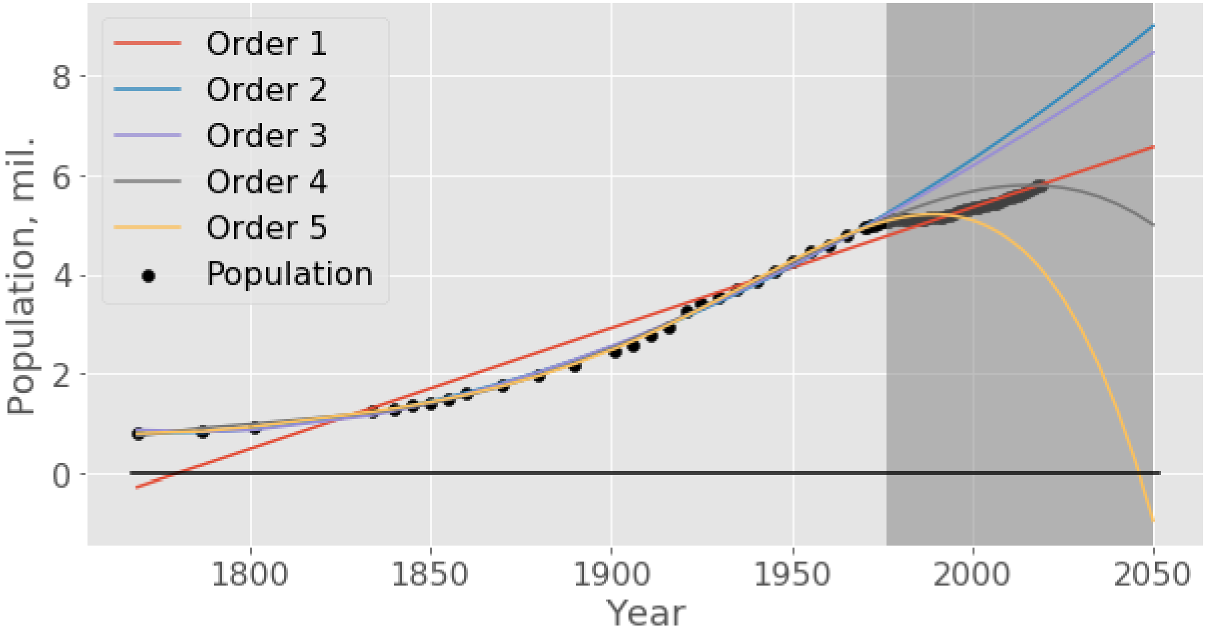
Model fragility (4)

What happens if we extend the prediction period until 2050? See the fifth order.

In [27]:

```
f_pop3
```

Out[27]:



Model fragility (5)

What trade off do we face in modelling?

- Making a model that is to simple and does not capture enough of data (`underfitting`)
- Making a model with great fit on estimation data, but poor out-of-sample prediction (`overfitting`)

The goal of machine learning is to find models that minimize these two problems simultaneously.

Machine learning overview

What is machine learning

Can you define machine learning, i.e. ML?

- Supervised learning
    - Models designed to infer a relationship between input and **labeled** data.
    - Requirement: labels on data
- Unsupervised learning
    - Find patterns and relationships from **unlabeled** data.
        - This may involve clustering, dimensionality reduction and more.

Why machine learning

How might this be useful for social scientists?

Supervised machine learning is important:

- Improve estimation by validating models (not only theory)
- We can generate new data (impute missing)
- Better predictive models
- Use in hybrid models that leverage machine learning for causal estimation
    - (e.g. causal forest, neural instrumentation)

Supervised ML problems (2)

How can we categorize a supervised learning model?

