Session 11:

Machine learning introduction

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Taking stock

What have we learned until now?

-

Some coding advice

- *How do I extract an object from my function?* Print or return?
- Solving complex problems: One thing at a time
- Is joining datasets difficult?
    - Check out the pandas documentation on merging (https://pandas.pydata.org/pandas-docs/stable/user_guide/merging.html)
    - Or the guide available from Jake Van der Plas (https://jakevdp.github.io/PythonDataScienceHandbook/03.07-merge-and-join.html)

Agenda

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.

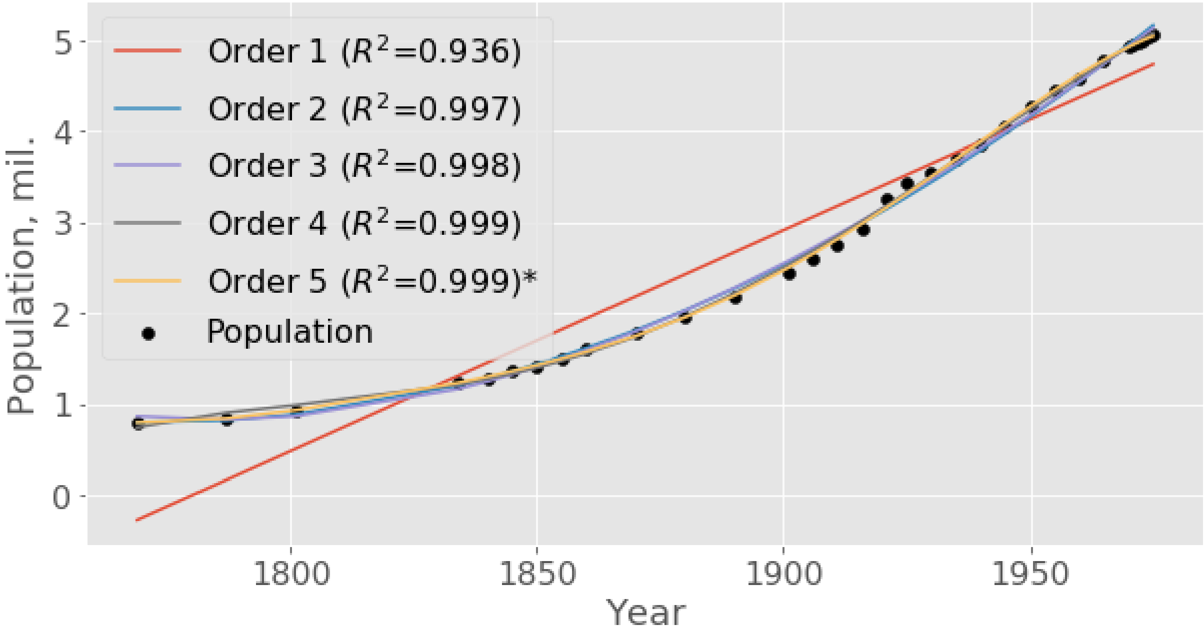
Model fragility (2)

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]:



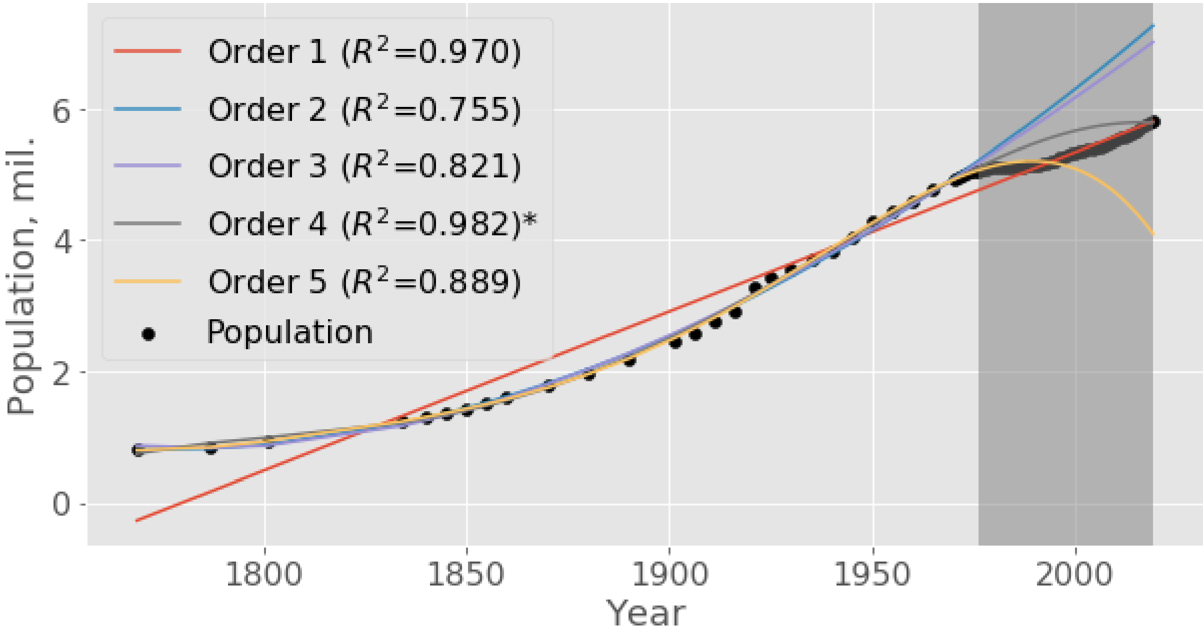
Model fragility (3)

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

In [26]:

```
f_pop2
```

Out[26]:

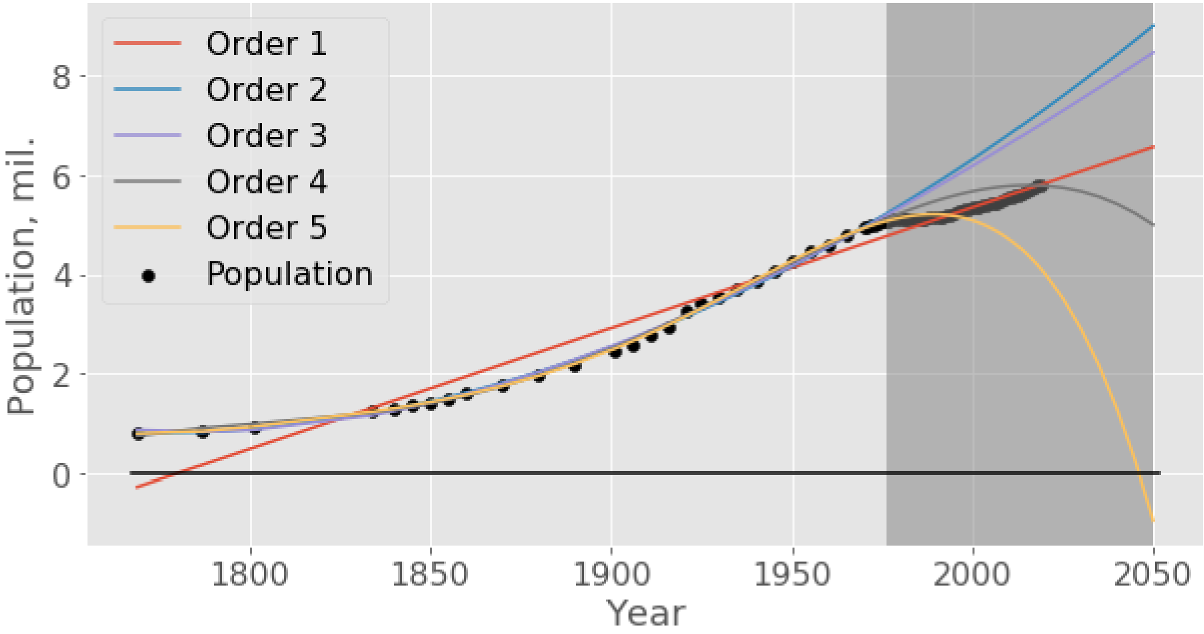


Model fragility (4)

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 too 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.

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!

Machine learning overview

Machine learning outline for this course

ML: short for machine learning

- Problems: ***supervised*** vs unsupervised
- Linear supervised ML models
    - classification and regression
    - regularization
    - **getting hands dirty with implementing solver**
- Fundamental concepts of ML
    - overfitting, underfitting, model validation
    - model selection and hyperparameters
- Emphasize differences and synergies between ML and statistics
- Brief intro of non-linear models

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.
    - We define the `target` as labels in data we wish to model.
        - Example: population as a function of year.
- Unsupervised learning
    - Find patterns and relationships from **unlabeled** data.
    - This may involve clustering, dimensionality reduction and more.
    - Not part of the course.

Why machine learning

How might this be useful for social scientists?

Supervised machine learning is important (elaborated in Lecture 14):

- 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

How can we categorize a supervised ML model?

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

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

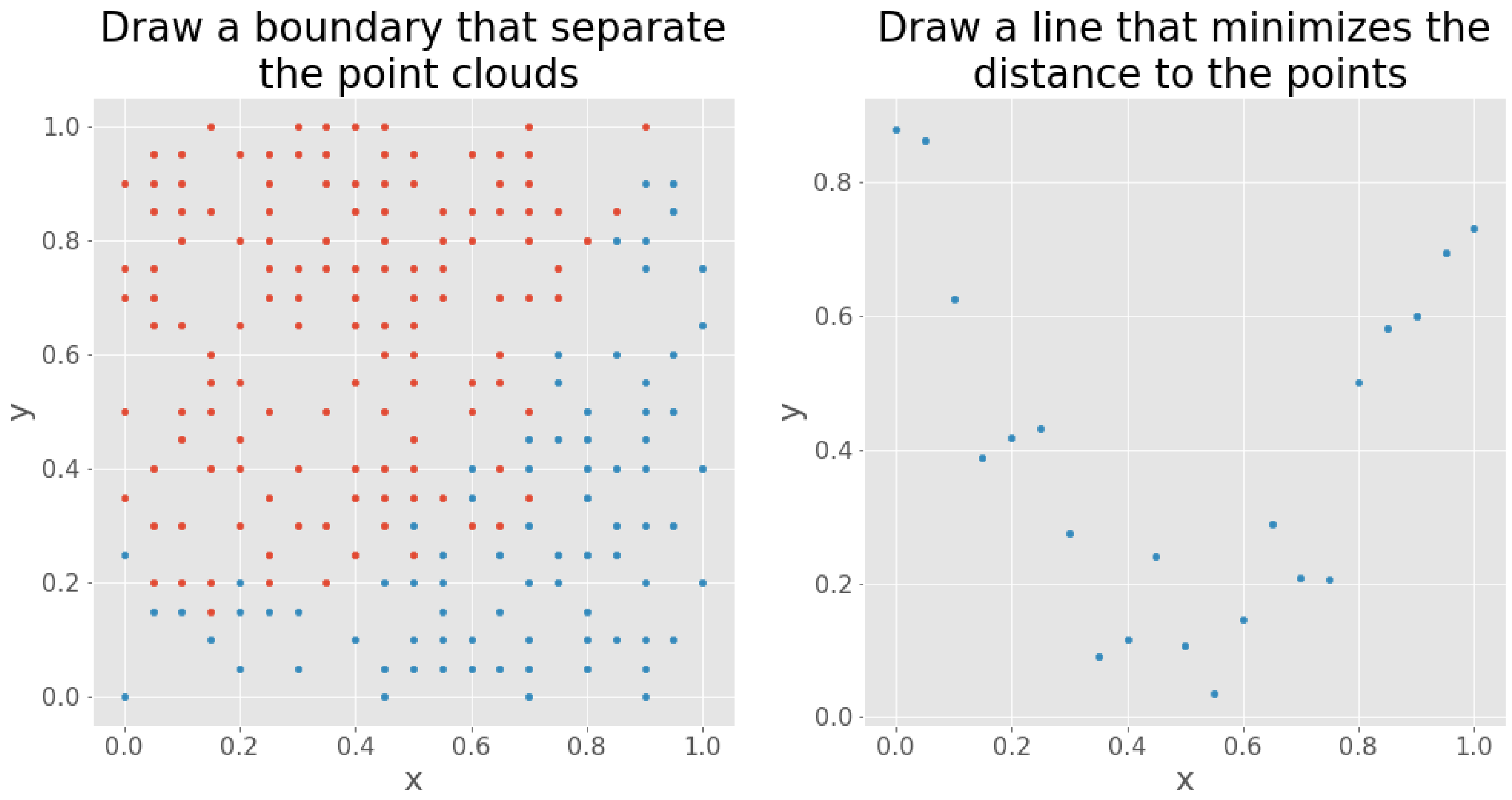
- **regression**: predict a numeric value
- **classification**: distinguish between target categories (non-numeric data)

