Elements Of Data Science - S2022

# Week 5: Intro to Machine Learning Models

2/15/2022

# TODOs

- Readings:
  - Recommended: **https://scikit-learn.org/stable/supervised_learning.html**
  - **Read** PDSH Chap 5 In Depth: Linear Regression
  - **Read** PDSH Chap 5 In Depth: Support Vector Machines
  - **Read** PDSH Chap 5 In Depth: Decision Trees and Random Forests
  - **Read** Chapter 3 from HOML
  - **Read** Chapter 4 from HOML
- Quiz 5, Due Mon Feb 21st, 11:59pm
- HW1 Due Fri Feb 18th, 11:59pm ET

# Today

- Intro to Machine Learning Models
- Various types of ML
- Linear models
- Next week:
    - One Vs. Rest For Multiclass/Multilabel Classification
    - Distance Based: kNN
    - Tree Based: Decision Tree
    - Ensembles: Bagging, Boosting, Stacking

Questions?

# Environment Setup

In [1]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns

sns.set_style('darkgrid')

%matplotlib inline
```

# Modeling and ML

- What is a Model?
  - Specification of a mathematical (or probabilistic) relationship between different variables.
- What is Machine Learning?
  - Creating and using models that are learned from data.

# Questions for Models

In [2]:

```
df_wine = pd.read_csv('../data/wine_dataset.csv',usecols=['alcohol','ash','proline','hue','class'])
df_wine.sample(4,random_state=1)
```

Out[2]:

| | alcohol | ash | hue | proline | class |
|---|---|---|---|---|---|
| 161 | 13.69 | 2.54 | 0.96 | 680.0 | 2 |
| 117 | 12.42 | 2.19 | 1.06 | 345.0 | 1 |
| 19 | 13.64 | 2.56 | 0.96 | 845.0 | 0 |
| 69 | 12.21 | 1.75 | 1.28 | 718.0 | 1 |

- Can we predict target/label "class" from the other columns? **(Classification)**
- Can we predict target/label "hue" from the other columns? **(Regression)**
- What are the important features when predicting "hue"? **(Feature Selection)**
- Can a model tell us about how the features and target/label interact? **(Interpretation)**
- Do the observations group together in feature space? **(Clustering)**

# Data Vocabulary for ML

In [3]:

```
df_wine.sample(5,random_state=1)
```

Out[3]:

| | alcohol | ash | hue | proline | class |
|---|---|---|---|---|---|
| 161 | 13.69 | 2.54 | 0.96 | 680.0 | 2 |
| 117 | 12.42 | 2.19 | 1.06 | 345.0 | 1 |
| 19 | 13.64 | 2.56 | 0.96 | 845.0 | 0 |
| 69 | 12.21 | 1.75 | 1.28 | 718.0 | 1 |
| 53 | 13.77 | 2.68 | 1.13 | 1375.0 | 0 |

- $X$, features, attributes, independent/exogenous/explanatory variables
    - Ex: alcohol, trip_distance, company_industry
- $y$, target, label, outcome, dependent/endogenous/response variables
    - Ex: class, hue, tip_amount, stock_price
- $f(X) \rightarrow y$, Model that maps features $X$ to target $y$

# Variations of ML Tasks

- **Supervised** vs **Unsupervised**
  - is there a target/label?
- **Regression** vs **Classification**
  - is the target numeric or categorical?
- **Prediction** vs **Interpretation**
  - generate predictions or understand interactions?
- Model Families
  - Linear, Tree, Distance, Probability, Neural Net, Ensemble, ...

# Supervised vs Unsupervised vs Reinforcement Learning

Is there a target, $y$?

- Yes:
  - **Supervised Learning:** Data consists of $(X, y)$ pairs
  - Uses: Classification, Regression
  - Ex: What is the relationship between length of ride and tip amount?
- No:
  - **Unsupervised Learning:** Data consists only of $(X)$
  - Uses: Clustering, Topic Modeling, etc.
  - Ex: Are there any clusters in length of ride?
- Eventually:
  - **Reinforcement Learning**
  - After a series of predictions (path) get a reward from a reward function
  - Ex. Poker player

# Other Learning Paradigms

- Do we have a mix of labeled and unlabeled?
    - **Semi-Supervised Learning**
    - Can we use structure of unlabeled data along with labeled?
- Will we continue getting new data?
    - **Online Learning**
    - Is there an oracle (ground truth) we can consult?
    - Can we select which points to make predictions on?

# Supervised Learning: Regression vs Classification

- **Regression** -> predict a numeric value
  - Ex: tip_amount, stock_price, wine_hue
- **Classification** -> predict a discrete class/category
  - Ex: class of wine, face/not face, object labels in image
- Note: convert a regression problem into classification with binning/thresholding

```
<td><img src="images/regression.png" width="350px"></td>
<td><img src="images/classification.png" width="350px"></td>
</tr></table></div>
```

From PML

# Prediction vs Interpretation

- Do we care more about: the accuracy when generating predictions?
    - Ex: For a given taxi trip, what will the tip size likely be?
    - Ex: For a given loan, will there be a default?
- Do we care more about: understanding how $X$ relates to $y$?
    - Ex: What happens to tip size as taxi trip length increases?
    - Ex: What is the relationship between debt and loan default?

# Model Families for Supervised Learning

- Linear
    - Simple/Multiple Linear Regression
    - Logistic Regression (for Classification)
    - Support Vector Machines
    - Perceptron
- Tree Based
    - Decision Tree
- Distance Based
    - K-Nearest Neighbor

# Model Families for Supervised Learning Continued

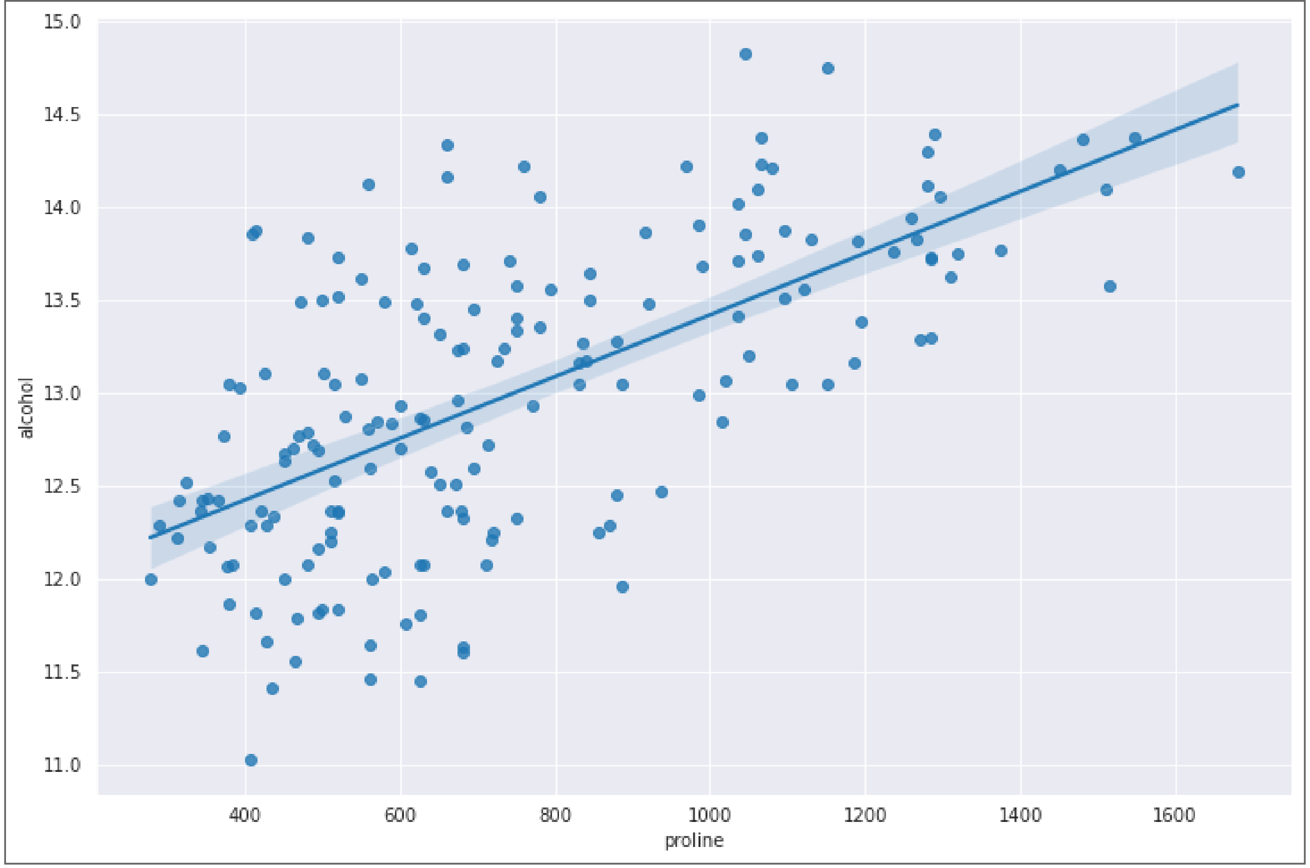
- Probability
  - Naive Bayes
  - Bayes Net
- Ensemble
  - Random Forest
  - Gradient Boosted Trees
  - Stacking
- Network
  - Multi-layer Perceptron
  - Deep Neural-Networks
  - Convolutional Neural Nets
  - Recurrant Neural Nets

# Example: Regression with a Linear Model

What is the relationship between 'proline' (an amino-acid) and 'alcohol' in wine?

In [4]:

```
fig,ax = plt.subplots(1,1,figsize=(12,8))
sns.regplot(x='proline', y='alcohol', data=df_wine);
```



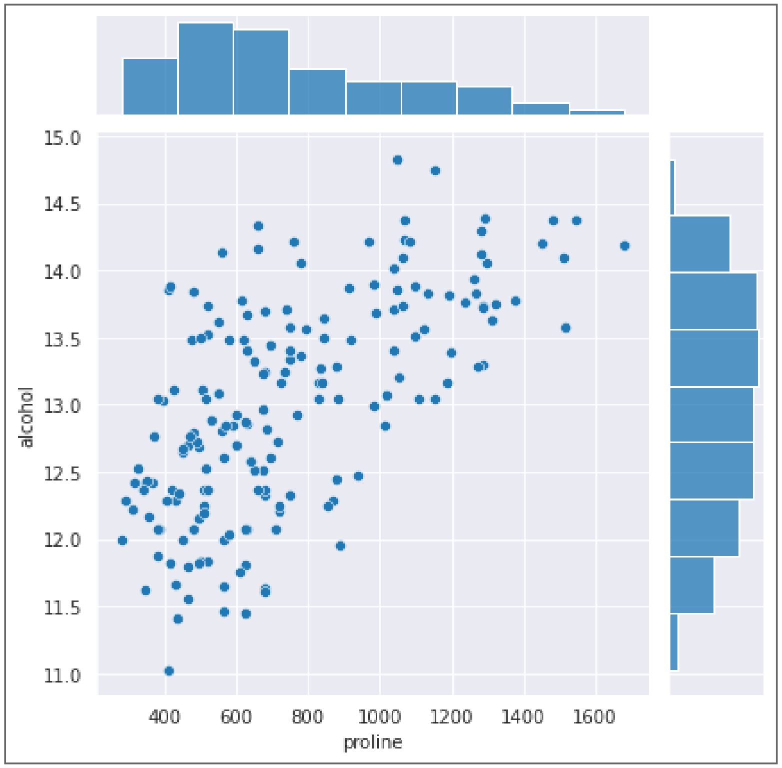
15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
alcohol
400
600
800
1000
1200
1400
1600
proline

# Aside: Correlation

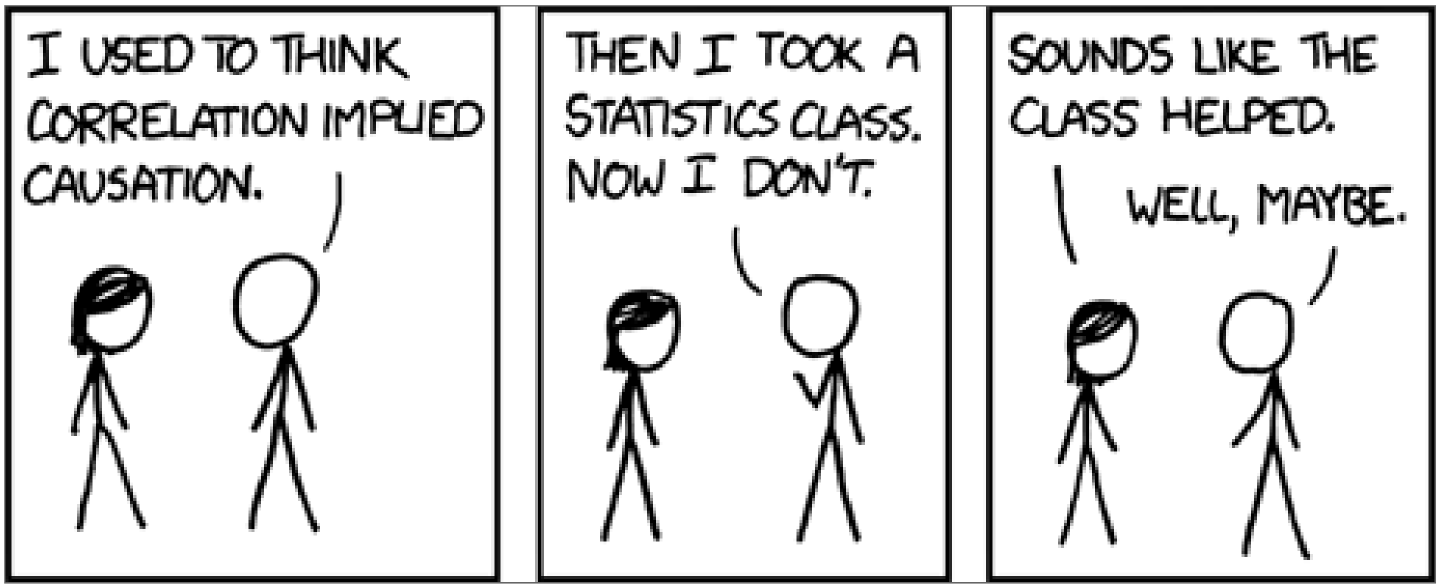
**Question:** are total_bill and tips correlated?

In [5]:

```
sns.jointplot(x='proline',y='alcohol',data=df_wine);
```



# Obligitory Correlation vs. Causation

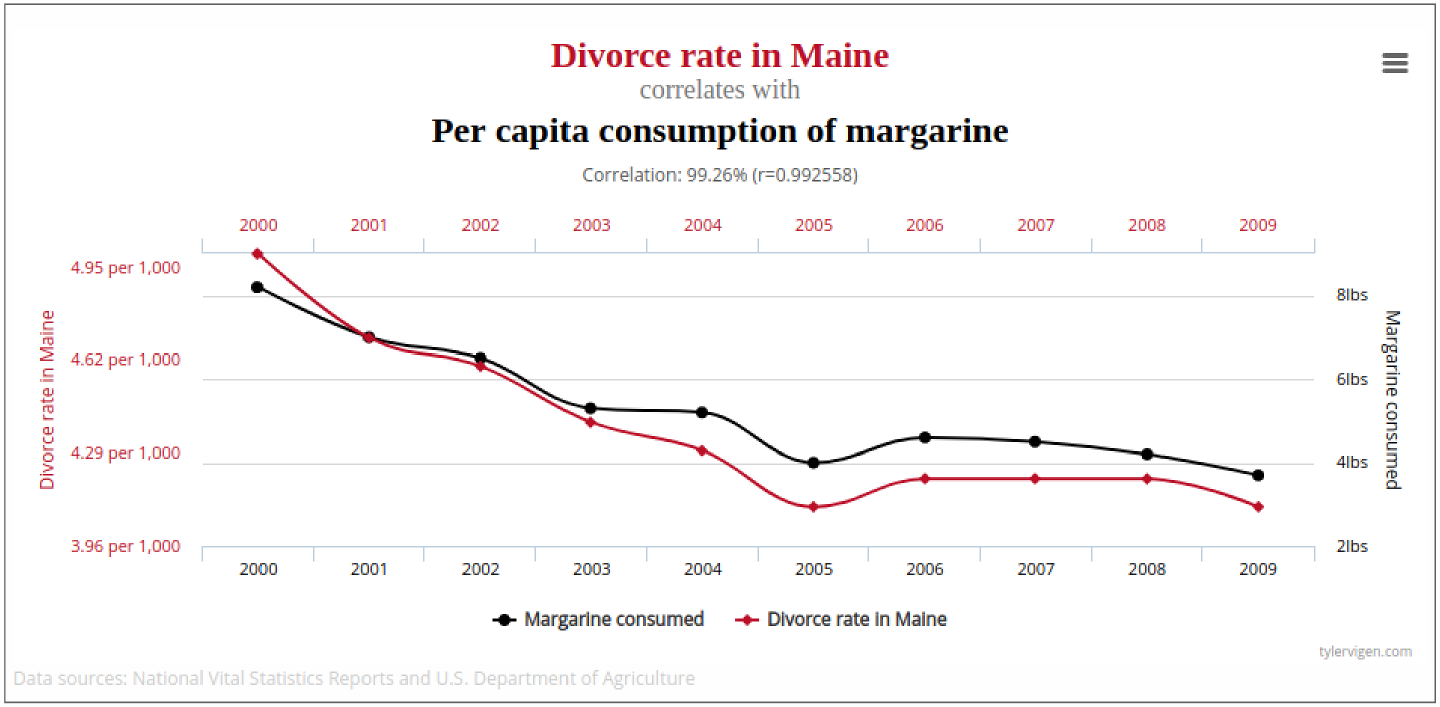



**https://imgs.xkcd.com/comics/correlation.png**

- Correlation does not mean causation!
- Causal Inference
  - controlled experiment
  - control for confounding variables

# Spurious Correlation

- Also, look hard enough and you'll find correlation.
  - See **spurious correlations** for examples



# Aside: Correlation

- Could calculate Pearson Correlation Coefficient
- Assumes normally distributed data! (which is not true here)
    - **On the Effects of Non-Normality on the Distribution of the Sample Product-Moment Correlation Coefficient](https://www.jstor.org/stable/2346598?seq=1#page_scan_tab_contents**)

In [6]:

```
from scipy.stats import pearsonr
r,p = pearsonr(df_wine.proline,df_wine.alcohol)
print(f'r: {r:.2f}, p: {p:.2f}')
```

```
r: 0.64, p: 0.00
```

- We know that as proline goes up alcohol goes up, but by how much?

# Python Modeling Libraries

## Prediction - scikit-learn

### Interpretation - scikit-learn and statsmodels

### Additional Tools - mlxtend

# Aside: MLxtend and conda-forge

- **MLxtend:** (machine learning extensions) is a Python library of useful tools for the day-to-day data science tasks.

- **Conda-Forge:** A community-led collection of recipes, build infrastructure and distributions for the conda package manager.

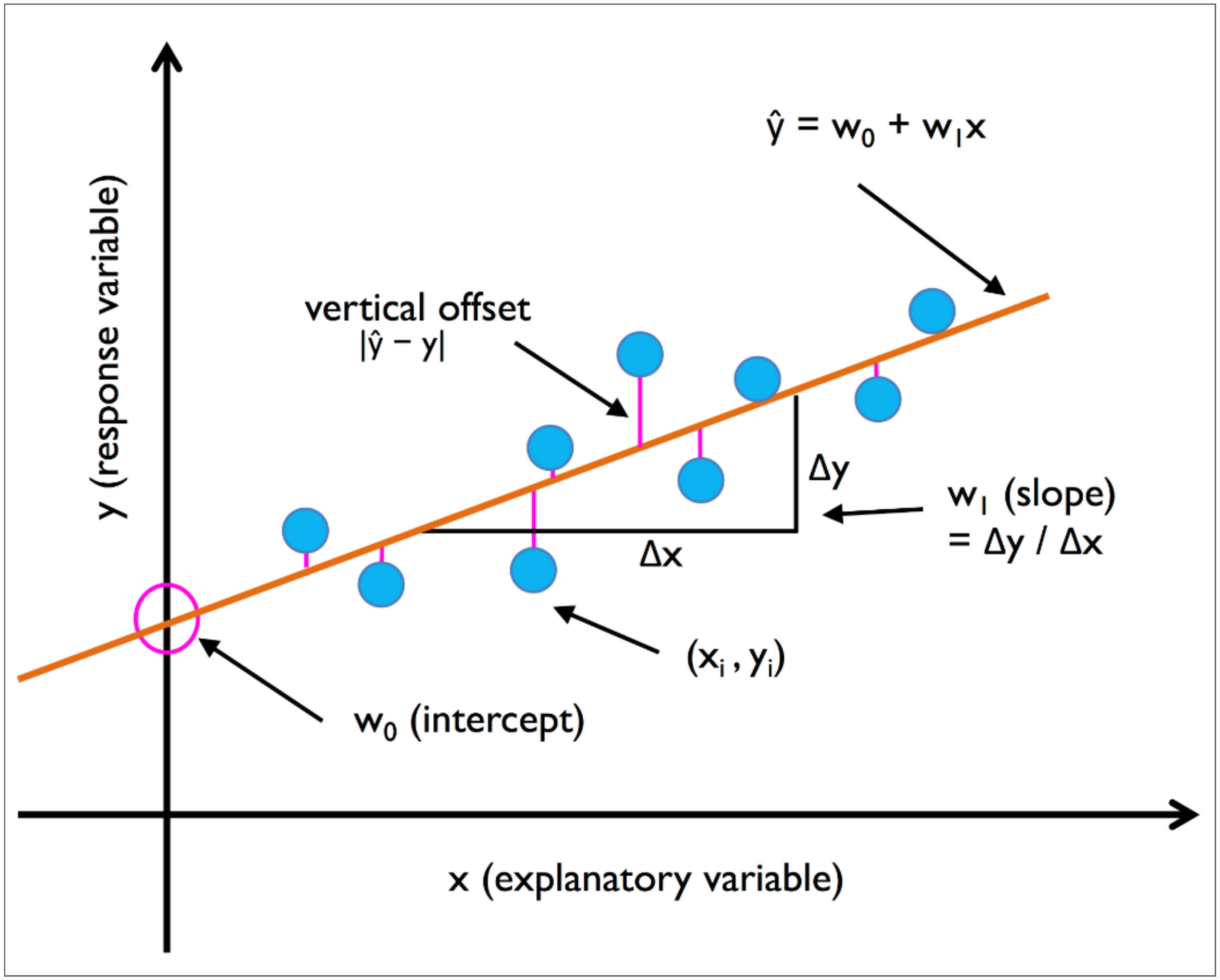
```
# NOTE: just an example, don't need to run, already installed
$ conda install --name eods-s22 --channel conda-forge mlxtend
```

# Simple Linear Regression

$$y = w_1 x + w_0 + \varepsilon_i$$

- $y$ : dependent/endogenous response, target, label (Ex: `alcohol`)
- $x_i$ : independent/exogenous/explanatory feature, attribute (Ex: `proline`)
- $w_1$ : coefficient, slope
- $w_0$ : bias term, intercept
- $\varepsilon_i$ : error, hopefully small, often assumed $\mathcal{N}(0, \varsigma^2)$
- Want to find values for $w_1$ and $w_0$ that best fit the data.
- Find a line as close to our observations as possible

# Simple Linear Regression




from PML

# Finding $w_1$ and $w_0$ with Ordinary Least Squares

- **prediction**: $\hat{y}_i = f(x_i) = w_1 x_i + w_0$
- **error**: $error(y_i, \hat{y}_i) = y_i - \hat{y}_i$
- **sum of squared errors**: $\sum_{i=1:n} (y_i - \hat{y}_i)^2$
- **least squares**: make the sum of squared errors as small as possible
- **gradient descent**: minimize error by following the gradient wrt $w_1, w_0$
    - can sometimes be optimized in closed form
    - often done iteratively

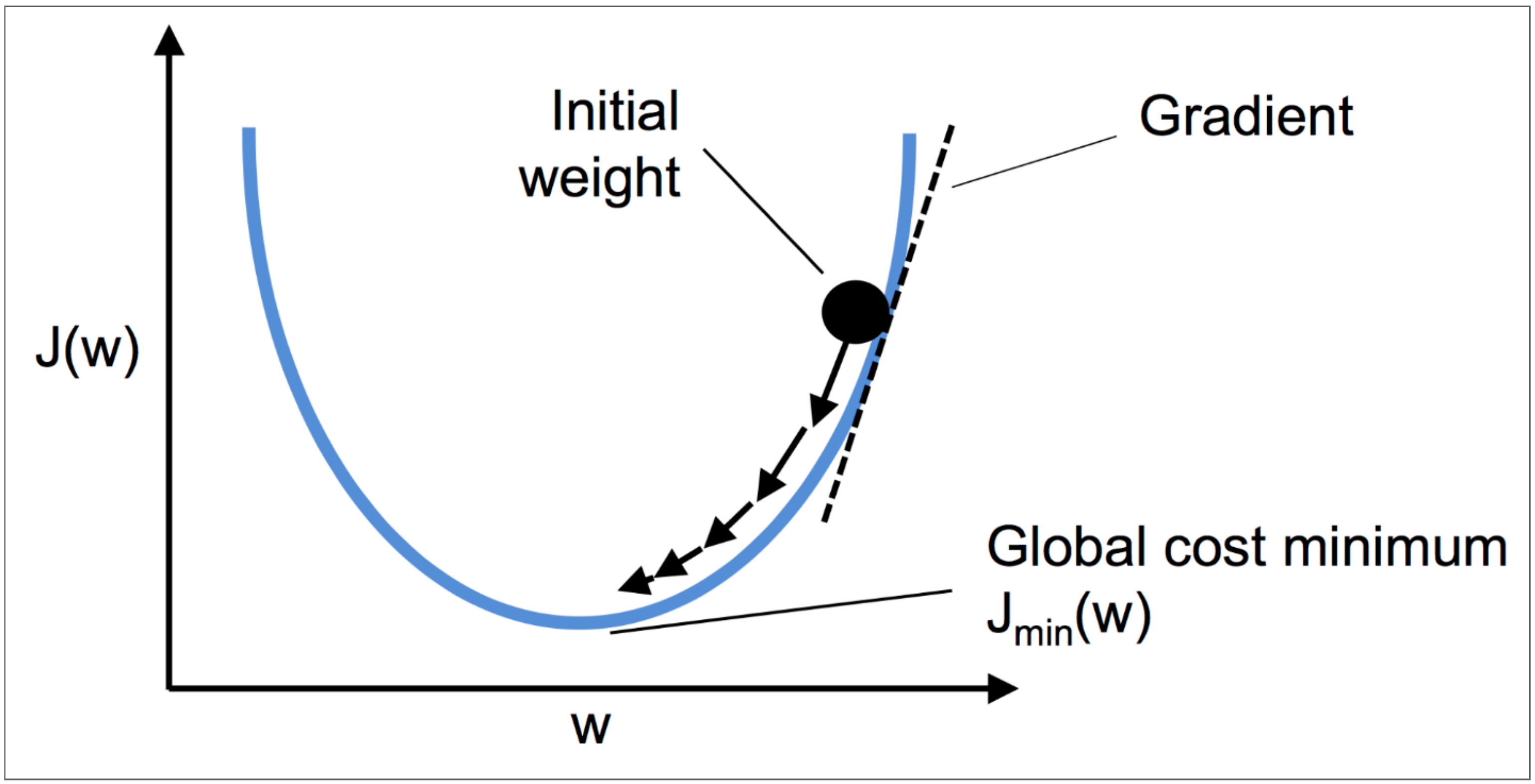
# Aside: Gradient Descent

- Want to maximize or minimize something (Ex: squared error)
- **Gradient** : direction, vector of partial derivatives
  - can get complicated, often estimated

- **Gradient Descent** : take steps wrt the direction of the gradient
  - **maximize** : in the direction of the gradient
  - **minimize** : in the opposite direction of the gradient

- **Global Maximum/Minimum** : the single best solution
- **Local Maximum/Minimum** : the best solution in the neighborhood

# Aside: Gradient Descent Cont.



# Simple Regression Using scikit-learn

In [7]:

```
# import the model from sklearn
from sklearn.linear_model import LinearRegression
```

In [8]:

```
 # instantiate the model and set hyperparameters
lr = LinearRegression(fit_intercept=True, # by default
                      normalize=False)    # by default
```

In [9]:

```
# fit the model
lr.fit(X=df_wine.proline.values.reshape(-1, 1), y=df_wine.alcohol);
```

In [10]:

```
# display learned coefficients (trailing underscore indicates learned values)
print(lr.coef_)
print(lr.intercept_)
```

```
[0.0016595]
11.761148483143145
```

In [11]:

```
# predict given new values for proline
X = np.array([1000,2000]).reshape(-1,1)
lr.predict(X)
```

Out[11]:

```
array([13.42064866, 15.08014884])
```

# Why .reshape(-1,1)?

## scikit-learn models expect the input features to be 2 dimensional

In [12]:

```
df_wine.proline.values[:5]
```

Out[12]:

```
array([1065., 1050., 1185., 1480.,  735.])
```

In [13]:

```
df_wine.proline.values.shape
```

Out[13]:

```
(178,)
```

In [14]:

```
df_wine.proline.values.reshape(-1,1).shape # -1 means "infer from the data"
```

Out[14]:

```
(178, 1)
```

## Alternatives:

In [15]:

```
df_wine.loc[:,['proline']].shape
```

Out[15]:

```
(178, 1)
```

In [16]:

```
df_wine[['proline']].shape
```

Out[16]:

```
(178, 1)
```

# Interpreting Coefficients

In [17]:

```
print(f'w_1 = {lr.coef_[0]:0.3f}, w_0 = {lr.intercept_:0.3f}')
```

```
w_1 = 0.002, w_0 = 11.761
```

In [18]:

```
print(f'alchohol = {lr.coef_[0]:0.3f}*proline + {lr.intercept_:0.3f}')
```

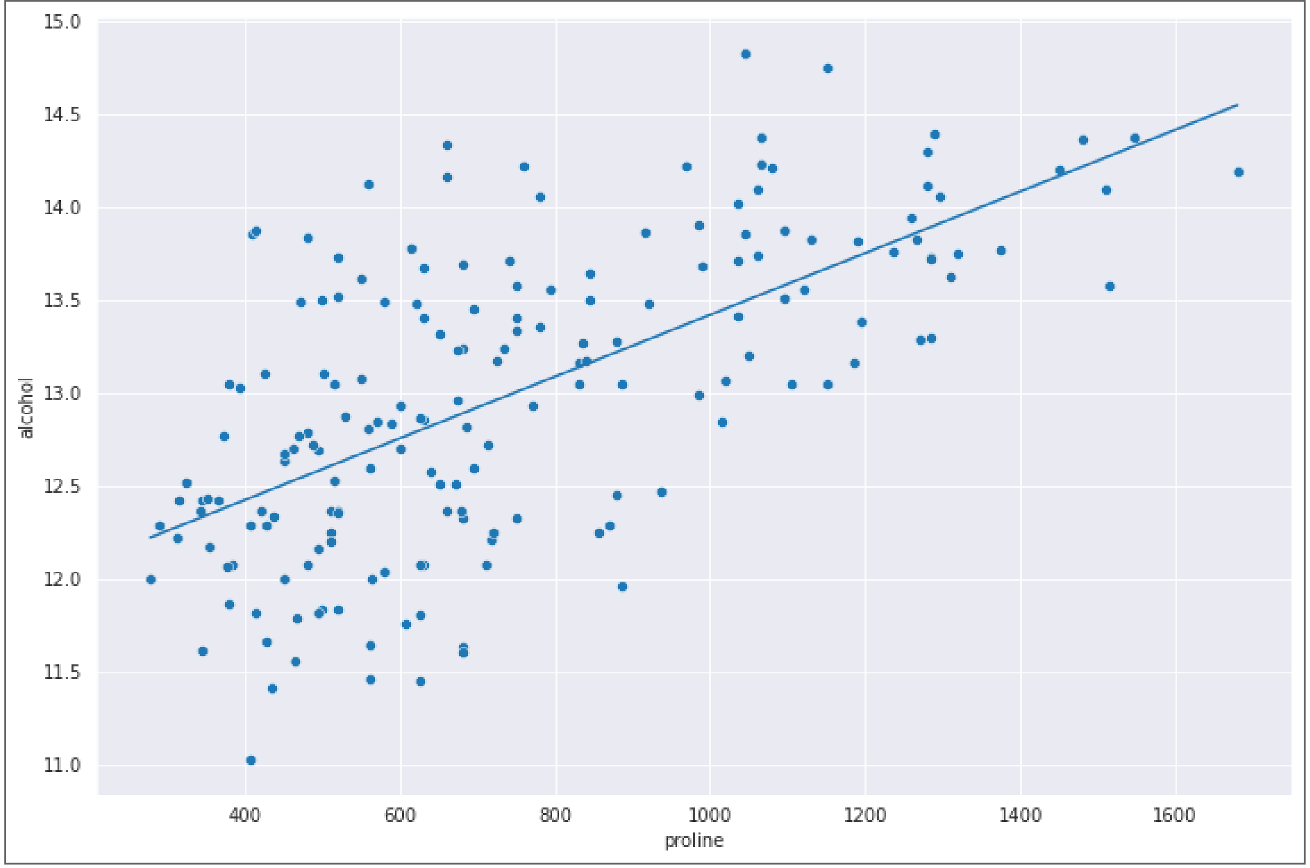
```
alchohol = 0.002*proline + 11.761
```

- When proline goes up by 1, alcohol goes up by .002
- When proline is 0, alcohol is 11.761

# Plotting The Model

In [19]:

```
x_predict = [df_wine.proline.min(),df_wine.proline.max()]
y_hat = lr.predict(np.array(x_predict).reshape(-1,1))

fig,ax = plt.subplots(1,1,figsize=(12,8))
ax = sns.scatterplot(x=df_wine.proline,y=df_wine.alcohol);
ax.plot(x_predict,y_hat);
```



15.0
14.5
14.0
13.5
13.0
12.5
12.0
11.5
11.0
alcohol
400
600
800
1000
1200
1400
1600
proline

# Multiple Linear Regression

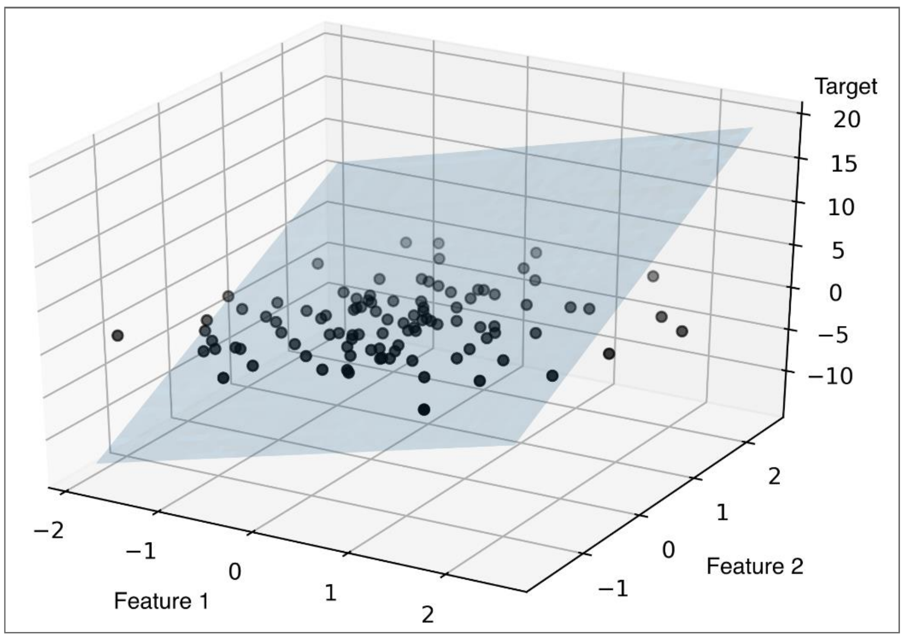
- Including multiple independent variables

$$y_i = w_0 + w_1 x_{i1} + w_2 x_{i2} + \ldots + w_m x_{im} + \varepsilon_i$$

Ex:

alcohol = w_0 + w_1*proline + w_2*hue

Objective: Find a *plane* that falls as close to our points as possible



# Multiple Linear Regression in scikit-learn

In [20]:

```
mlr = LinearRegression()
mlr.fit(df_wine[['proline','hue']],y=df_wine.alcohol);

for (name,coef) in zip(['proline','hue'],mlr.coef_):
    print(f'{name:10s} : {coef: 0.3f}')
print(f'{"intercept":10s} : {mlr.intercept_:0.3f}')
```

```
proline    :  0.002
hue        : -0.842
intercept  : 12.459
```

- If we hold everything else constant, what effect does each variable have?
  - If hue is held constant, a rise of 1 proline -> rise of .002 in alcohol
  - If proline is held constant, a rise of 1 hue -> decrease of .842 in alcohol
- Can add interaction terms to allow both to move
  - Ex: hue * proline

- more complicated to interpret

# Multiple Linear Regression in statsmodels

In [21]:

```
import statsmodels.api as sm

X = df_wine[['proline','hue']].copy()
X['const'] = 1 # or use sm.add_constant(X)
y = df_wine.alcohol
sm_mlr = sm.OLS(y,X).fit() # Note: X,y passed as parameters to object, not fit
sm_mlr.summary()
```

Out[21]:

OLS Regression Results

| | | | |
|---|---|---|---|
| **Dep. Variable:** | alcohol | **R-squared:** | 0.467 |
| **Model:** | OLS | **Adj. R-squared:** | 0.461 |
| **Method:** | Least Squares | **F-statistic:** | 76.79 |
| **Date:** | Mon, 11 Oct 2021 | **Prob (F-statistic):** | 1.15e-24 |
| **Time:** | 18:56:48 | **Log-Likelihood:** | -158.89 |
| **No. Observations:** | 178 | **AIC:** | 323.8 |

| | | | |
|---|---|---|---|
| **Df Residuals:** | 175 | **BIC:** | 333.3 |
| **Df Model:** | 2 | | |
| **Covariance Type:** | nonrobust | | |

| | coef | std err | t | P>\|t\| | [0.025 | 0.975] |
|---|---|---|---|---|---|---|
| **proline** | 0.0018 | 0.000 | 12.325 | 0.000 | 0.002 | 0.002 |
| **hue** | -0.8418 | 0.202 | -4.175 | 0.000 | -1.240 | -0.444 |
| **const** | 12.4593 | 0.203 | 61.347 | 0.000 | 12.058 | 12.860 |

| | | | |
|---|---|---|---|
| **Omnibus:** | 0.751 | **Durbin-Watson:** | 1.734 |
| **Prob(Omnibus):** | 0.687 | **Jarque-Bera (JB):** | 0.606 |
| **Skew:** | 0.142 | **Prob(JB):** | 0.739 |
| **Kurtosis:** | 3.028 | **Cond. No.** | 4.96e+03 |

Notes:
[1] Standard Errors assume that the covariance matrix of the errors is correctly specified.
[2] The condition number is large, 4.96e+03. This might indicate that there are strong multicollinearity or other numerical problems.

## Dealing With the Intercept/Bias

- Two ways of keeping track of the bias term

1. Keep it as a separate parameter:
    - $y = w_0 + w_1x_1 + w_2x_2 + \ldots + w_mx_m$
    - $y = w_0 + \sum_{i=1}^{m} w_ix_i$

1. Append a constant of $x_0 = 1$ so $x$ and $w$ are the same length
    - $y = w_0x_0 + w_1x_1 + w_2x_2 + \ldots + w_mx_m$
    - $y = \sum_{i=0}^{m} w_ix_i$

## Standardizing/Normalizing Features for Interpretation

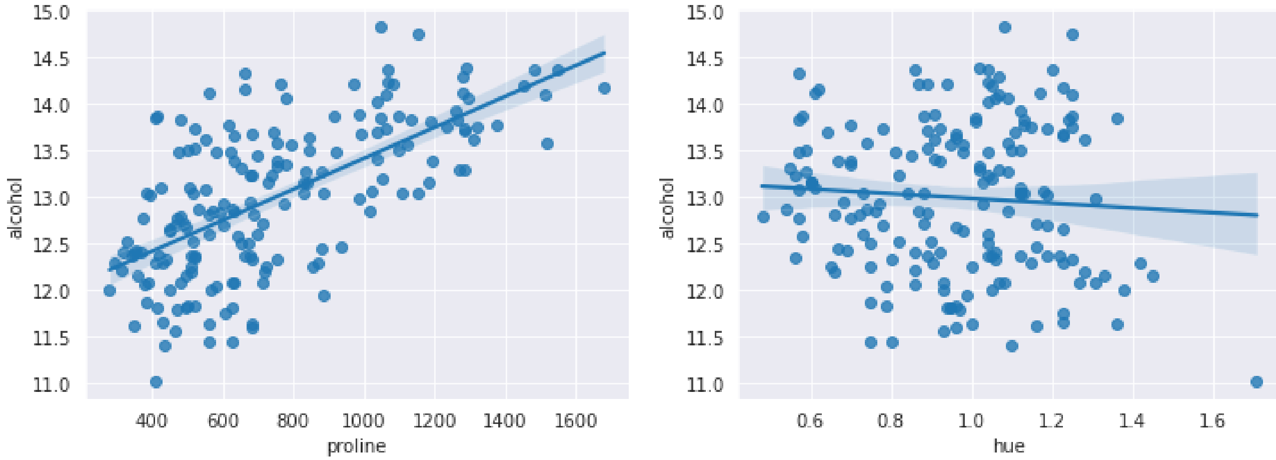
In [22]:

```
for (name,coef) in zip(['proline','hue'],mlr.coef_):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    :  0.002
hue        : -0.842
```

In [23]:

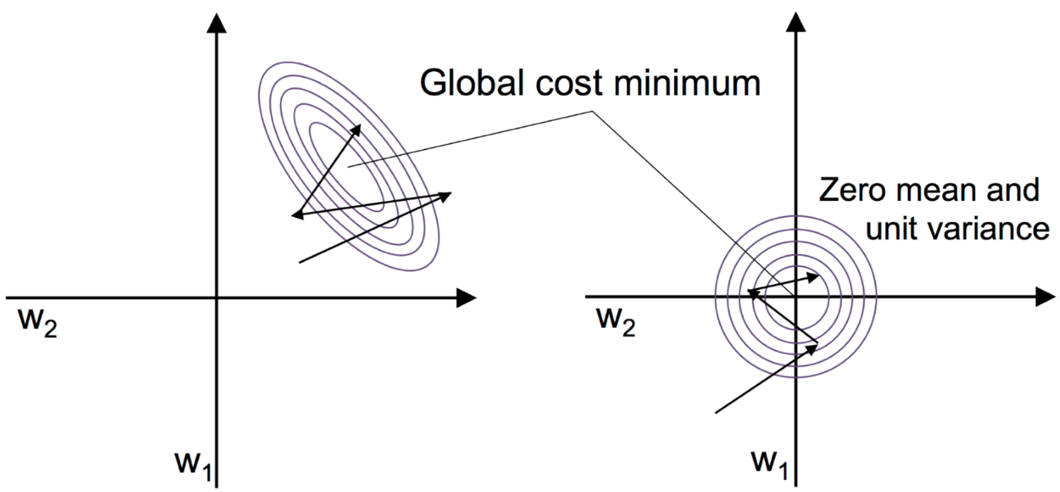
```
fig,ax = plt.subplots(1,2,figsize=(12,4))
sns.regplot(x='proline',y='alcohol',data=df_wine,ax=ax[0])
sns.regplot(x='hue',y='alcohol',data=df_wine,ax=ax[1]);
```




What would the coefficents look like if the features were on the same scale?

# Standardizing/Normalizing Features for Gradient Descent

$$z = \frac{x - \bar{x}}{s}$$



# Multiple Linear Regression with Standardization/Normalization

- `DataFrame.apply()`: apply a function across rows (axis=0) or columns (axis=1)

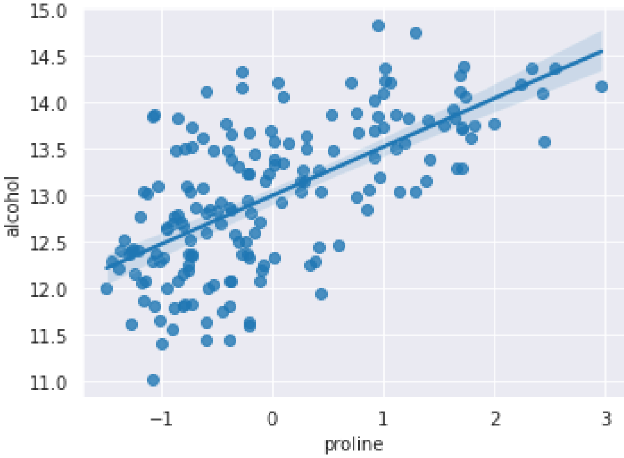
In [24]:

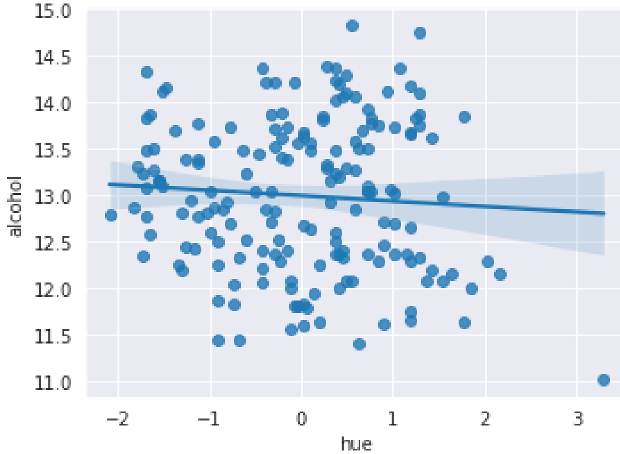
```
X_zscore = df_wine[['proline','hue']].apply(lambda x: (x-x.mean())/x.std(), axis=0) # or use StandardScaler

mlr_n = LinearRegression()
mlr_n.fit(X_zscore, df_wine.alcohol)
for (name,coef) in zip(X_zscore.columns,mlr_n.coef_):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    :  0.568
hue        : -0.192
```

In [25]:

```
fig,ax = plt.subplots(1,2,figsize=(12,4))
sns.regplot(x=X_zscore.proline,y=df_wine.alcohol,ax=ax[0]);
sns.regplot(x=X_zscore.hue,y=df_wine.alcohol,ax=ax[1]);
```




# Aside: apply(axis=), rows vs columns

| | proline | hue |
|---|---|---|
| 0 | 1065.0 | 1.04 |
| 1 | 1050.0 | 1.05 |
| 2 | 1185.0 | 1.03 |
| 3 | 1480.0 | 0.86 |
| 4 | 735.0 | 1.04 |

axis=0
or
axis='rows'

| | proline | hue |
|---|---|---|
| 0 | 1065.0 | 1.04 |
| 1 | 1050.0 | 1.05 |
| 2 | 1185.0 | 1.03 |
| 3 | 1480.0 | 0.86 |
| 4 | 735.0 | 1.04 |

axis=1
or
axis='columns'

## Colinarity

- MLR assumes features are linearly independent
  - eg: Can't rewrite one column as a weighted sum of the others
  - Ex: at a restaurant number, of entrees ordered will likely be linearly related to table size
- Issue: Model won't know how to estimate $w$
  - If we add to one $w_i$ and subtract from another, there will be no change in error
- Try to remove obvious colinearity
  - can use correlation and linear regression to detect
  - Important to consider when constructing categorical features (feature engineering)

In [26]:

```python
df_wine.corr()
```

Out[26]:

| | alcohol | ash | hue | proline | class |
|---|---|---|---|---|---|
| alcohol | 1.000000 | 0.211545 | -0.071747 | 0.643720 | -0.328222 |
| ash | 0.211545 | 1.000000 | -0.074667 | 0.223626 | -0.049643 |
| hue | -0.071747 | -0.074667 | 1.000000 | 0.236183 | -0.617369 |
| proline | 0.643720 | 0.223626 | 0.236183 | 1.000000 | -0.633717 |
| class | -0.328222 | -0.049643 | -0.617369 | -0.633717 | 1.000000 |

# Aside: Interpretation vs. Prediction

- Interpretation: Explain how observed features relate to observed target
- Prediction: Given new features, can we generate a prediction
- Often asked to do one or the other, be clear which is most important
- In prediction, may not worry about interpreting the model!
- There is increased attention on interpretability

## Questions re Regression with Linear Models?

# Classification

- **Regression** -> predict a numeric value
- **Classification** -> predict a discrete class, category
- **Binary classification** : two categories
  - pos/neg, cat/dog, win/lose
- **Multiclass classification** : more than two categories/classes
  - red/green/blue, flower type, integer 0-10
- **Multilabel classification** : can assign more than one label to an instance
  - paper topics, entities in image

## Wine as Binary Classification

In [27]:

```
df_wine['class'].value_counts() # originally multiclass
```

Out[27]:

```
1    71
0    59
2    48
Name: class, dtype: int64
```

In [28]:

```
# only keep classes 0 and 1
df_wine_2class = df_wine[df_wine['class'] < 2]

# rename 'class' as 'target', since class is a reserved python word
df_wine_2class = df_wine_2class.rename({'class':'target'},axis=1)

df_wine_2class.target.value_counts()
```

Out[28]:

```
1    71
0    59
Name: target, dtype: int64
```

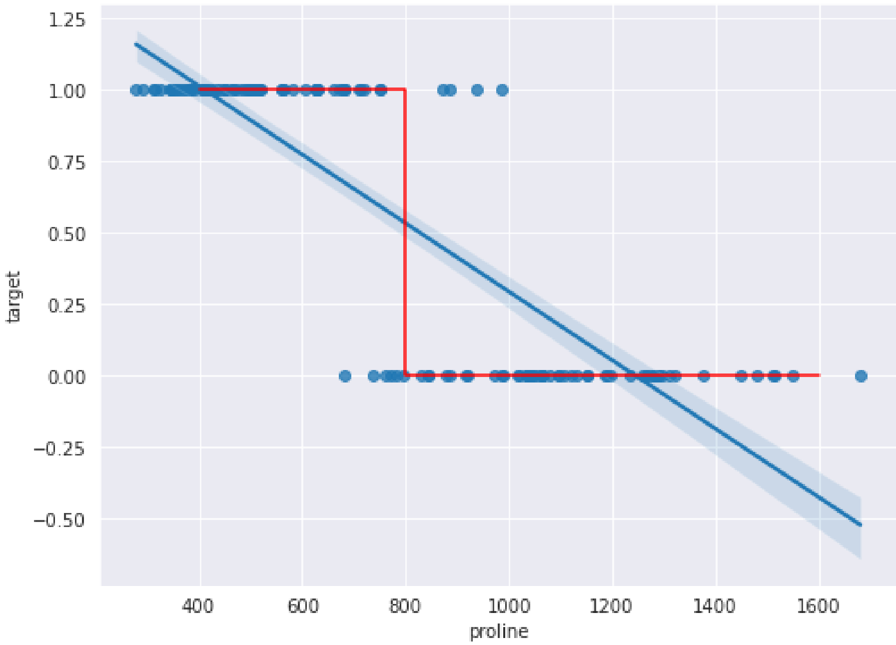
# Classifying Wine with a Linear Model

- Can't use our linear regression model directly

In [29]:

```
fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.regplot(x=df_wine_2class.proline,y=df_wine_2class.target);
```

```
ax.plot([400,800,800,1600],[1,1,0,0],c='r');
```




- Want something with that looks like a threshold
- Would like a prediction between 0 and 1

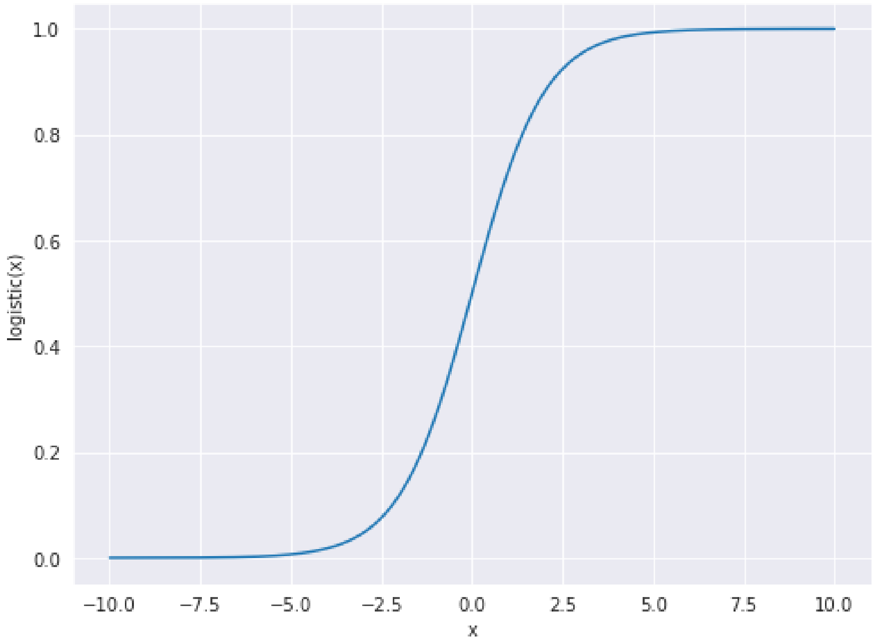
# Logistic Regression

$$logistic(x) = \frac{1}{1+e^{(-x)}}$$

In [30]:

```
def logistic(x,w1=1,w0=0):
    return 1 / (1+np.exp(-(w0+w1*x)))

x = np.linspace(-10,10,1000) # generate 1000 numbers evenly spaced between -10 and 10
fig,ax = plt.subplots(1,1,figsize=(8,6))
```

```
ax.plot(x,logistic(x));
ax.set_xlabel('x');ax.set_ylabel('logistic(x)');
```




# Logistic Regression with sklearn

- Our problem becomes: $P(y_i = 1|x_i) = logistic(w_0 + w_1 x_i) + \varepsilon_i$

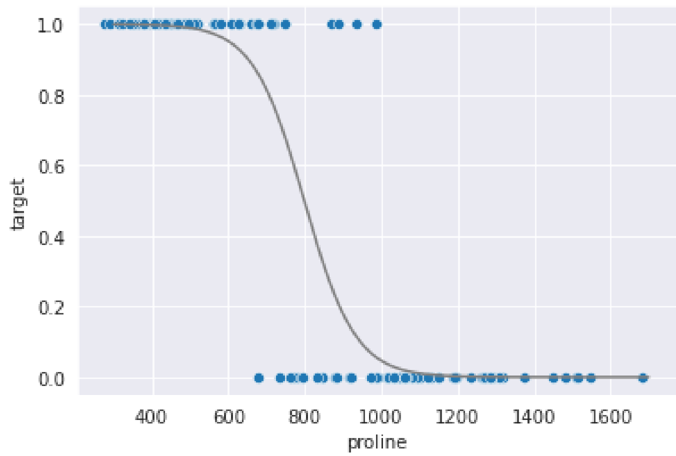
In [31]:

```
from sklearn.linear_model import LogisticRegression

X = df_wine_2class.proline.values.reshape(-1,1)
y = df_wine_2class.target

logr = LogisticRegression(fit_intercept=True).fit(X,y)
print(f'w_0 = {logr.intercept_[0]:0.2f}')
print(f'w_1 = {logr.coef_[0][0]:0.2f}')
```

```
w_0 = 11.97
w_1 = -0.01
```

In [32]:

```
fig,ax = plt.subplots(1,1,figsize=(6,4))
x = np.linspace(300,1700,1000)
logistic_x = logistic(x,logr.coef_[0],logr.intercept_)
ax.plot(x,logistic_x,c='gray');
sns.scatterplot(x=df_wine_2class.proline,y=df_wine_2class.target, ax=ax);
```



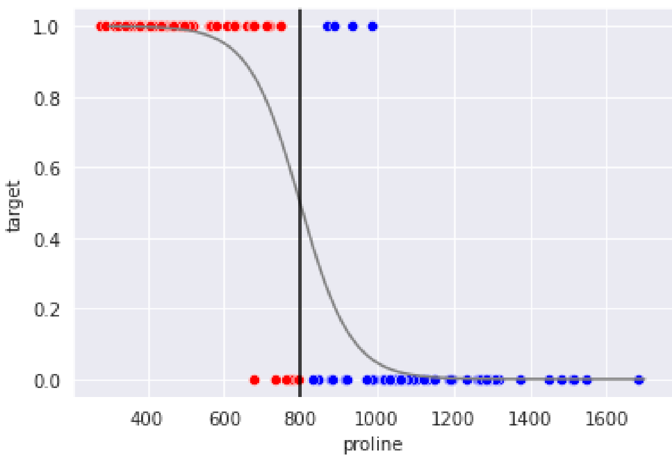

# Adding the Threshold

- Can treat the output of the logistic function as $P(y=1|x)$
- Threshold at .5 (50%) to get class prediction

In [33]:

```
threshold = x[np.argmin(np.abs(logistic_x - .5))]

predicted_0 = df_wine_2class[df_wine_2class.proline <= threshold]
predicted_1 = df_wine_2class[df_wine_2class.proline > threshold]
```

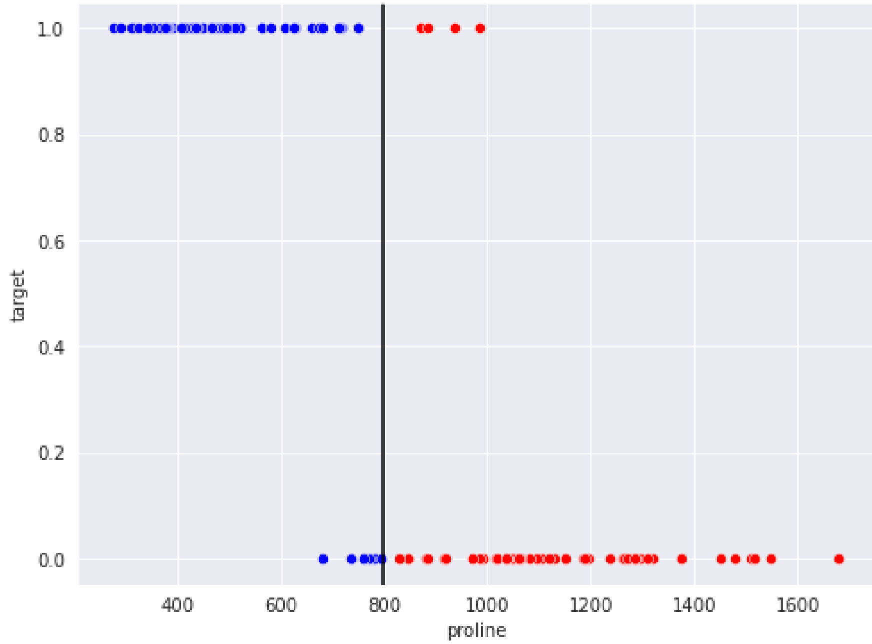
```
fig,ax = plt.subplots(1,1,figsize=(6,4))
sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
ax.plot(x,logistic_x,c='gray');
ax.axvline(threshold,c='k');
```




# Getting Predictions from sklearn

In [34]:

```
yhat = logr.predict(X)

predicted_0 = df_wine_2class[yhat==0]
predicted_1 = df_wine_2class[yhat==1]

fig,ax = plt.subplots(1,1,figsize=(8,6))
sns.scatterplot(x='proline',y='target', data=predicted_0, color='r',ax=ax);
sns.scatterplot(x='proline',y='target', data=predicted_1, color='b',ax=ax);
ax.axvline(threshold,c='k');
```




Note we have some errors!

# Getting Probabilities from sklearn

- said we could use output of logistic as $P(y = 1|x)$

In [35]:

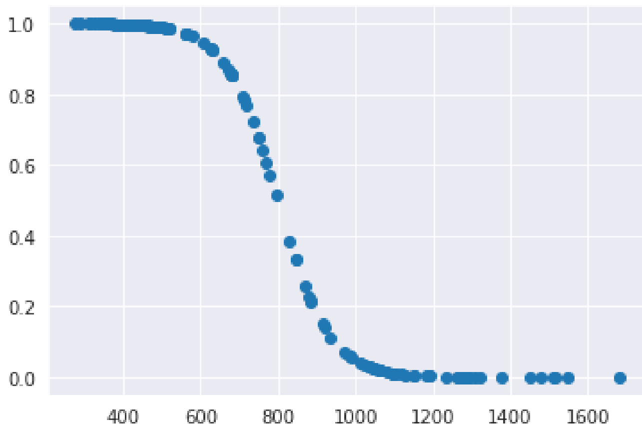
```
p_y = logr.predict_proba(X)
p_y[:5] # p(y=0|x), p(y=1|x)
```

Out[35]:

```
array([[9.81833759e-01, 1.81662409e-02],
       [9.77356984e-01, 2.26430157e-02],
       [9.96947414e-01, 3.05258552e-03],
       [9.99963234e-01, 3.67664871e-05],
       [2.77482032e-01, 7.22517968e-01]])
```

In [36]:

```
plt.scatter(df_wine_2class.proline,p_y[:,1]);
```




# Interpreting Logistic Regression Coefficients

- After some math

$$\log\left(\frac{y_i}{1-y_i}\right) = w_0 + w_1 x_{i1}$$

- this is the **log odds ratio** of p(y=1)/p(y=0)
- odds range from 0 to positive infinity
- odds(5) -> 5/1 -> 5 out of 6 times -> .83
- odds(.2) -> 1/5 -> 1 out of 6 times -> .16

See **here** for a good explanation

# Logistic Regression with Multiple Features

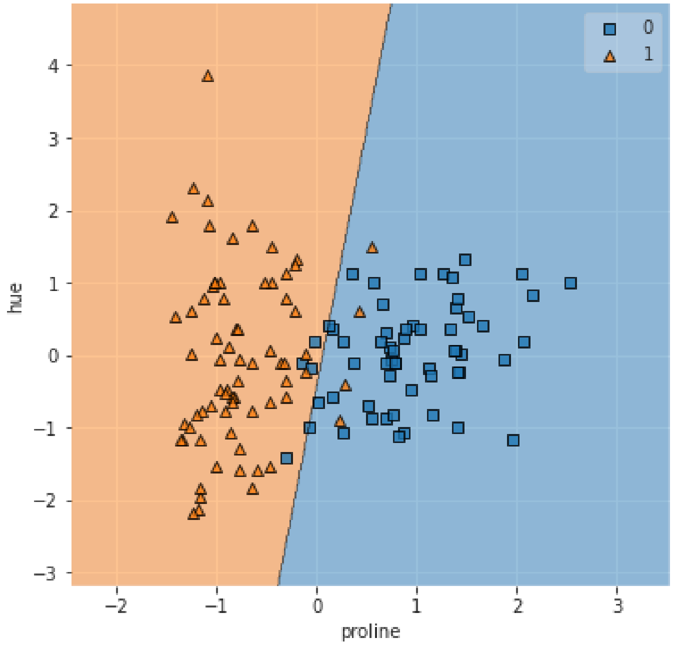
In [37]:

```
X = df_wine_2class[['proline','hue']]
X_zscore = X.apply(lambda x: (x-x.mean())/x.std())

logrm = LogisticRegression().fit(X_zscore,y)
for (name,coef) in zip(X.columns,logrm.coef_[0]):
    print(f'{name:10s} : {coef: 0.3f}')
```

```
proline    : -3.464
hue        :  0.488
```

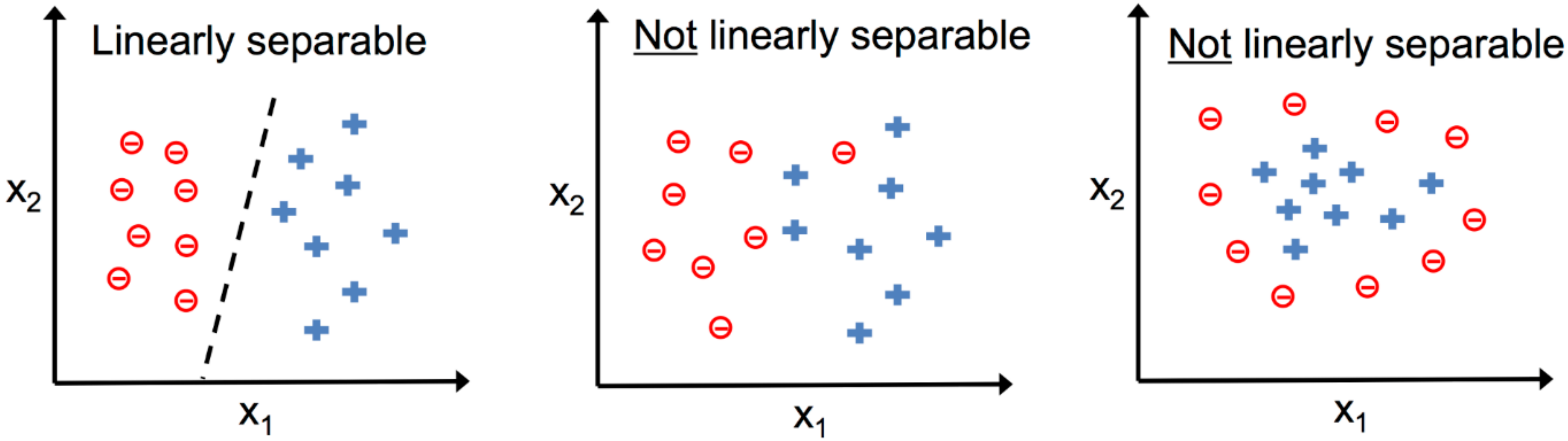
In [38]:

```
# need to have run: conda install -n eods-f20 -c conda-forge mlxtend
from mlxtend.plotting import plot_decision_regions