Suppose we have model $y = g(X\beta)$

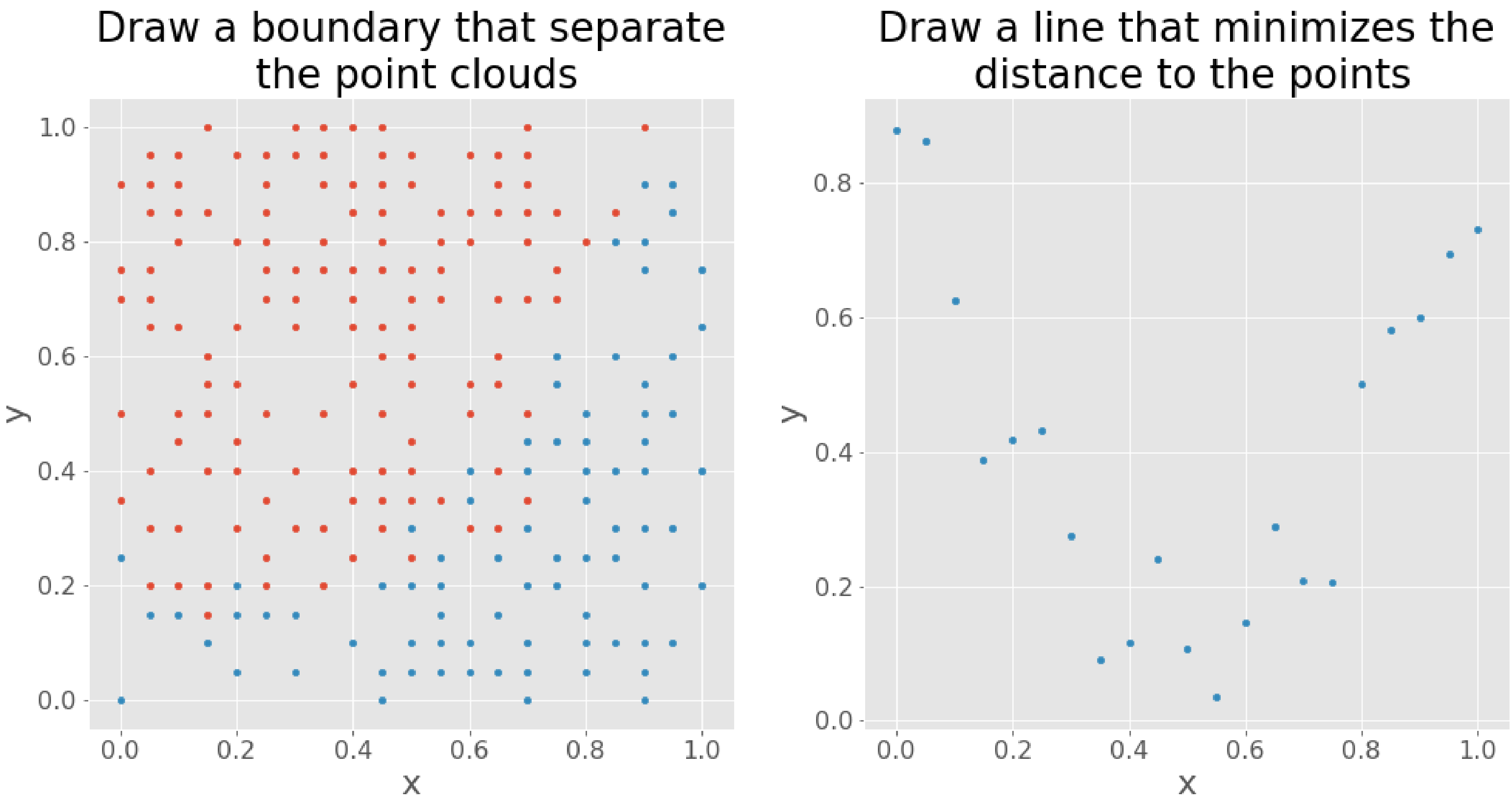
- We distinguish by type of the `target` variable y

Supervised ML problems (3)

Which one is classification, which one is regression?

In [28]:
```
f_identify_question
```

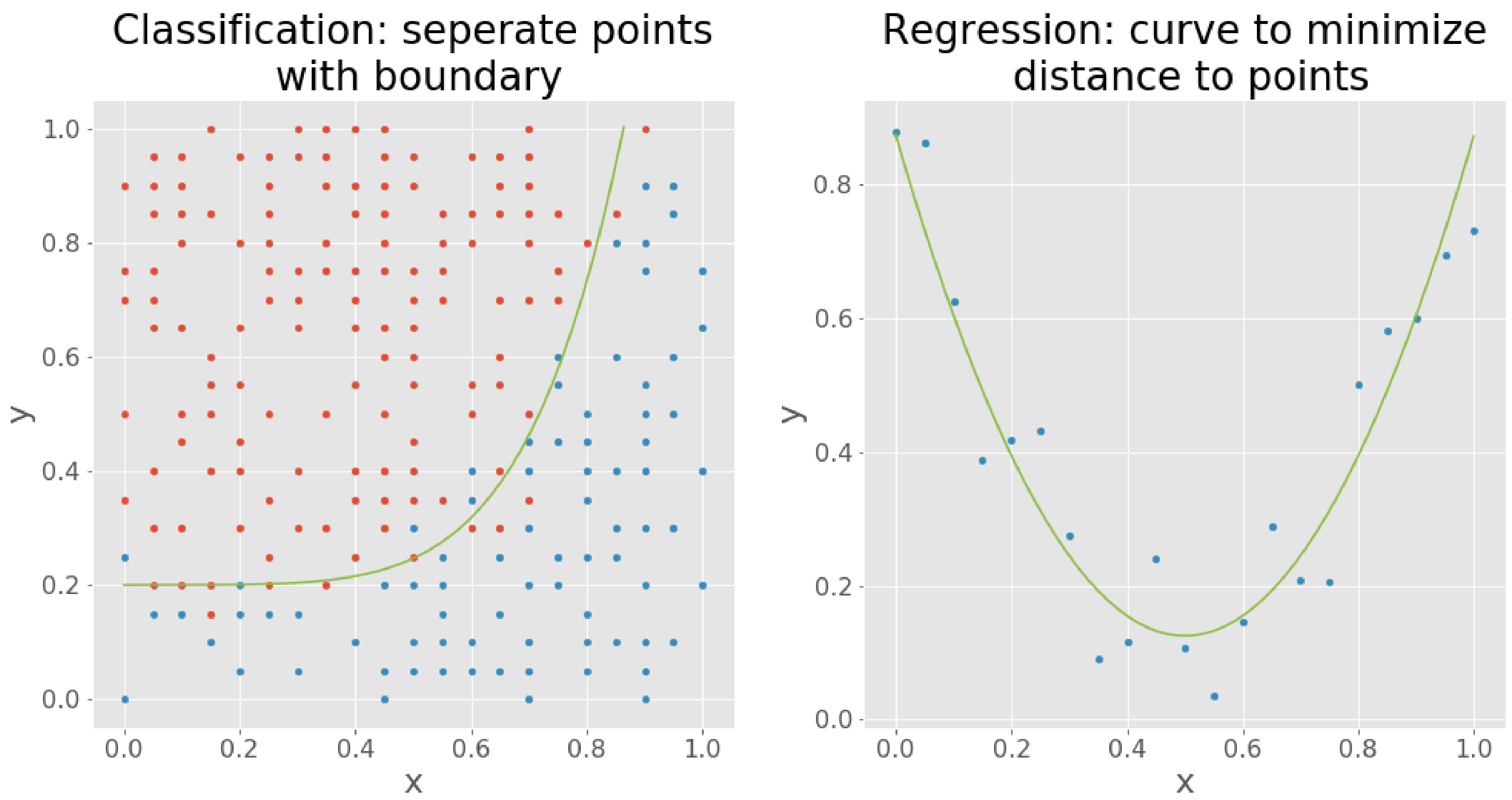
Out[28]:



Supervised ML problems (4)

In [29]:
```
f_identify_answer
```

Out[29]:



Regression models

What are examples of regressions models?