Supervised ML problems (2)

Which one is classification, which one is regression?

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

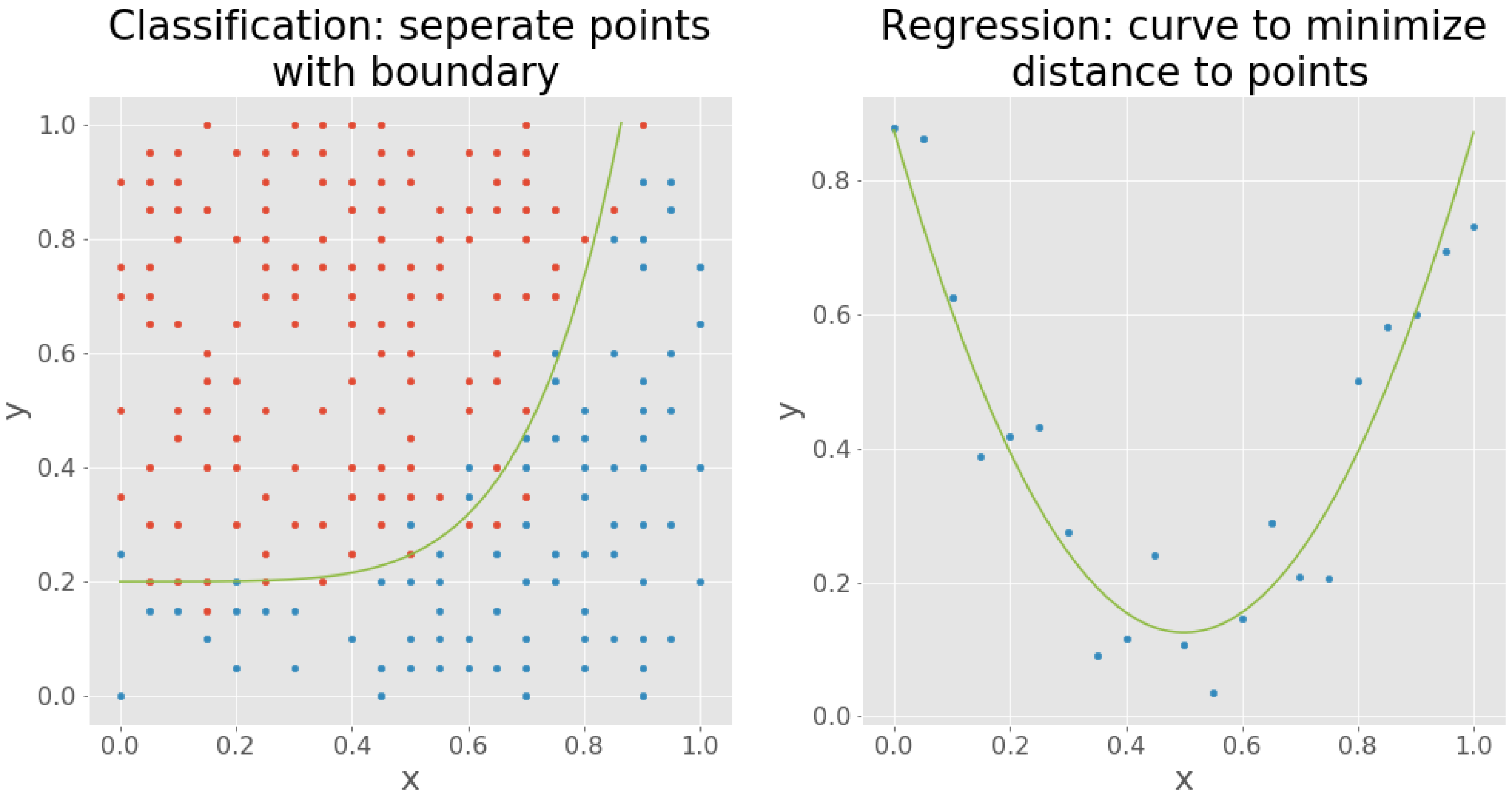
Out[28]:



Supervised ML problems (3)

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

Out[29]:



Regression models

What are examples of regressions models?

- Example of targets: 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?

- Targets are categories
    - sometimes known as `factor` in statistics
    - (work for `str`, `bool`, `int`, `float` which are then interpreted as categories)
- Examples of target: kind of education (linguistics, math), mode of transportation

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.