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=logrm, ax=ax);
ax.set_xlabel(X.columns[0]); ax.set_ylabel(X.columns[1]);
```




# Linearly Seperable Data

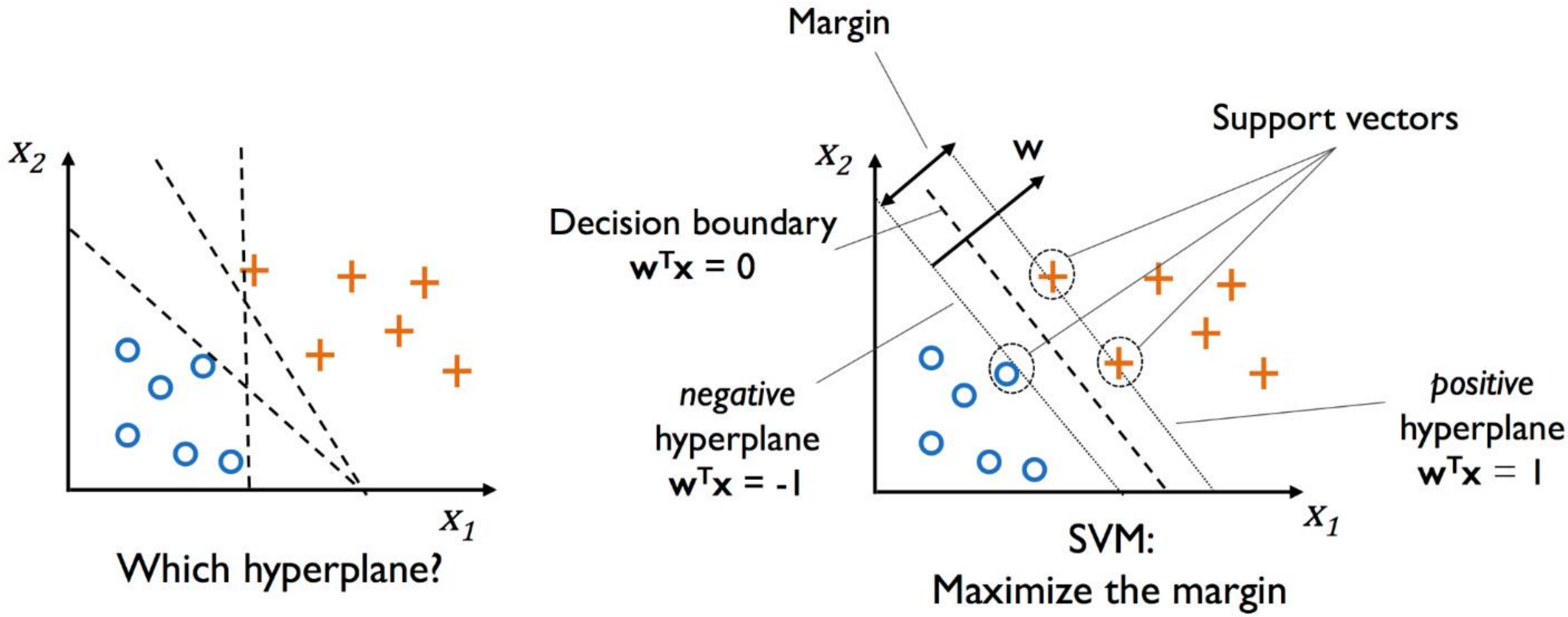
- Logistic Regression depends on data being linearly seperable




From PML

## Which boundary to choose? Support Vector Machines (SVMs)

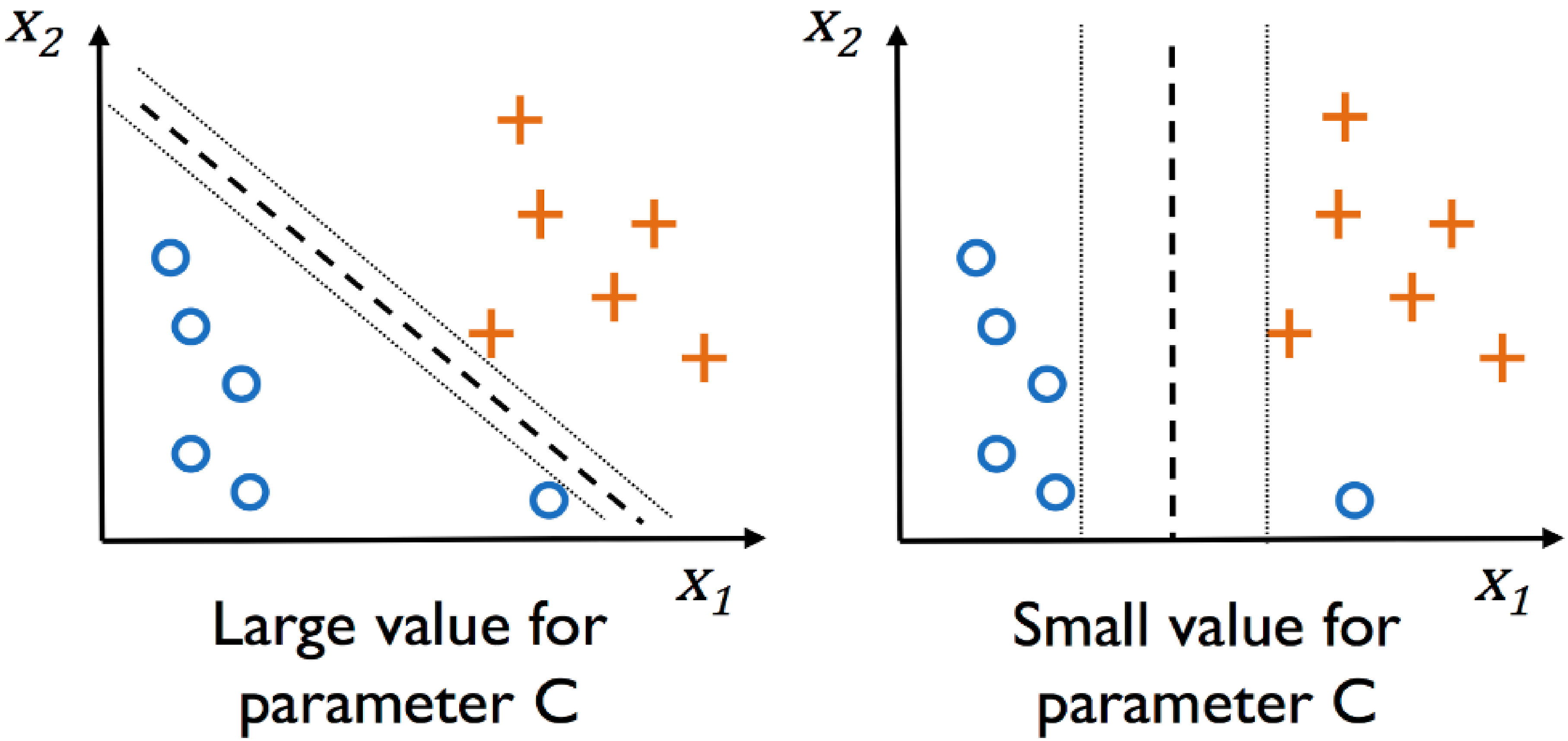
- For a linearly seperable dataset, where should we place the decision boundary?
- Support Vector Machine (SVM) tries to "maximize the margin" between classes




From PML

## SVM Hyperparameter C

- **Hyperparameter**: Something we set

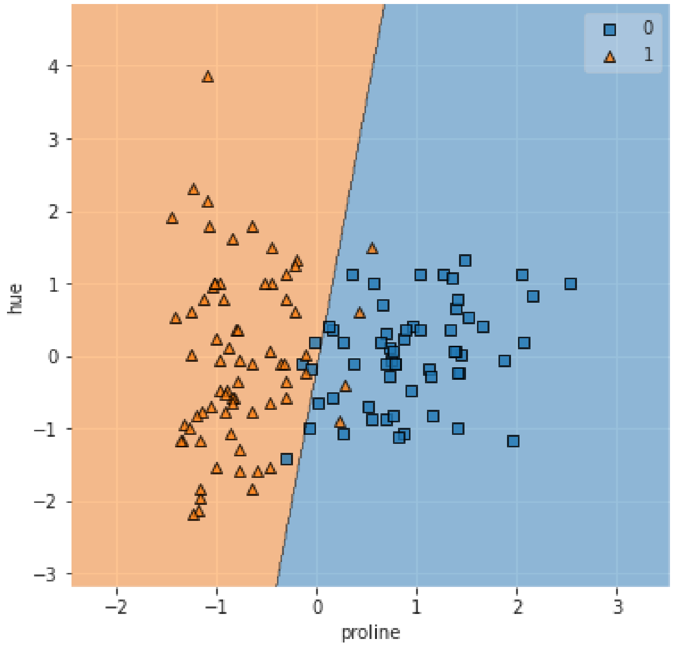



From PML

## SVM with sklearn

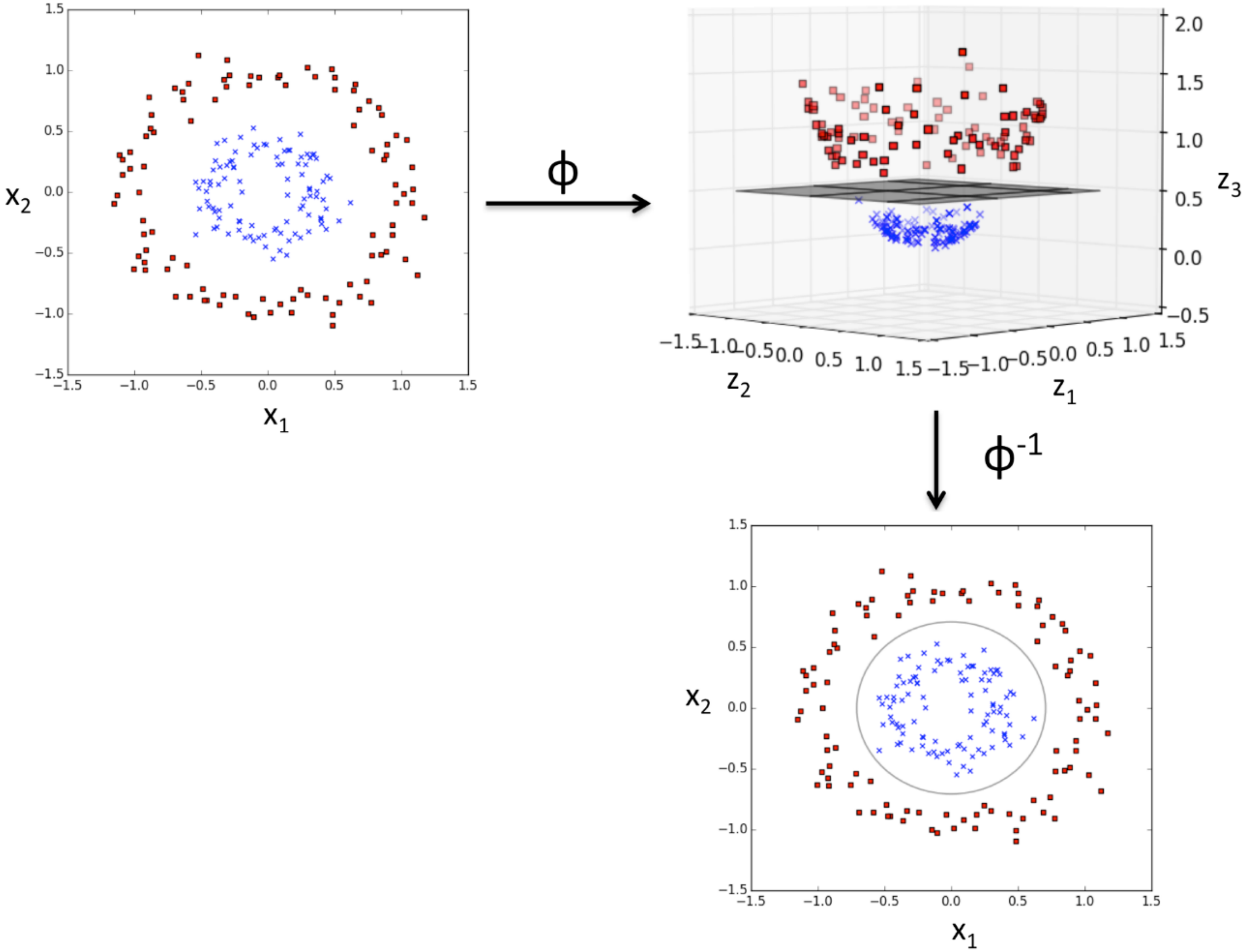
In [39]:

```
from sklearn.svm import SVC
svm_linear = SVC(kernel='linear')
svm_linear.fit(X_zscore,y);

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=svm_linear);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```




# Non-Linear Boundaries with SVMs Kernel Trick

- **Kernel Trick**: Map data to a higher dimensional space and find linear boundary there



