Methods 3: Multilevel Statistical Modeling and Machine Learning

Week 7: *Linear regression revisited (machine learning)*

November 9, 2021

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Last time – Mid-way evaluation

1) Write something you liked about the course so far

2) Write something you did not like about the course so far

3) What would you change?

Summary

summary of student feedback

LIKE
Good amount of practical exercises (n=3)
Hands-on coding (n=8)
GitHub introduction (n=3)
Lau is answering questions (n=9)
That we go into depth (n=1)
Peer-review (n=1)
Good readings (n=5)
Involvement of students (n=2)
Lectures are interesting (n=2)
Good structure of classes (n=4)
Lau is engaged (n=4)
Exercises tied with papers (n=1)
Allow more time for clarification (n=1)
Easy to get help (n=3)
Pace too slow (n=1)
Explaining lecture goals (n=1)
Demystifying math (n=2)

DID NOT LIKE
Portfolio too challenging or too many questions (n=8)
GitHub is not worth it (n=1)
Math is hard - Explain math more (n=5)
Coding is hard (n=2)
Too many slides, not enough time (n=4)
Questions not clear enough in portfolio (n=9)
Connection between lecture and readings (n=5)
Bad structure of classes (n=1)
Exercises that have not been explicitly covered in class (n=5)
Not clear why we are doing the assignments (n=1)
That Lau is not in all classes (n=2)
Methods 1, 2 and 3 are not well connected (n=2)
Lau talking too fast and not loud enough (n=1)

CHANGE
Closer match between lectures and classes (n=2)
List main concepts in syllabus (n=1)
Better deadlines needed (n=5)
More explanation on portfolios (n=1)
More feedback on exercises (n=3)
Programming together (n=1)
Go through papers that exercises are based on (n=1)

Total n = 29

https://github.com/ualsbombe/github_methods_3/blob/main/week_07/mid-way_evaluation.pdf

Summary – what you liked

- Top 3
  1) Lau is answering questions (n=9)
  2) Good readings (n=5)
  3) Lau is engaged (n=4) Good structure of classes (n=4)

Total n = 29

Summary – what you did not like

- Top 3
  1) Questions not clear enough in portfolio (n=9)
  2) Portfolio too challenging or too many questions (n=8)
  3) Math is hard – explain math more (n=5)
     Connection between lecture and readings (n=5)
     Exercises not explicitly covered in class (n=5)

Total n = 29

Summary – to change

CHANGE

Closer match between lectures and classes (n=2)

List main concepts in syllabus (n=1)

Better deadlines needed (n=5)

More explanation on portfolios (n=1)

More feedback on exercises (n=3)

Programming together (n=1)

Go through papers that exercises are based on (n=1)

Summary – what I promise to change

I will be very careful and aim at writing questions that are easy to understand

Exercise for you: In tomorrow’s exercise: For each question indicate whether you understood what was required of you.

Summary – what I promise to change

Connection between lectures and class will be closer – we will be following the textbook more closely

Summary – a discussion

Lau is answering questions (n=9)

Too many slides, not enough time (n=4)

This is a classic conundrum (which we should still try to solve)

Summary – a discussion

What is the optimal balance between me going through the slides and me answering questions?

Discuss for 3-5 minutes

What should our balance be?