Target is: ...?

In [4]:
```
import numpy as np
import pandas as pd
import seaborn as sns

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 and econometric equivalents

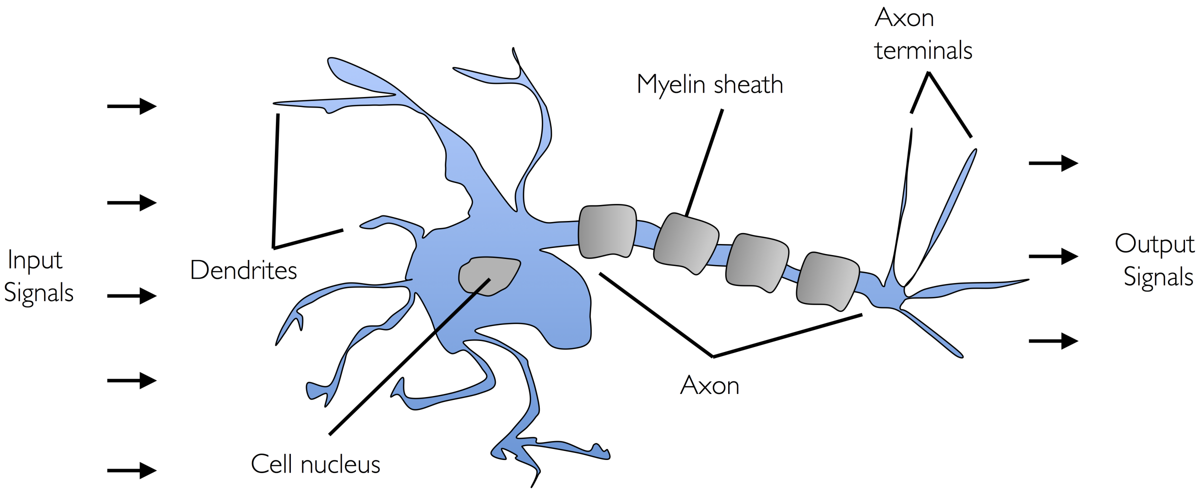
- `feature` vector, $\mathbf{x}_i$, i.e a row of input variables
    - = explanatory **variables** in econometrics
- `weight` vector, $\mathbf{w}$, i.e model parameters
    - = **coefficients** in econometrics where denoted β
- `bias` term, w_0, i.e. the model intercept
    - = the **constant** variable in denoted β_0

The perceptron model

The artificial neuron

A real neuron maps stimulus (input) to output.

[Research estimates (https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5063692)](https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5063692) there are 55–70 billion neurons in the brain.



The artificial neuron (2)

We are interested in making a decision rule that takes arbitrary input and outputs either positive or negative.

Mathematically we define this map as $\phi : \mathbb{R}^p \rightarrow \{-1, 1\}$.

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

- `net-input`, $z_i = \underbrace{\boldsymbol{w}^T \boldsymbol{x}_i}_{vector\ form} = \underbrace{1 \cdot w_0 + w_1 x_{i,1} + \ldots + w_k x_{i,k}}_{expanded\ form}$
- `unit step function`, ϕ, checks if value exceeds threshold

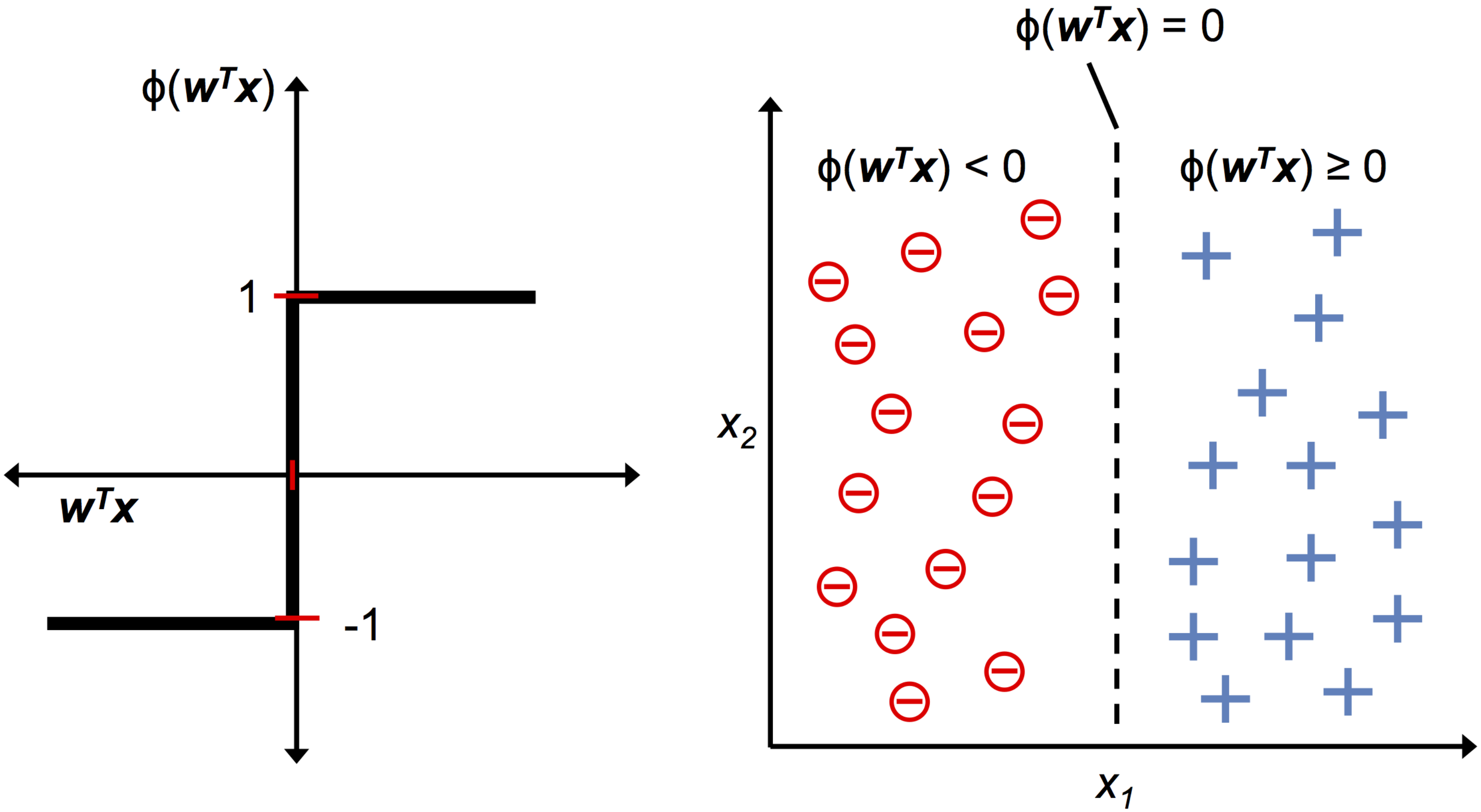
The artificial neuron (3)