- Output is income, life expectancy, education length (years)

What is the underlying data of the target, y?

- target is `continuous`

Classications models

What are examples of classication models?

What is the underlying data of the target, y?

- target is `categorical`
    - sometimes known as`factor`
    - can also be `bool` or `int`

Example of supervised ML

Classification or regression?

We load the titanic data. We select variables and make dummy variables from categorical. We split into target and features.

In [66]:
```
titanic = sns.load_dataset('titanic')
cols = ['survived','class', 'sex', 'sibsp', 'age', 'alone']
titanic_sub = pd.get_dummies(titanic[cols].dropna(), drop_first=True).astype(np.int64)

X = titanic_sub.drop('survived', axis=1)
y = titanic_sub.survived
```

Definitions

ML lingo, notation and concepts

- `net-input`, $z_i = \underbrace{\boldsymbol{w}^T \boldsymbol{x}_i}_{vector\ form} = \underbrace{1 \cdot w_0 + w_1 x_{i,1} + \ldots + w_k x_{i,k}}_{expanded\ form}$
- `feature` vector, $\mathbf{x}_i$, i.e a row of input variables
    - = explanatory variables in econometrics
- `weight` vector, $\mathbf{w}$, i.e model parameters
    - = coefficients in econometrics where denoted β
- `bias` term, w_0, i.e. the model intercept
    - = the constant variable in denoted β_0

The perceptron model

The artificial neuron (1)

We are interested in making a decision rule $\phi : \mathbb{R}^p \to \{-1, 1\}$.

$$\phi(z_i) = \begin{cases} 1, & z_i > 0 \\ -1, & z_i \leq 0 \end{cases}$$

- `unit step function`, ϕ, checks if value exceeds threshold

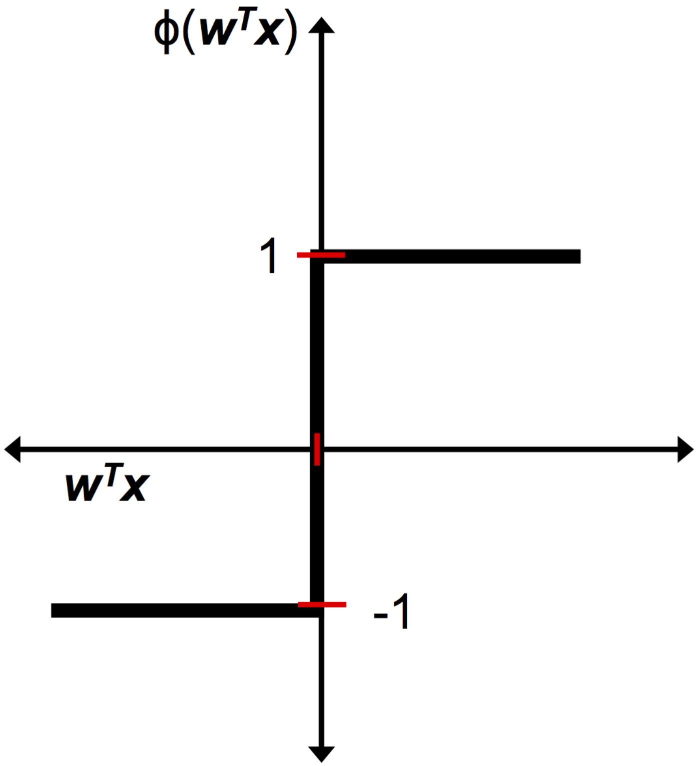
The artificial neuron (2)

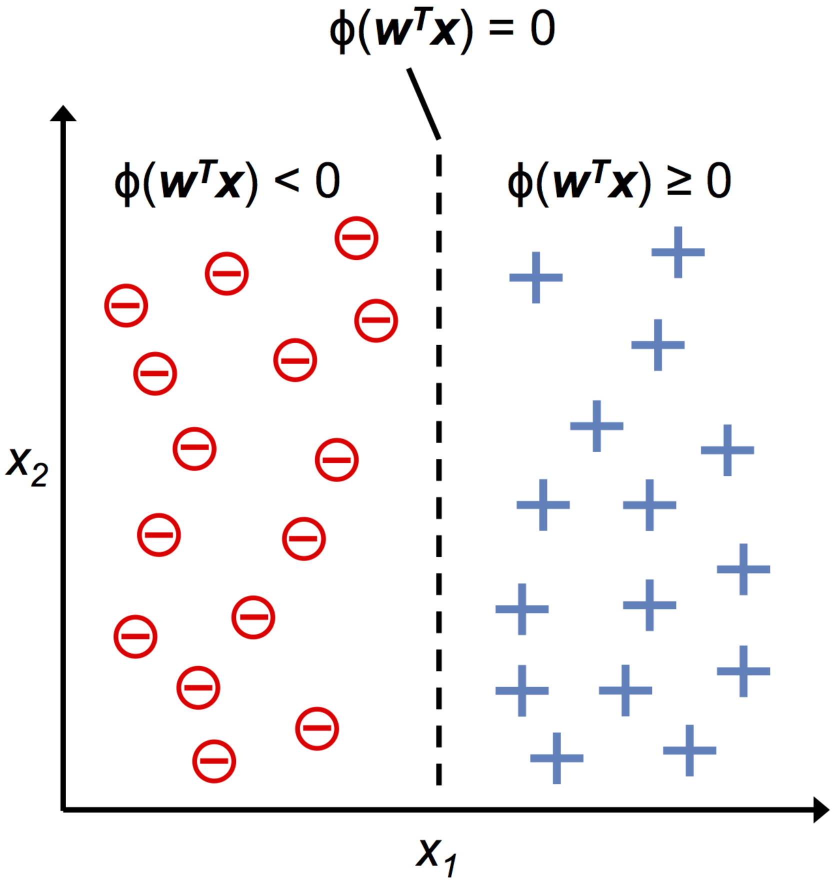
Quiz: what are the input dimensions of the neuron, what is the output dimension?