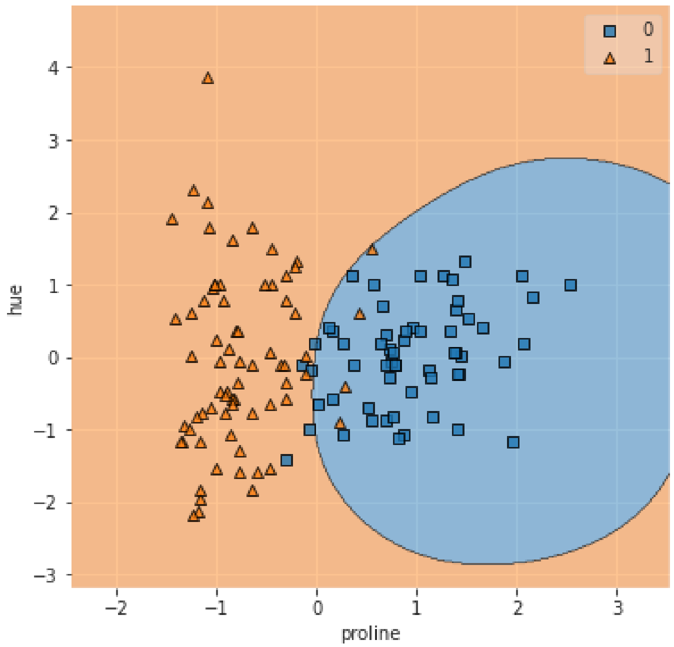

From PML

## SVM Kernel Trick with RBF Kernel

- RBF (Radial-Basis Function) kernel

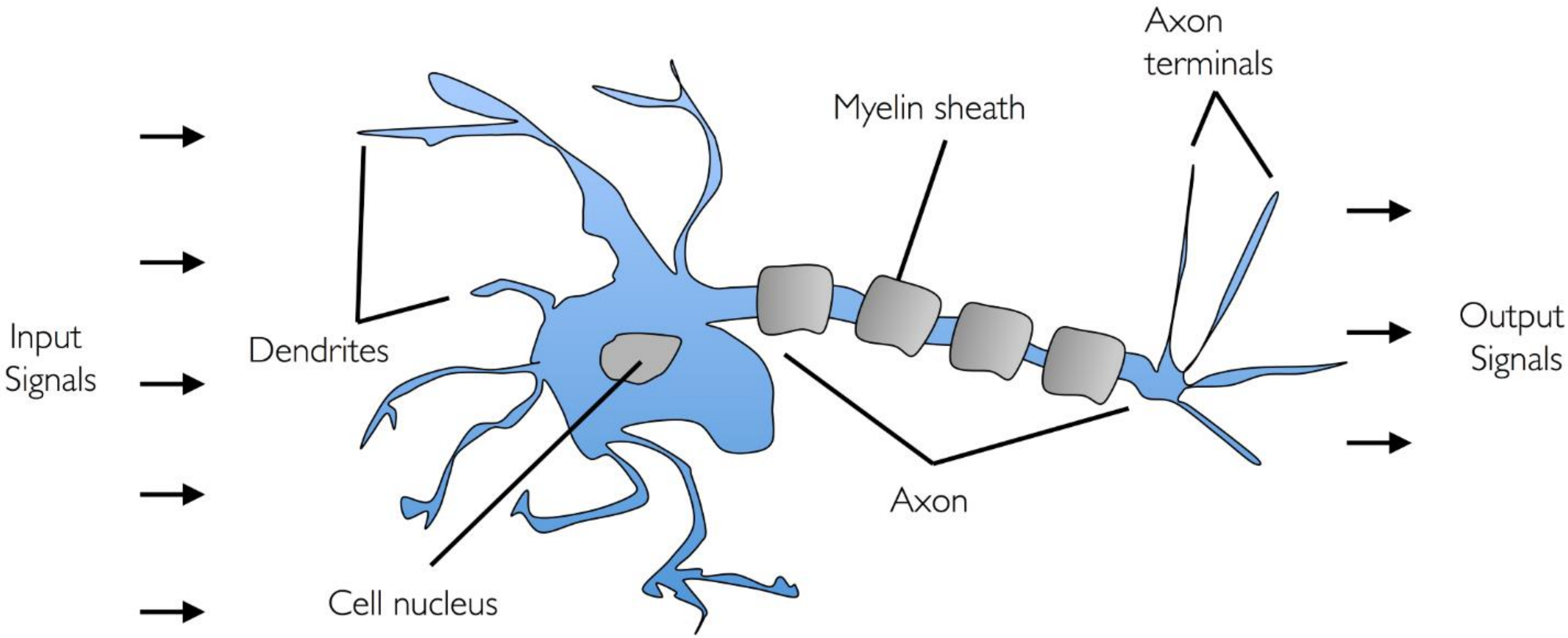
In [40]:

```
svm_rbf = SVC(kernel='rbf')
svm_rbf.fit(X_zscore,y);

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=svm_rbf);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```



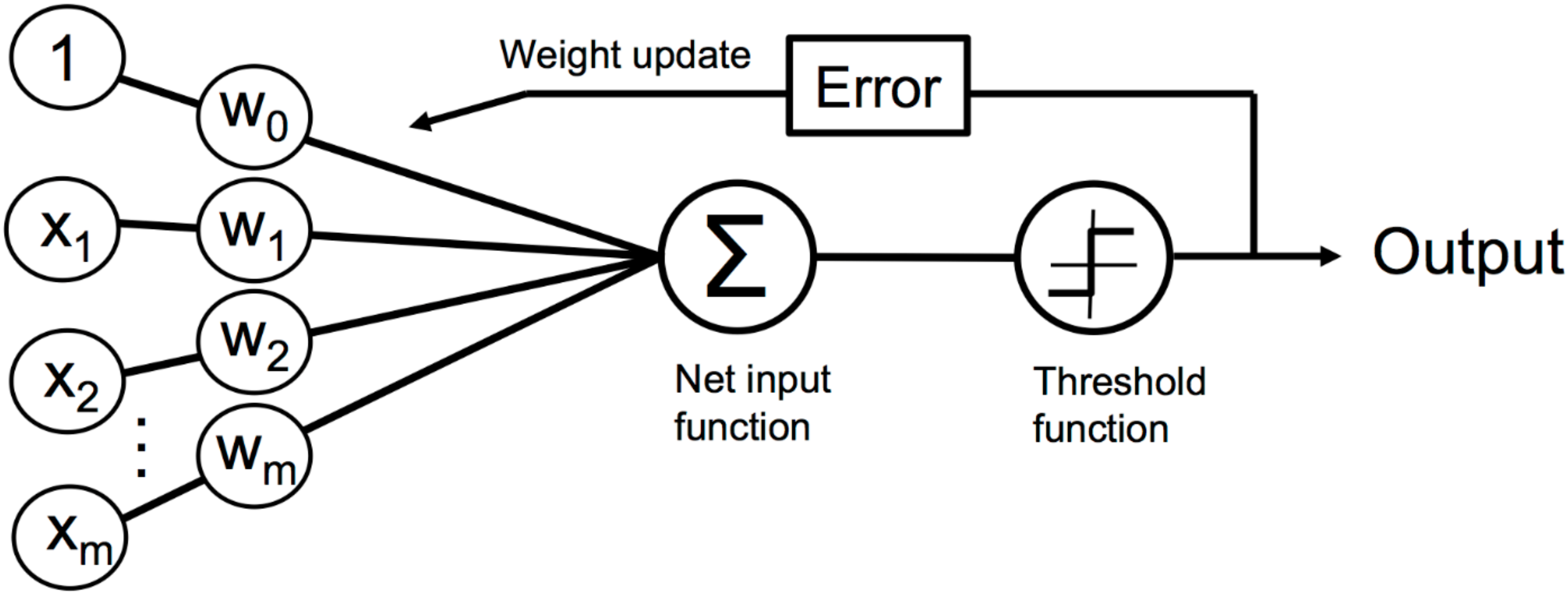

# If we have time...

# From Perceptron to Artificial Neural Network




From PML

# Perceptron: Early Neuron Model

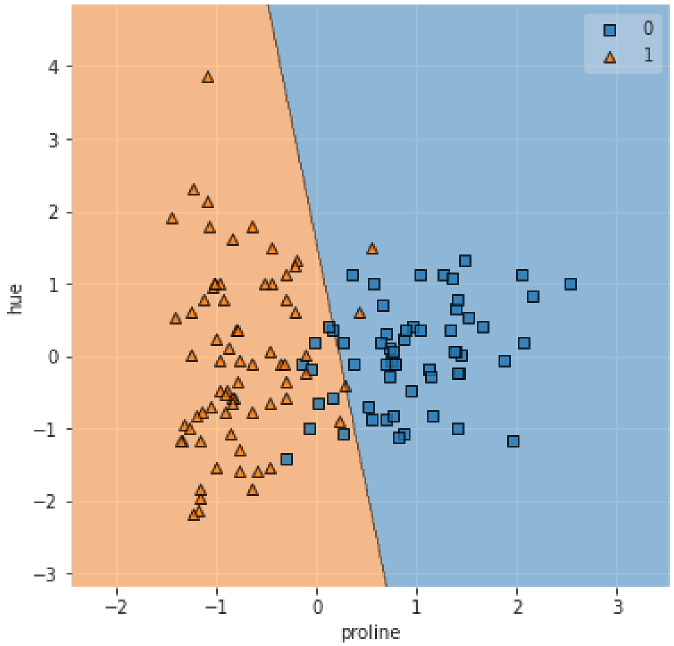



From PML

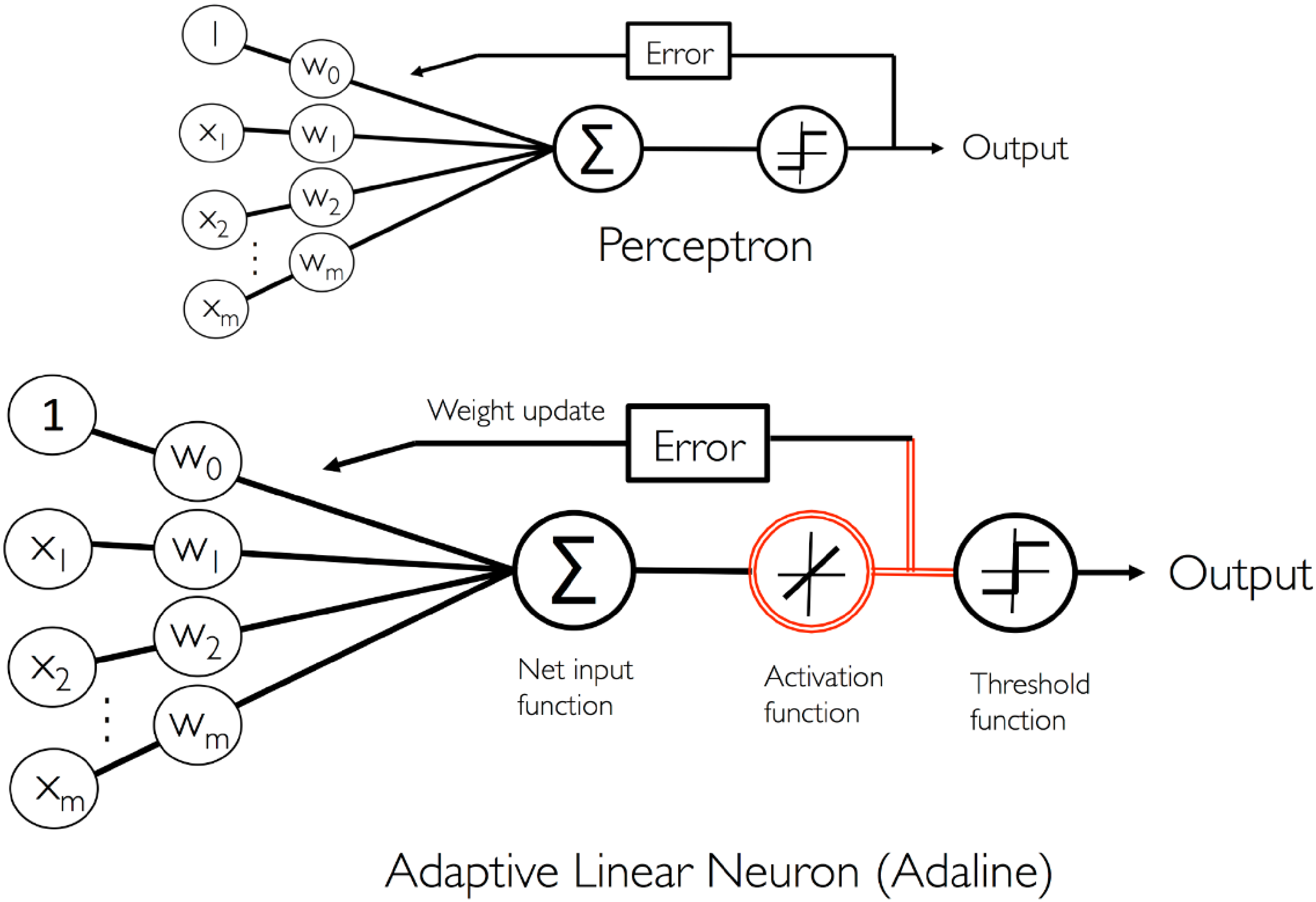
## Perceptron in sklearn

In [43]:

```
from sklearn.linear_model import Perceptron
perceptron = Perceptron()
perceptron.fit(X_zscore,y);

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=perceptron);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```




# Perceptron to Adaline

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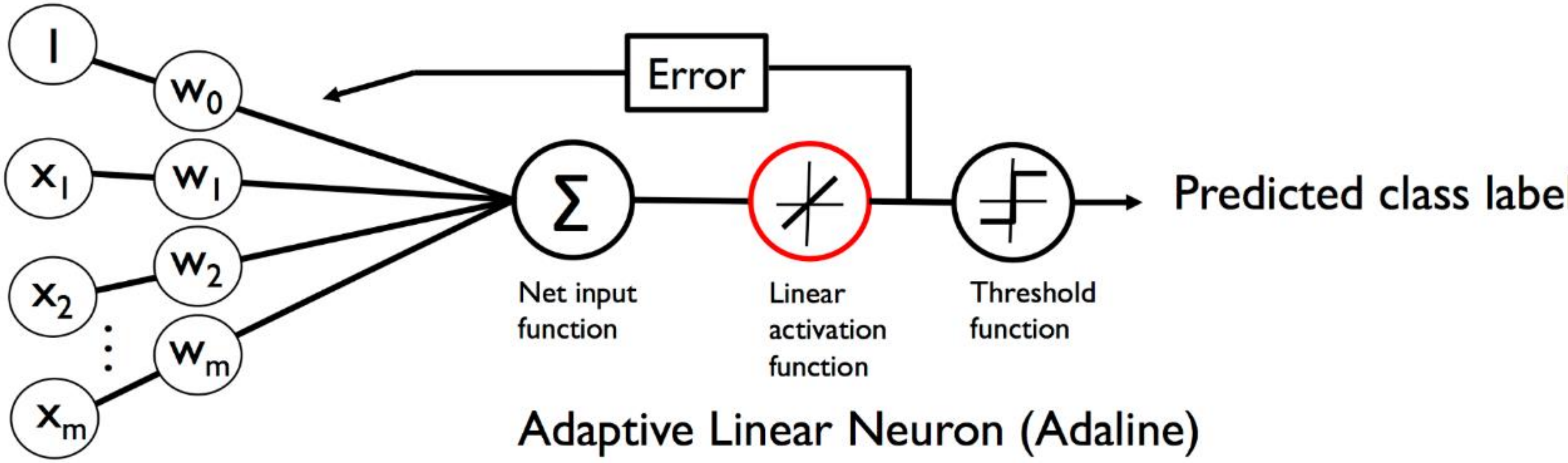
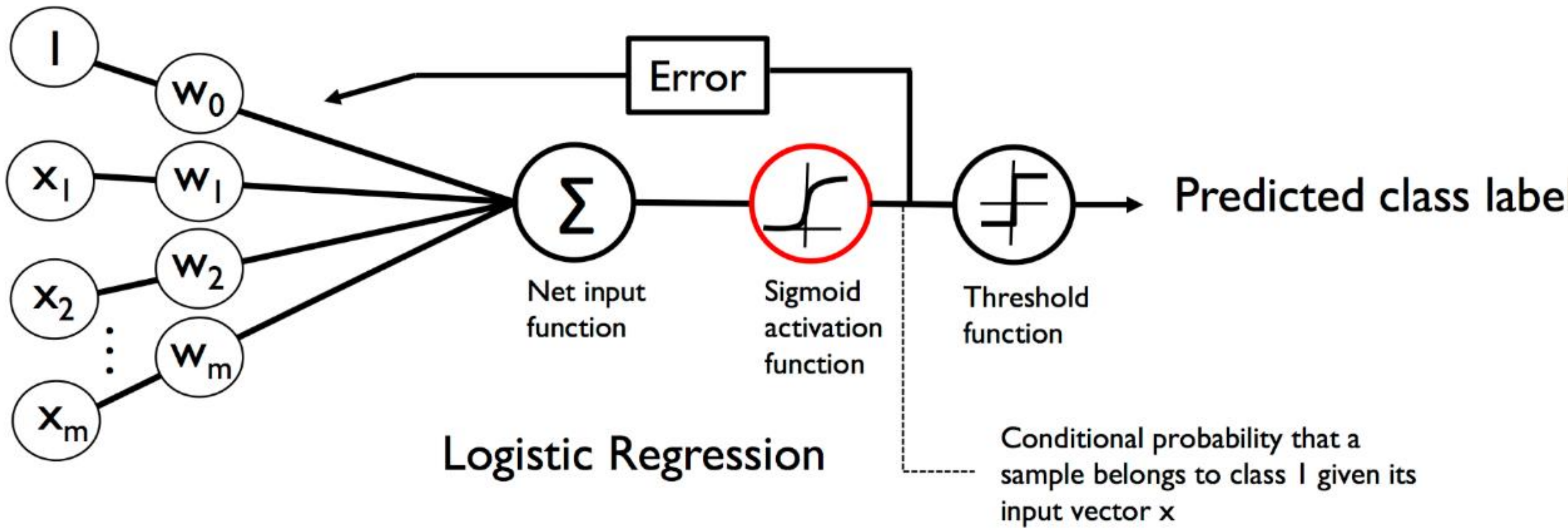
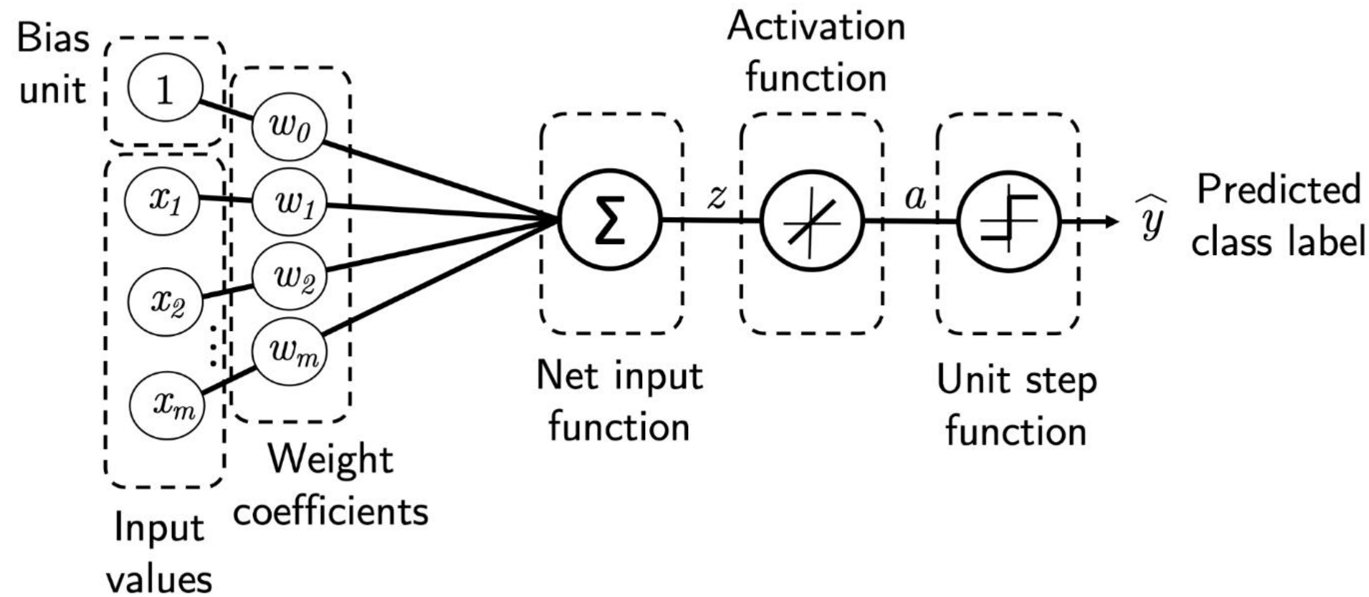
## Adaline to Logistic Regression