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 (4)

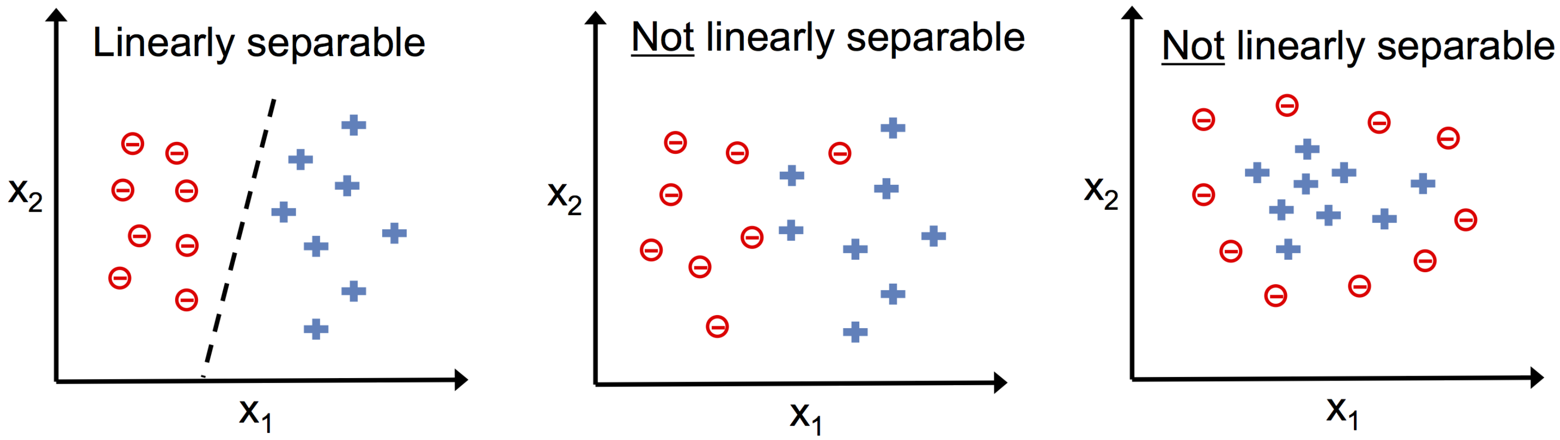
The unit step function (left) and the decision boundary (right)



The artificial neuron (5)

When does the artical 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 compute the predicted target $\hat{y}$?

We apply a transformation on the net-input :

- single observation, expanded notation:
  $$\hat{y}_i = \phi(z_i), \quad z_i = w_0 + w_1 \boldsymbol{x}_{i,1} + \ldots + w_k \boldsymbol{x}_{i,k}$$
- single observation, vector notation:
  $$\hat{y}_i = \phi(z_i), \quad z_i = \boldsymbol{w}^T \boldsymbol{x}_i$$
- multiple observations, matrix notation:
  $$\hat{\boldsymbol{y}} = \phi(\boldsymbol{z}), \quad \boldsymbol{z} = \boldsymbol{X}\boldsymbol{w}$$

The perceptron learning rule (3)

How do we update weights?

Weights are updated as follows:

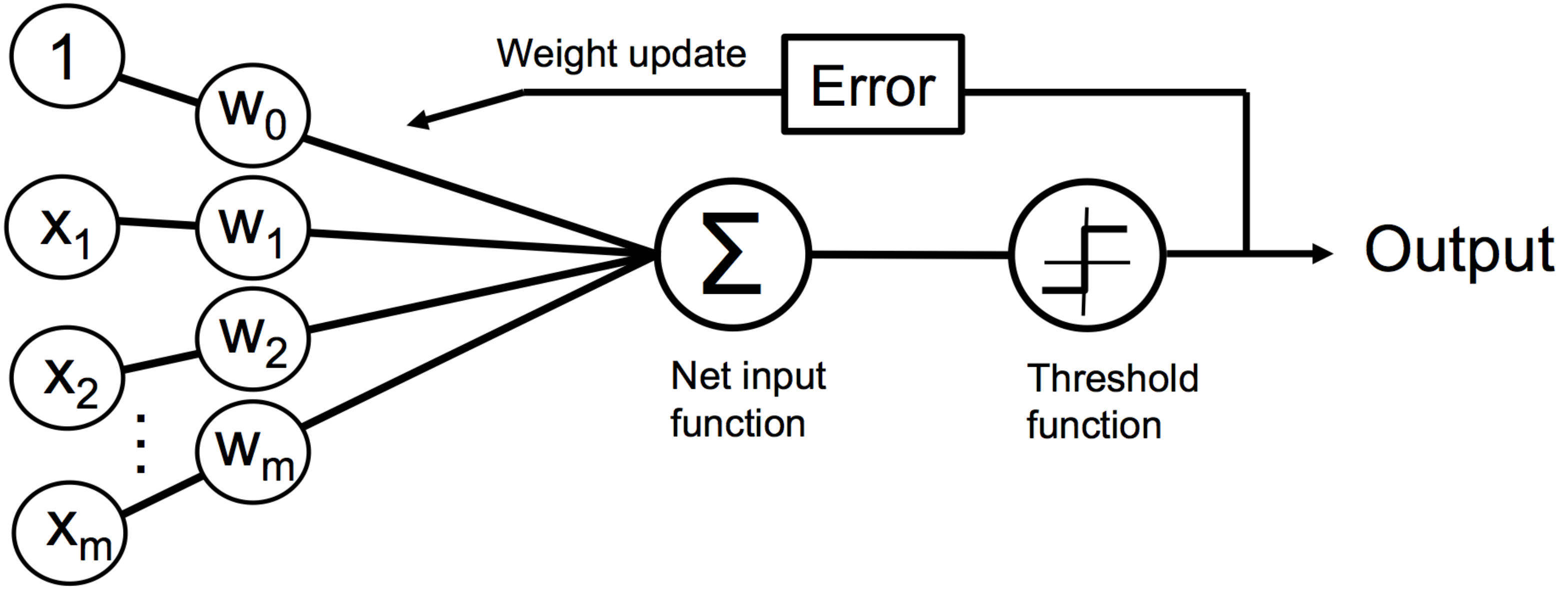
$$w = w + \Delta w$$
$$\Delta w = \eta \cdot (y_i - \phi(z_i)) \cdot \mathbf{x}_i$$

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

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

The perceptron learning rule (4)

The computation process



Implementation in Python (1)

Let's set some values of input and output

In [ ]:
```
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)
```

Implementation in Python (2)

How do we compute the errors vectorized?

In [6]:

```
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 [10]:
```
# learning rate
eta = 0.001

# negative first order derivative (FOD) of SSE wrt β
# FOD vector notation: = -ε'X = -(Y-Xβ)'X
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]:

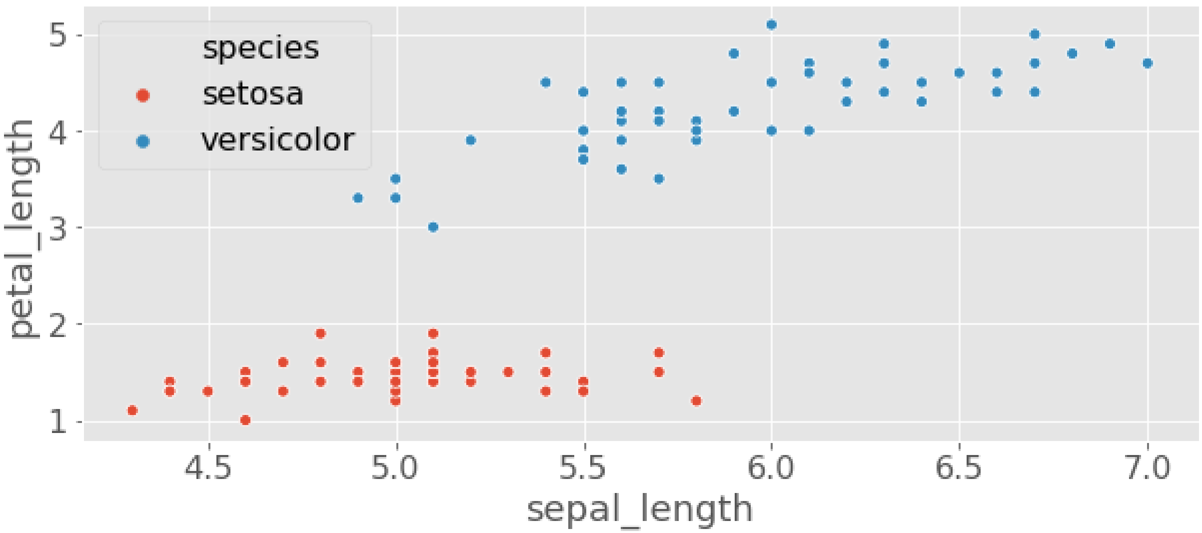
```
iris = sns.load_dataset('iris').iloc[:100] # drop virginica

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>
```

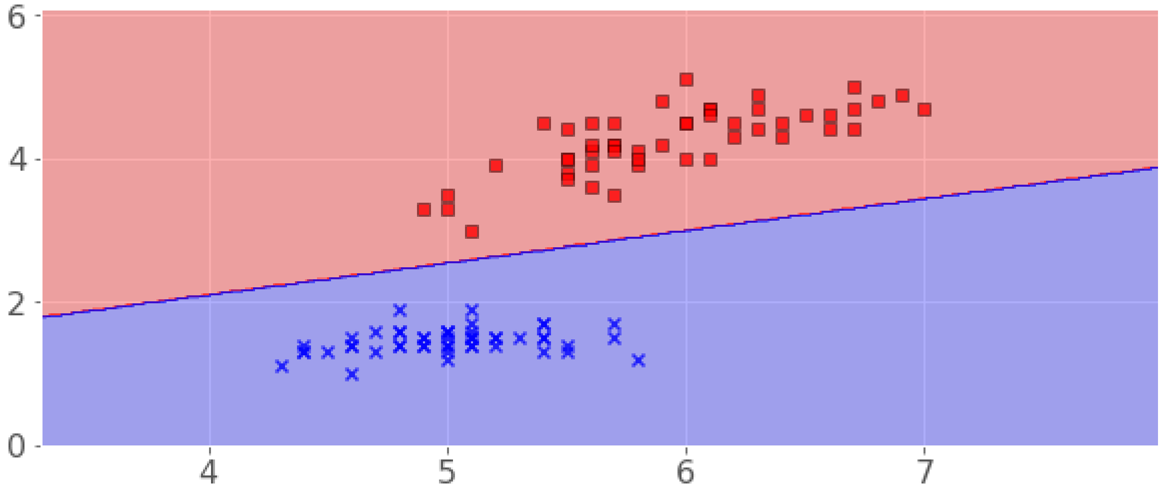
Working with the perceptron (3)

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
```