- Input is the p-dimensional space, $\mathbb{R}^p$.
- Output is binary, either -1 or 1.

The artificial neuron (3)

The unit step function (left) and the decision boundary (right)

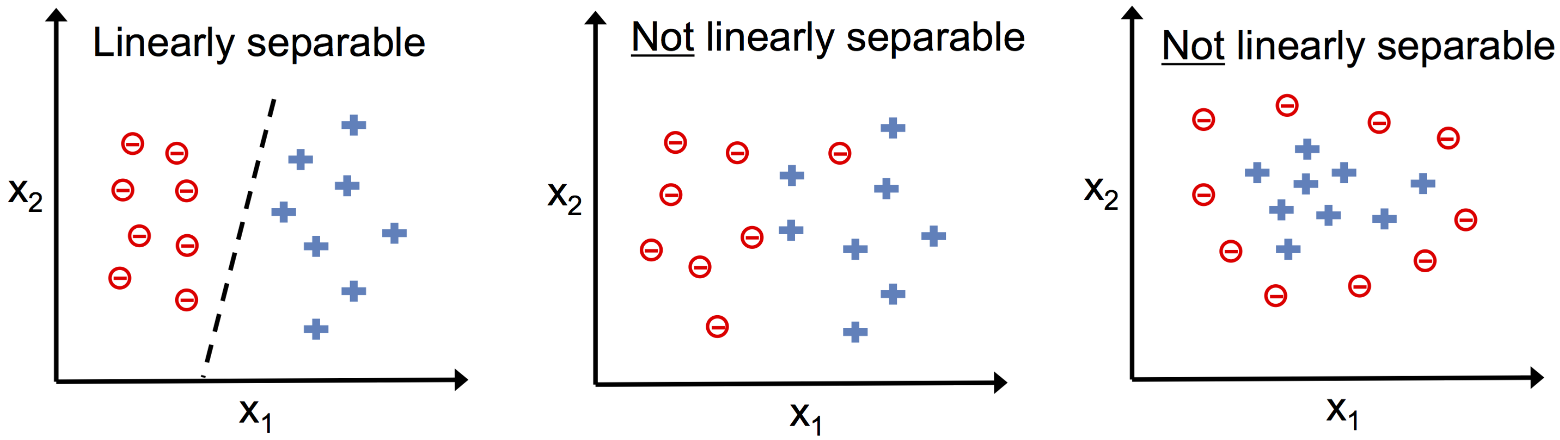




The artificial neuron (4)

When does the articial neuron work?

If the two target types are linearly separable:



The perceptron learning rule (1)

How do we estimate the model parameters?

1. initialize the weight with small random number
2. for each training observation, i=1,..,n
    A. compute predicted target, $\hat{y}_i$
    B. update weights $\hat{w}$

The perceptron learning rule (2)

How do we predict the target?

Single observation

- expanded notation:
$$\hat{y}_i = \phi(z_i), \quad z_i = w_0 + w_1 x_{i,1} + \ldots + w_k x_{i,k}$$

- vector notation:
$$\hat{y}_i = \phi(z_i), \quad z_i = \hat{\boldsymbol{w}}^T \boldsymbol{x}_i$$

Multiple observations (matrix notation)

$$\hat{\boldsymbol{y}} = \phi(\boldsymbol{z}), \quad \boldsymbol{z} = \boldsymbol{X}\hat{\boldsymbol{w}}$$

The perceptron learning rule (3)

How do we update weights?

Weights are updated as follows:

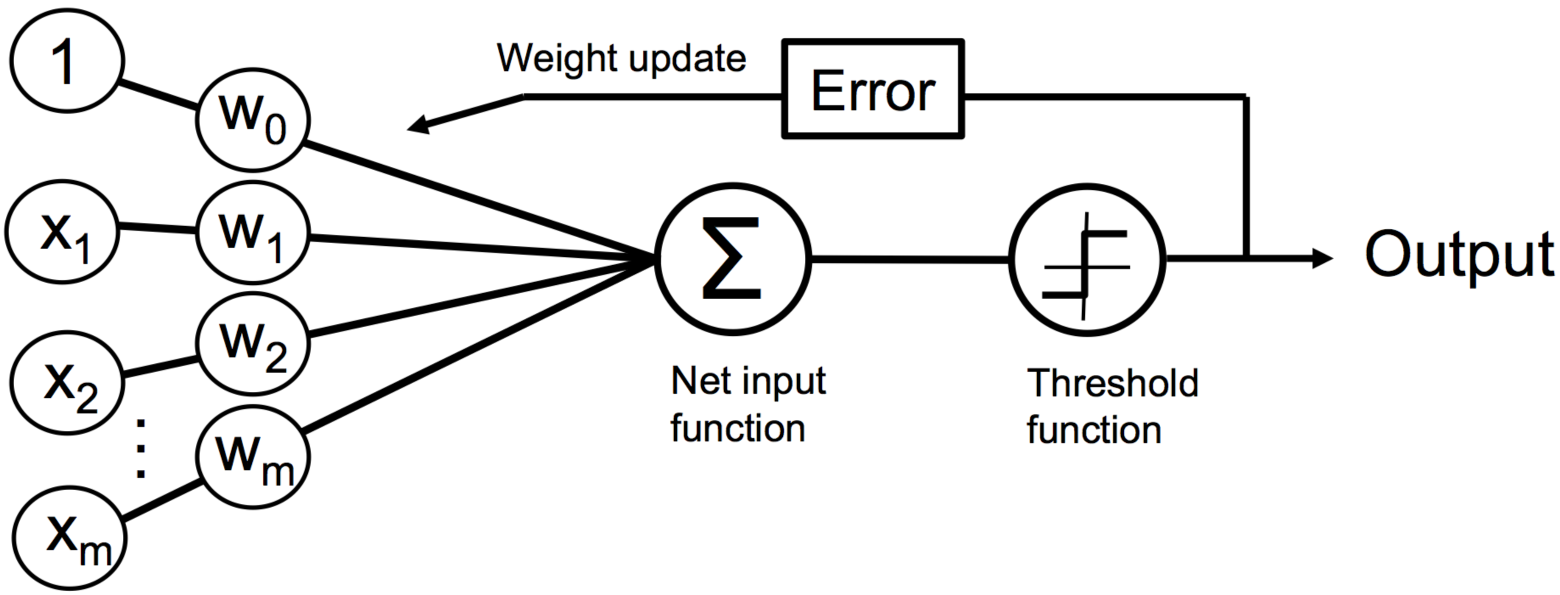
$$\hat{w} = \hat{w} + \Delta\hat{w}$$
$$\Delta\hat{w} = \eta \cdot (y_i - \phi(z_i)) \cdot \mathbf{x}_i$$

where η is the learning rate, and the first order derivative is:

$$\frac{\partial MSE}{\partial w} = \mathbf{X}^T\mathbf{e}$$

The perceptron learning rule (4)

The computation process



Implementation in Python (1)

How do we compute the net-input vectorized?

In [57]:
```
X = np.random.normal(size=(3, 2)) # feature matrix
y = np.array([1, -1, 1]) # target vector
w = np.random.normal(size=(3)) # weight vector
print('X:\n',X)
print('y:',y)
print('w:',w)
```

```
X:
 [[ 0.72485469  0.92849521]
 [ 0.65091101  0.49875232]
 [ 0.06184218 -0.93236388]]
y: [ 1 -1  1]
w: [ 0.22683369 -0.1328085   0.34351078]
```

Implementation in Python (2)

How do we compute the errors vectorized?

In [58]:
```
z = w[0] + X.dot(w[1:]) # compute net-input
positive = z>0 # compute prediction (boolean)

y_hat = np.where(positive, 1, -1)  # convert prediction
e = y - y_hat # compute errors
SSE = e.T.dot(e)
```

Implementation in Python (3)

How do we compute the updated weights?

In [59]:

```
# learning rate
eta = 0.001

# first order derivative
fod = X.T.dot(e) / 2

# update weights
update_vars = eta*X.T.dot(e) # insert fod
update_bias = eta*e.sum()/2
```

Working with the perceptron (1)

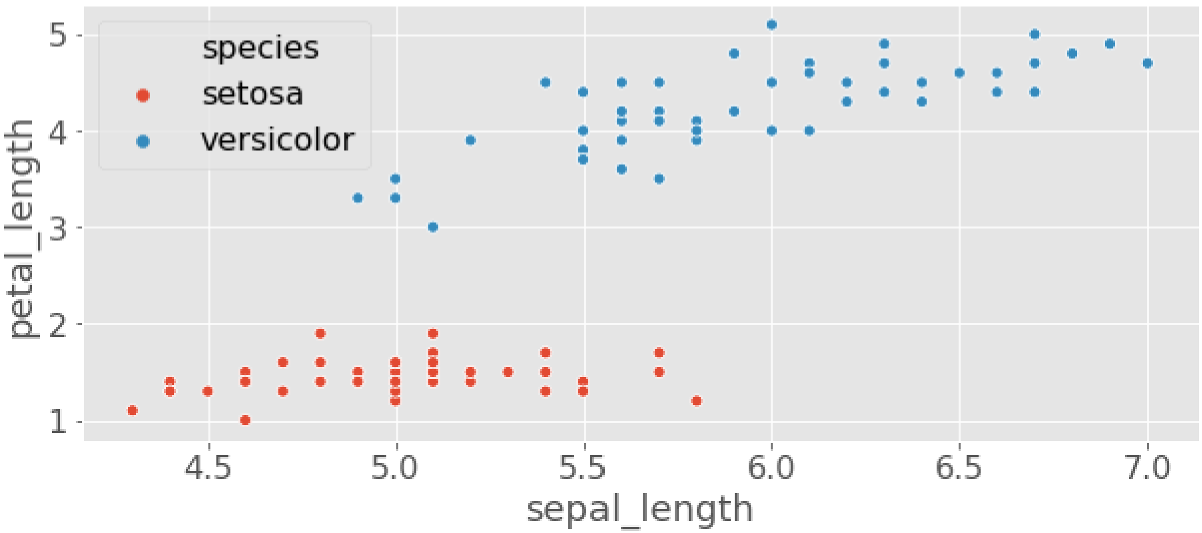
We load the iris data.