1
$w_0$
$x_1$
$w_1$
$x_2$
$w_2$
$x_m$
$w_m$
Error
Net input function
Linear activation function
Threshold function
Predicted class label
Adaptive Linear Neuron (Adaline)


1
$w_0$
$x_1$
$w_1$
$x_2$
$w_2$
$x_m$
$w_m$
Error
Net input function
Sigmoid activation function
Threshold function
Predicted class label
Logistic Regression
Conditional probability that a sample belongs to class 1 given its input vector x

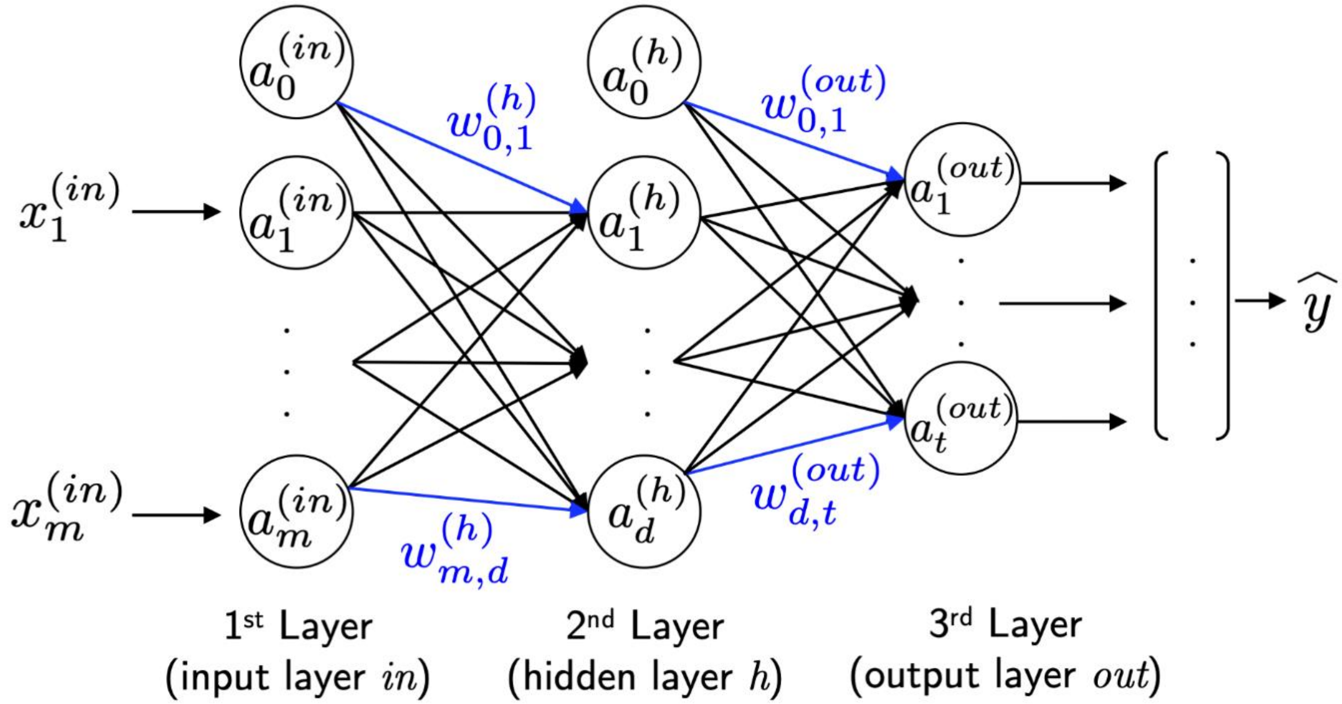
From PML

# Components of Single Layer Neural Net



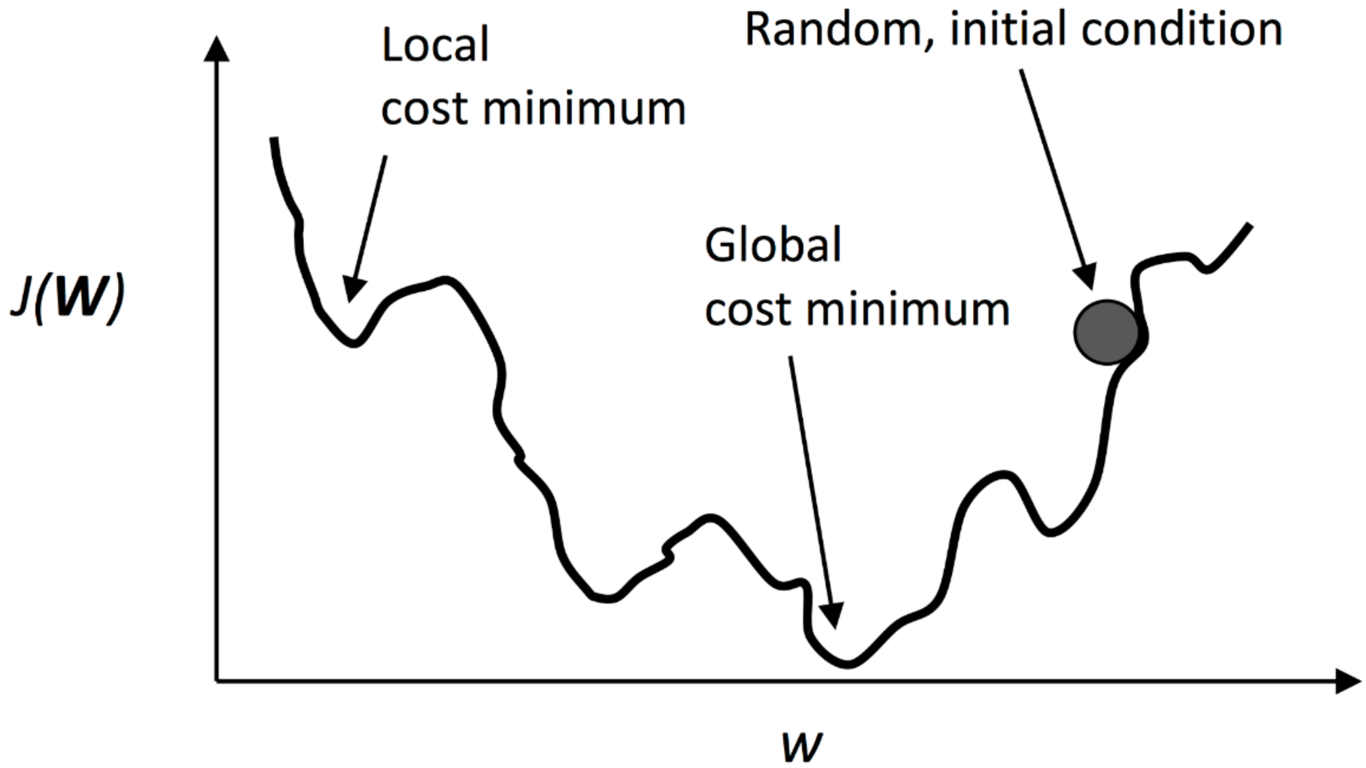

From PML

# Multi-Layer Neural Network



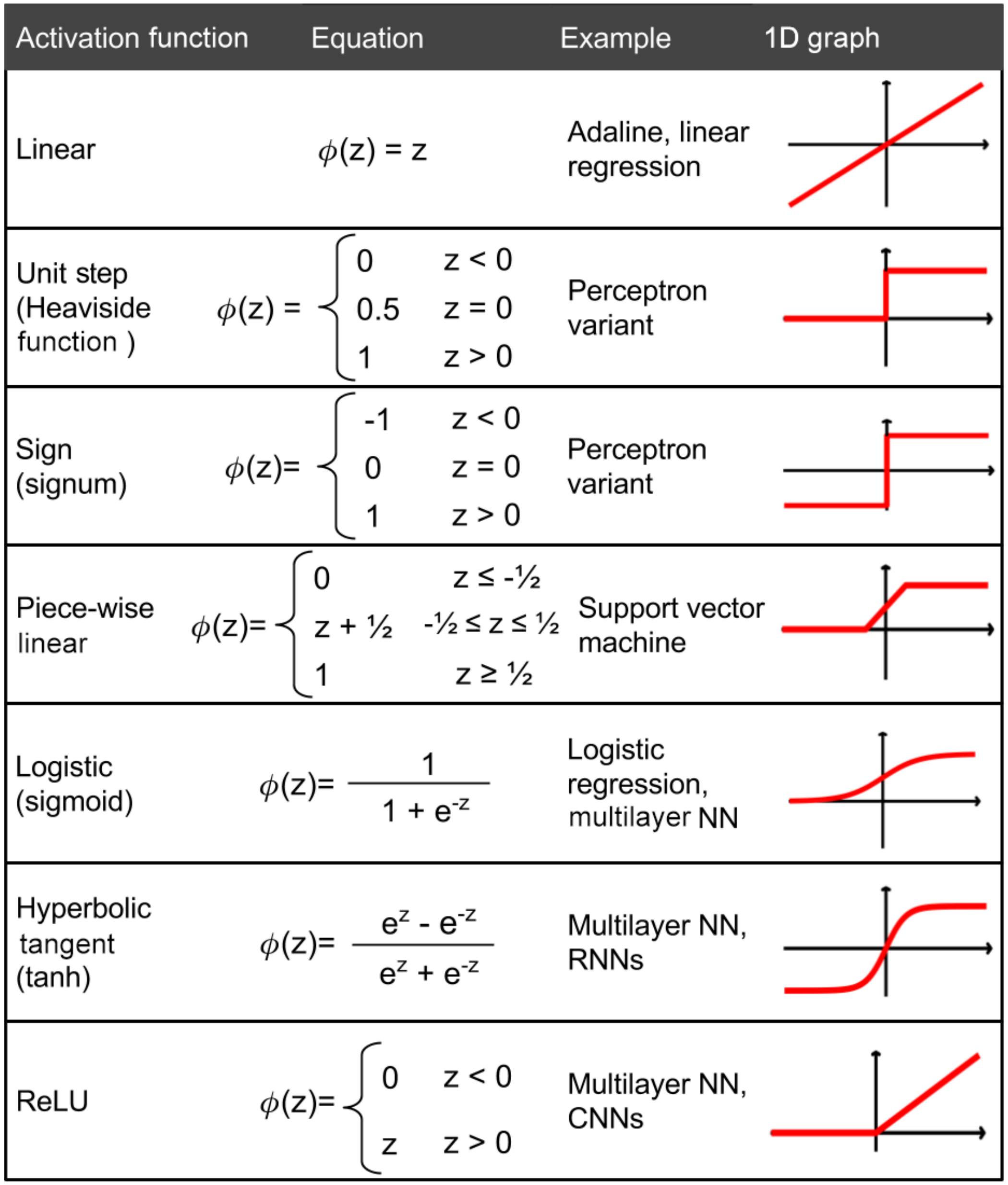

From PML

# Complex Optimization Space




From PML

## Activation Functions



| Activation function | Equation | Example | 1D graph |
|---|---|---|---|
| Linear | $\phi(z) = z$ | Adaline, linear regression | |
| Unit step (Heaviside function ) | $\phi(z) = \begin{cases} 0 & z < 0 \\ 0.5 & z = 0 \\ 1 & z > 0 \end{cases}$ | Perceptron variant | |
| Sign (signum) | $\phi(z)= \begin{cases} -1 & z < 0 \\ 0 & z = 0 \\ 1 & z > 0 \end{cases}$ | Perceptron variant | |
| Piece-wise linear | $\phi(z)= \begin{cases} 0 & z \le -\frac{1}{2} \\ z + \frac{1}{2} & -\frac{1}{2} \le z \le \frac{1}{2} \\ 1 & z \ge \frac{1}{2} \end{cases}$ | Support vector machine | |
| Logistic (sigmoid) | $\phi(z)= \dfrac{1}{1 + e^{-z}}$ | Logistic regression, multilayer NN | |
| Hyperbolic tangent (tanh) | $\phi(z)= \dfrac{e^z - e^{-z}}{e^z + e^{-z}}$ | Multilayer NN, RNNs | |
| ReLU | $\phi(z)= \begin{cases} 0 & z < 0 \\ z & z > 0 \end{cases}$ | Multilayer NN, CNNs | |

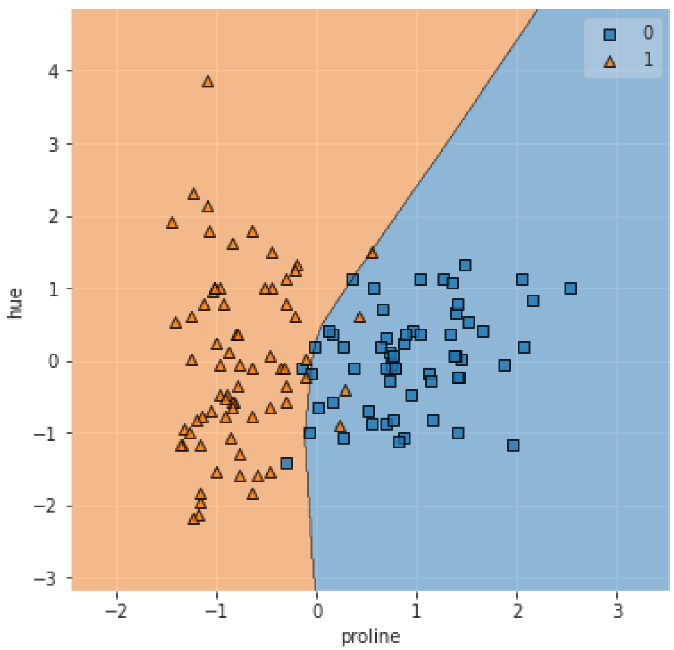
From PML

# Multi-Layer Perceptron with sklearn

In [42]:

```python
from sklearn.neural_network import MLPClassifier, MLPRegressor
mlp = MLPClassifier(hidden_layer_sizes=(100,),
                    max_iter=1000)
mlp.fit(X_zscore,y);

fig,ax = plt.subplots(1,1,figsize=(6,6))
plot_decision_regions(X_zscore.values, y.values, clf=mlp);
plt.xlabel(X.columns[0]); plt.ylabel(X.columns[1]);
```




# Questions re Classification with Linear Models?