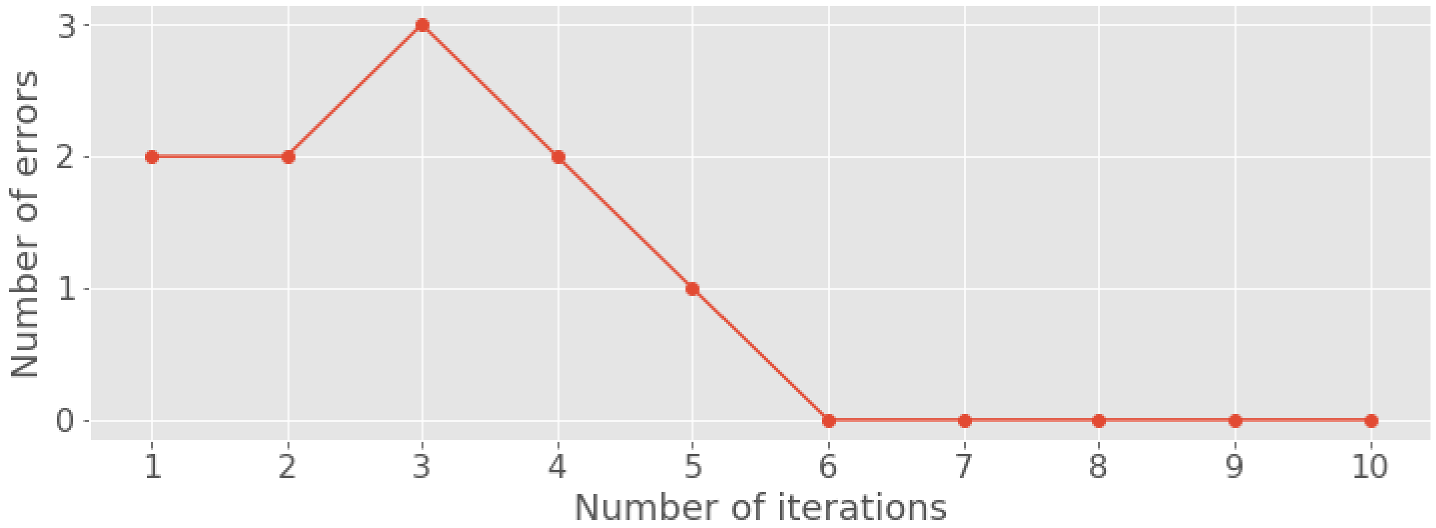


Working with the perceptron (4)

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 [ ]:
```
print(titanic_sub.head(3))
```

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

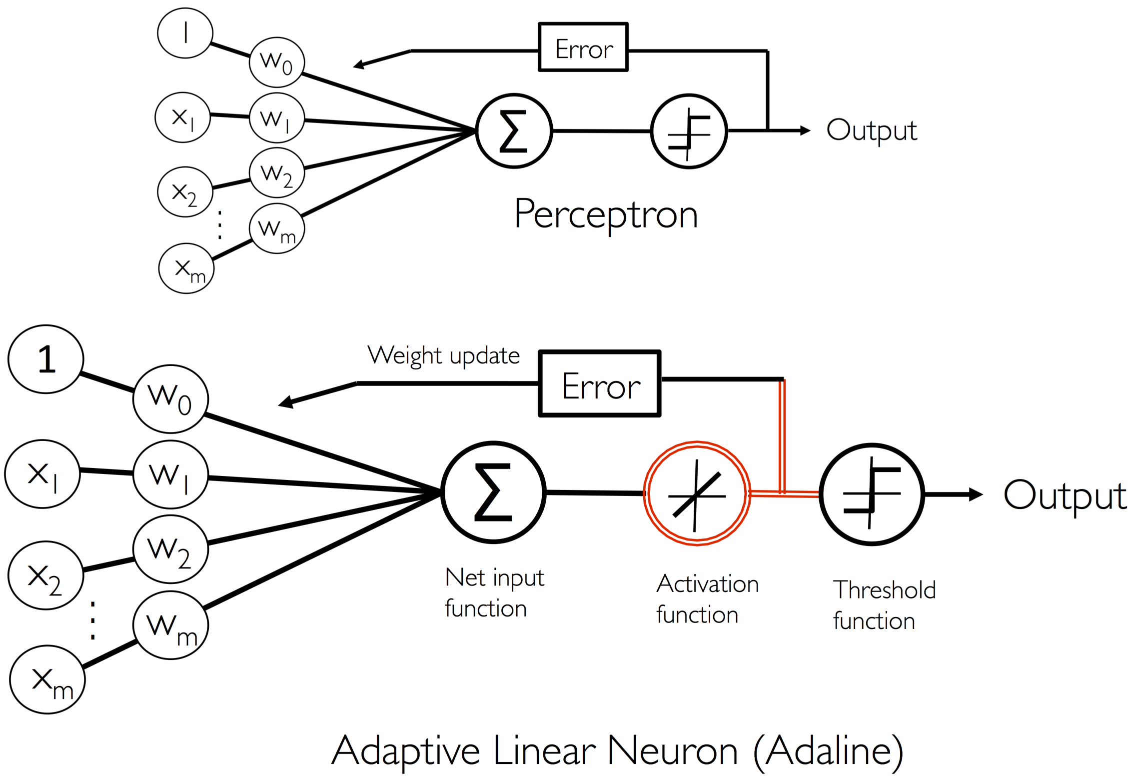
The activation function (1)