In [60]:
```
iris = sns.load_dataset('iris').iloc[:100] # drop virginica

X = iris.iloc[:, [0, 2]].values # keep petal_length and sepal_length
y = np.where(iris.species=='setosa', 1, -1) # convert to 1, -1

sns.scatterplot(iris.sepal_length, iris.petal_length, hue=iris.species)
```

Out[60]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x25648703240>
```



Working with the perceptron (2)

How do we fit the perceptron model? [perceptron definition]

In [61]:
```
# initialize the perceptron
clf = Perceptron(n_iter=10)

# fit the perceptron
# runs 10 iterations of updating the model
clf.fit(X, y)
```

Out[61]:
```
<ch02.Perceptron at 0x25649277438>
```

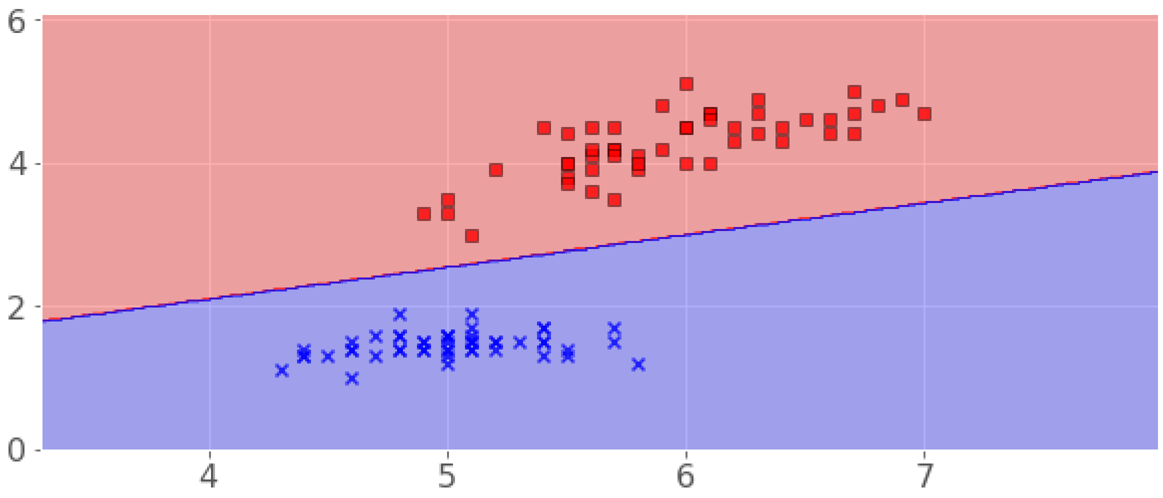
Working with the perceptron (3)

How can we evaluate the model??

In [62]:
```
print('Number of errors: %i' % sum(clf.predict(X)!=y))

# we plot the decisions
plot_decision_regions(X,y,clf)
```

```
Number of errors: 0
```

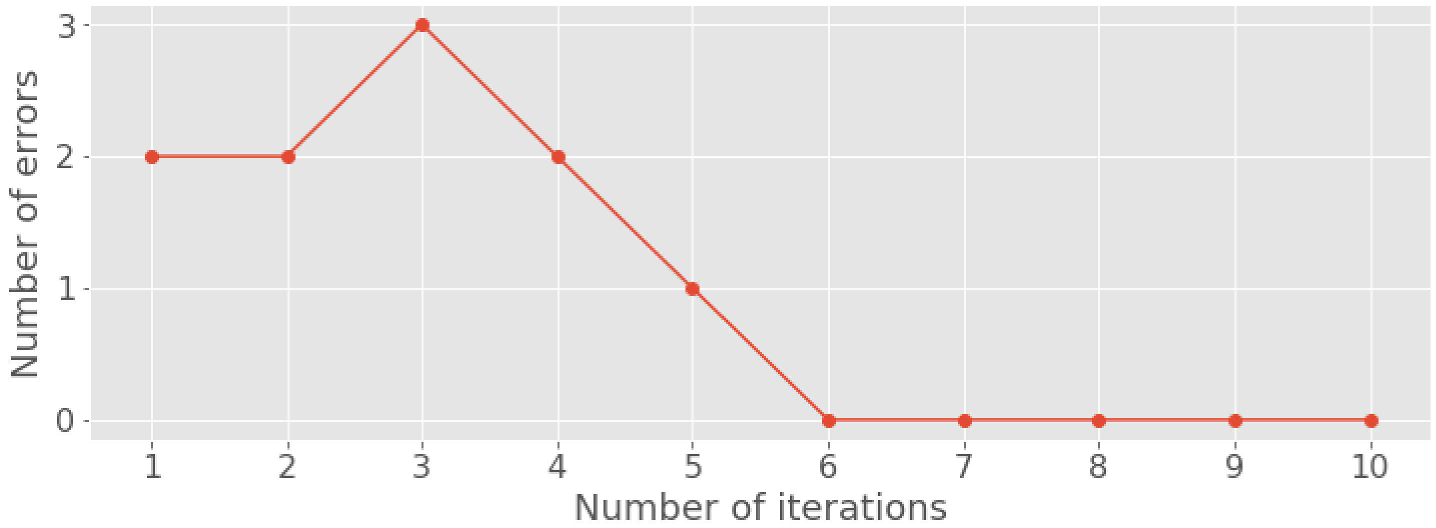


Working with the perceptron (4)

How does the model performance change??

In [63]:
```
f,ax = plt.subplots(figsize=(12, 4))
ax.set_xticks(range(11))
ax.plot(range(1, len(clf.errors_) + 1), clf.errors_, marker='o')
ax.set_xlabel('Number of iterations')
ax.set_ylabel('Number of errors')
```

Out[63]:
```
Text(0, 0.5, 'Number of errors')
```



Model validation

Model validation

How can we see how our model generalizes?

We can simulate out-of-sample prediction. How?

- Idea: Use some of our sample for model evaluation.
- Implementation - divide data randomly into two subsets:
    - `training data` for estimation;
    - `test data` for evaluation.
- Note: does not work for time series.

Model validation (2)

We revert to titanic, y : survived, X : everything else

In [68]:
```
titanic_sub.head(3)
```

Out[68]:

	survived	sibsp	age	alone	class_Second	class_Third	sex_male
0	0	1	22	0	0	1	1
1	1	1	38	0	0	0	0
2	1	0	26	1	0	1	0

We split the data into test and training samples

In [65]:
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=.5, random_state=0)
```