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)

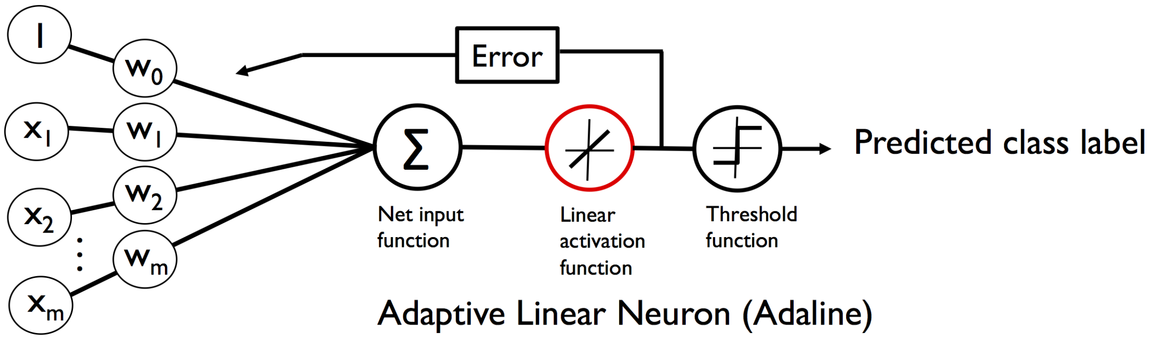
Which activation functions can be used?

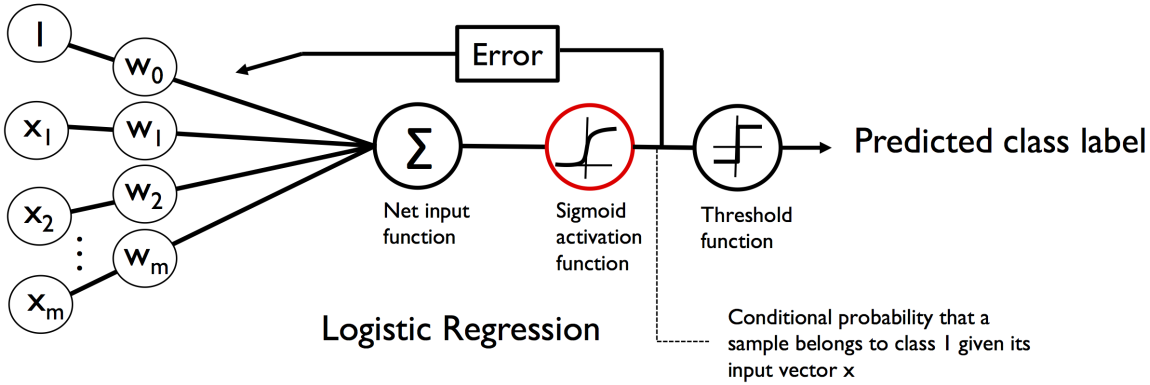
- Linear
- Logistic (Sigmoid)
- Unit step, sign

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. The difference:
  - OLS computes the exact solution with system of equations from first order conditions.
  - We make an approximate solution.

A new objective (2)

So how the hell do we make the approximate solution?

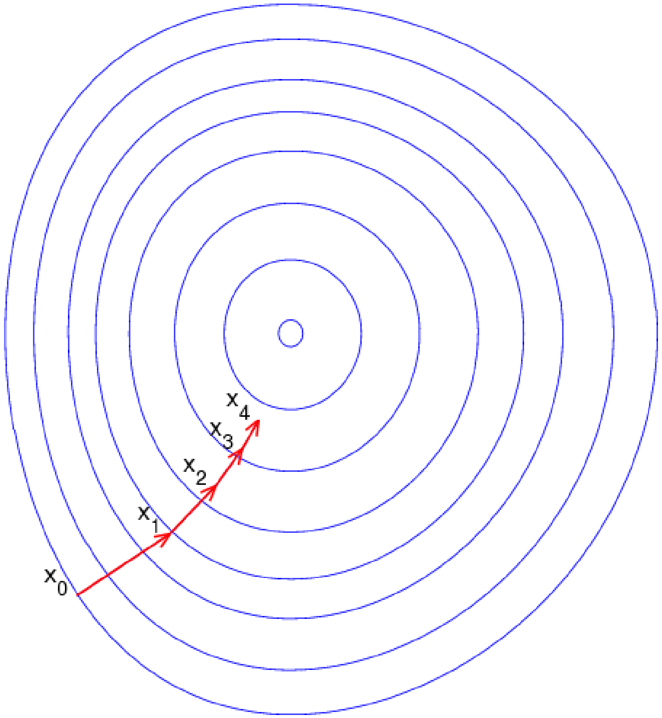
- Two general classes:
  - We approximate the first order derivative ~ gradient descent (GD)
  - We approximate both first and second order derivative ~ quasi Newton

- We take gradient descent - much simpler (often 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 wrt. weights in Adaline?

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

How do we update with GD in Adaline?

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

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. Two variants:
    - *stochastic gradient descent* (SGD): uses random subset of observations
    - *mini batch*: uses deterministic subset of observations (loop whole dataset)
- Idea: we converge faster by computing update for subset of data
    - Note: we may need a million repetitions.

Applying logistic regression

How difficult is it to use `LogisticRegression` ?

Very easy:

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