Beyond the perceptron

Motivation

What might we change about the perceptron?

1. Change from updating errors that are binary to continuous
2. Use more than one observation a time for updating

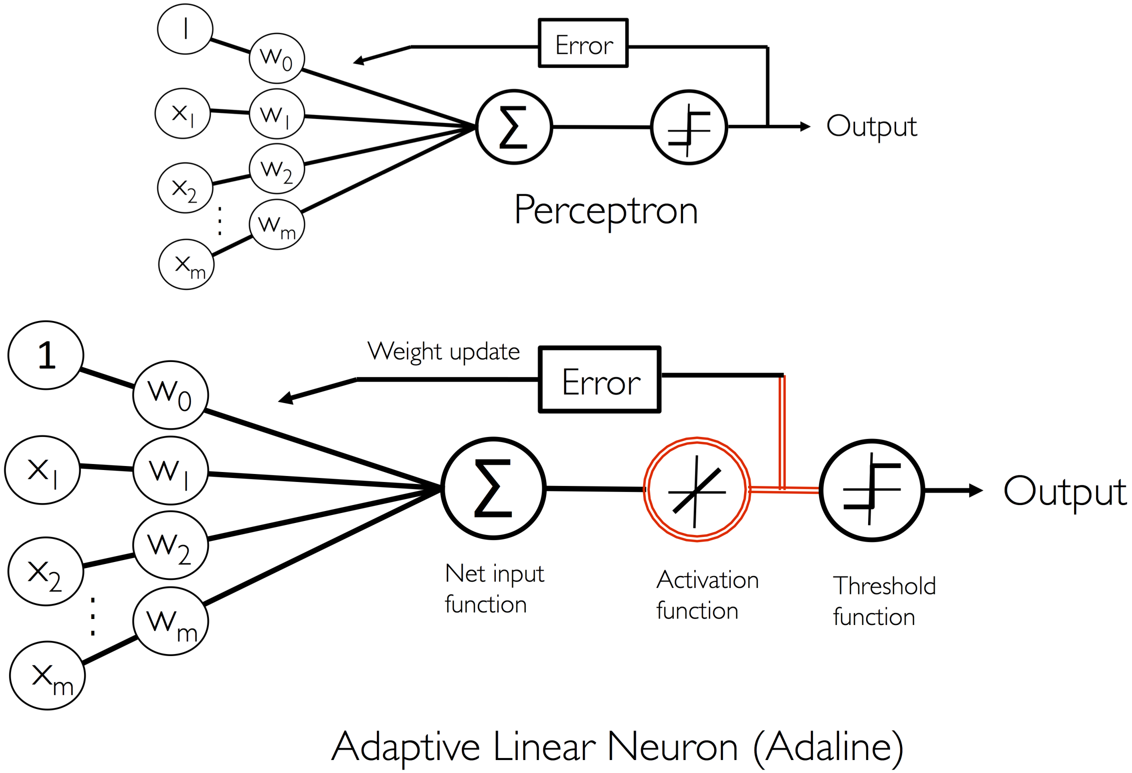
The activation function (1)

What else might we use to update errors?

- The most simple is **no transformation** of the net-input, i.e. $\phi(z_i) = z_i$.
- When we change this from perceptron we call it Adaptive Linear Neuron (**Adaline**).

The activation function (2)

How is this different from the Perceptron?



The activation function (3)

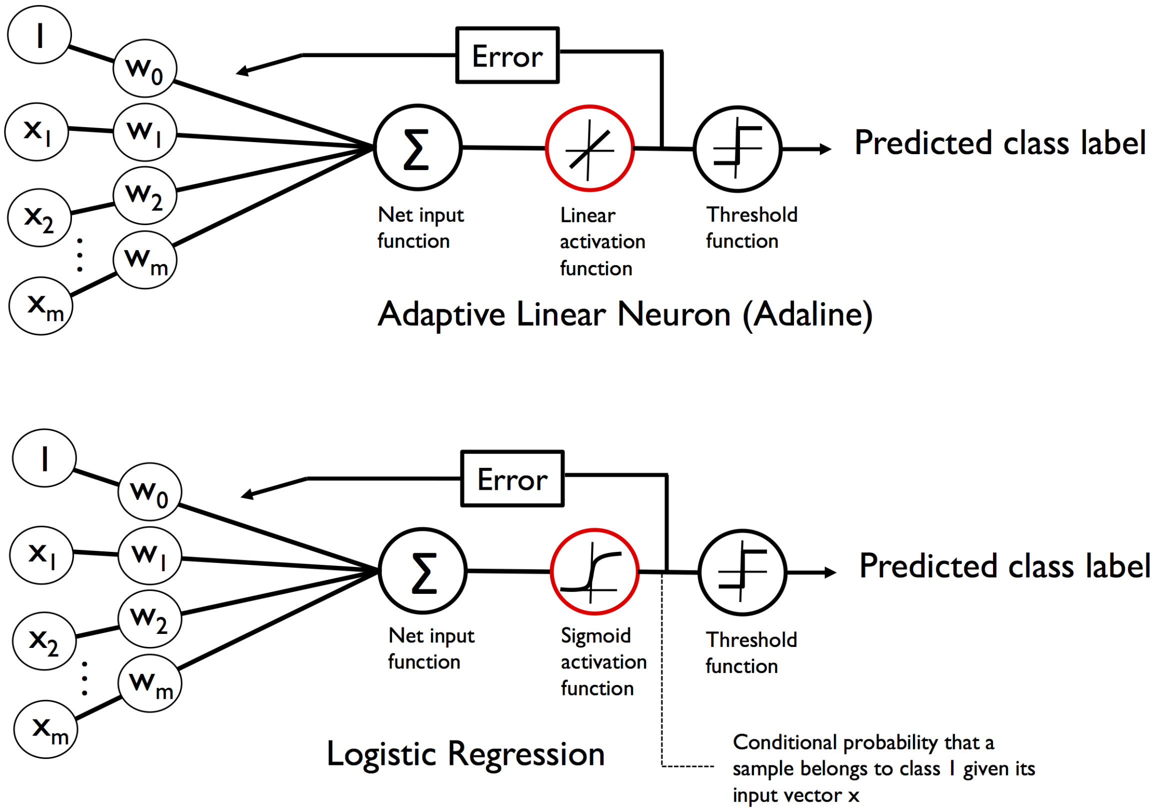
Which activation functions can be used?

- Linear
- Logistic (Sigmoid)
- Unit step, sign

See page 450 in Python for Machine Learning.

The activation function (4)

How do Adaline and Logistic regression differ?



A new objective (1)

The update rule in perceptron seems ad hoc, is there a more general way?

- Yes, we minimize the sum of squared errors (SSE). The SSE for Adaline is:

$$SSE = \boldsymbol{e}^T\boldsymbol{e} = e_1^2 + .. + e_n^2$$

$$\boldsymbol{e} = \mathbf{y} - \mathbf{X}\mathbf{w}$$

Doesn't the above look strangely familiar?

- Yes, it is the same objective as OLS.
- But no, we will not solve like OLS.

A new objective (2)

So how the hell do we solve the model?

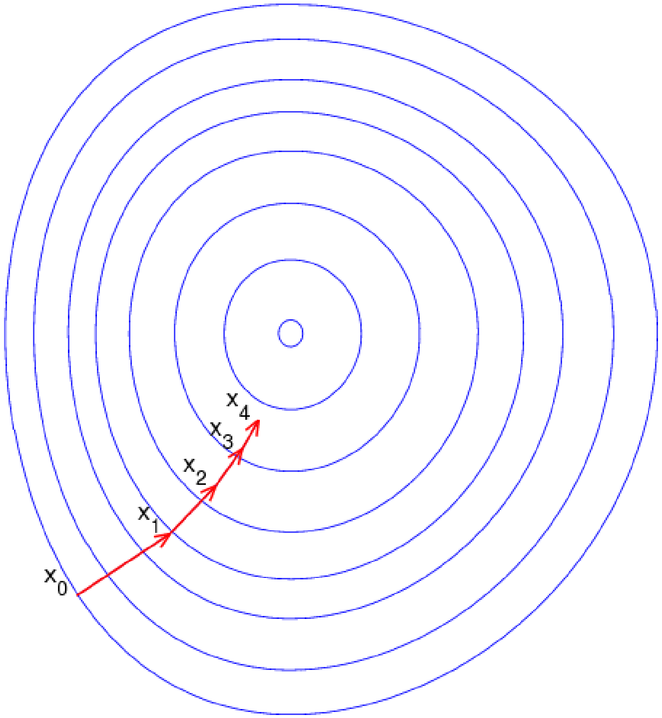
- We approximate the solution. Two options:
    - We approximate the first order derivative ~ gradient descent (GD)
    - We approximate both first and second order derivative ~ quasi Newton

- We take gradient descent - much simpler (sometimes faster)

A new objective (3)

How does a gradient descent look?

An algorithm that finds the direction where expected differences are largest. Attempt of satisfying first order condition (FOC).



A new objective (4)

What is the first order derivative of SSE in Adaline?

$$\frac{\partial SSE}{\partial \hat{w}} = \mathbf{X}^T\mathbf{e},$$

How do we update with GD in Adaline?

- Idea: take small steps to approximate the solution.
- $\Delta \hat{w} = \eta \mathbf{X}^T \mathbf{e} = \eta \cdot \mathbf{X}^T(\mathbf{y} - \hat{\mathbf{y}})$

A new objective (5)

The gradient descent algorithm we just learned uses the whole data.

- Often known as batch gradient descent.

What might be a smart way of changing (batch) gradient descent?

- we only use a subset of the data
- this called *stochastic gradient descent* (SGD)

Applying logistic regression

In [23]:
```
from sklearn.linear_model import LogisticRegression

# estimate model on train data, evaluate on test data
clf = LogisticRegression(solver='lbfgs')
clf.fit(X_train, y_train) # model training
y_hat = clf.predict(X_test)
accuracy = (y_hat==y_test).mean() # model testing
print('Model accuracy is:', np.round(accuracy,3))
```

```
Model accuracy is: 0.793
```

The end

Return to agenda