Learning goals

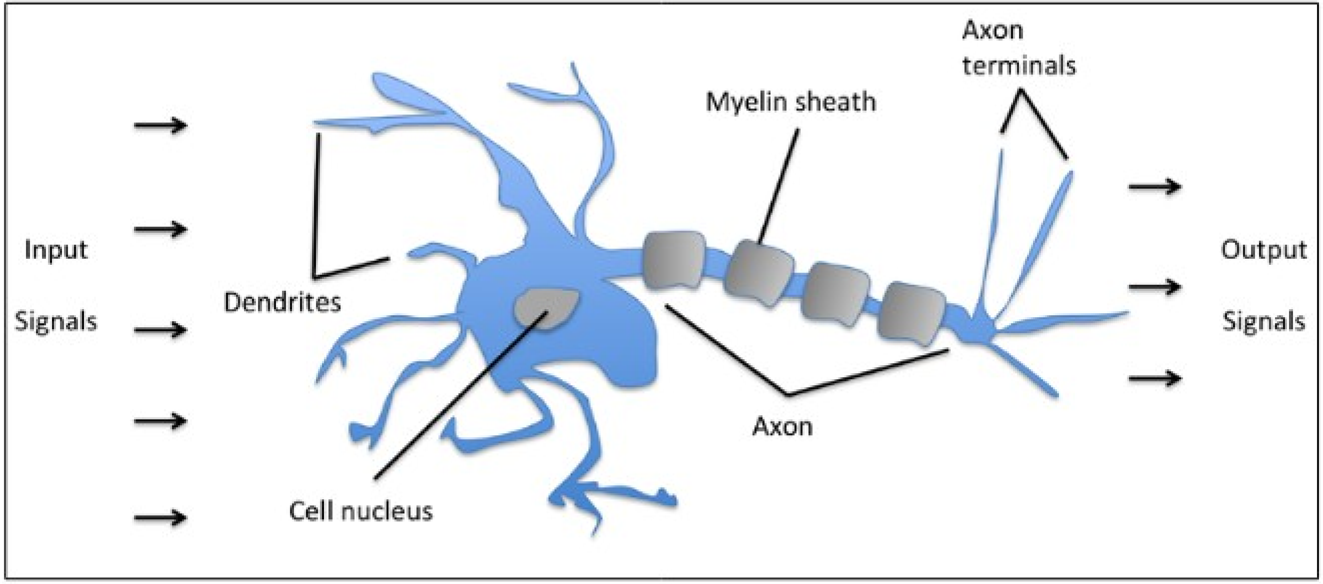
Linear regression revisited (machine learning)

1) Learning some early classification methods

2) Learning how linear regression (with biasing penalties) can be constructed and cross-validated

3) Understanding that biasing in-sample solutions can improve out-of-sample predictions

Black box idea



$$\boldsymbol{w} = \begin{bmatrix} w_1 \\ \vdots \\ w_m \end{bmatrix}, \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_m \end{bmatrix}$$

$$z = w_1 x_1 + \ldots + w_m x_m$$

Question: what do *x*, *w* and *z* correspond to in the above picture of the *Perceptron*?

(p. 18: Raschka, 2015)

Prediction/classification rule

$$\phi(z) = \begin{cases} 1 \; if \; z \geq \theta \\ -1 \; otherwise \end{cases}$$

Perceptron fires

Perceptron doesn’t fire

θ is a pre-specified threshold

(Raschka, 2015)

Prediction/classification rule

$$w_0 = -\theta$$
$$x_0 = 1$$

$$z = w_0 x_0 + w_1 x_1 + \ldots + w_m x_m = \boldsymbol{w}^T \boldsymbol{x}$$

$$z = -\theta + w_1 x_1 + \ldots + w_m x_m = \boldsymbol{w}^T \boldsymbol{x}$$

$$\phi(z) = \begin{cases} 1 & if\ z \geq 0 \\ -1 & otherwise \end{cases}$$

Perceptron fires

Perceptron doesn’t fire

(Raschka, 2015)

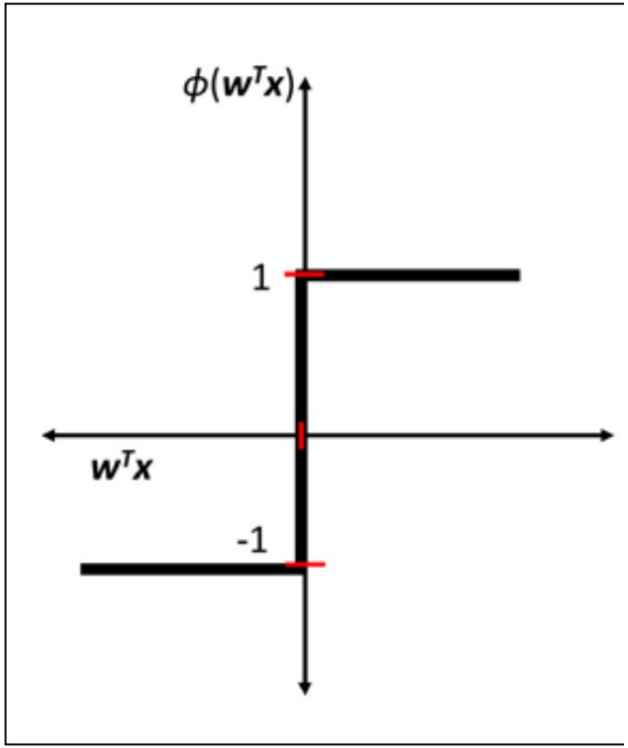
Perceptron classification

Bonus info

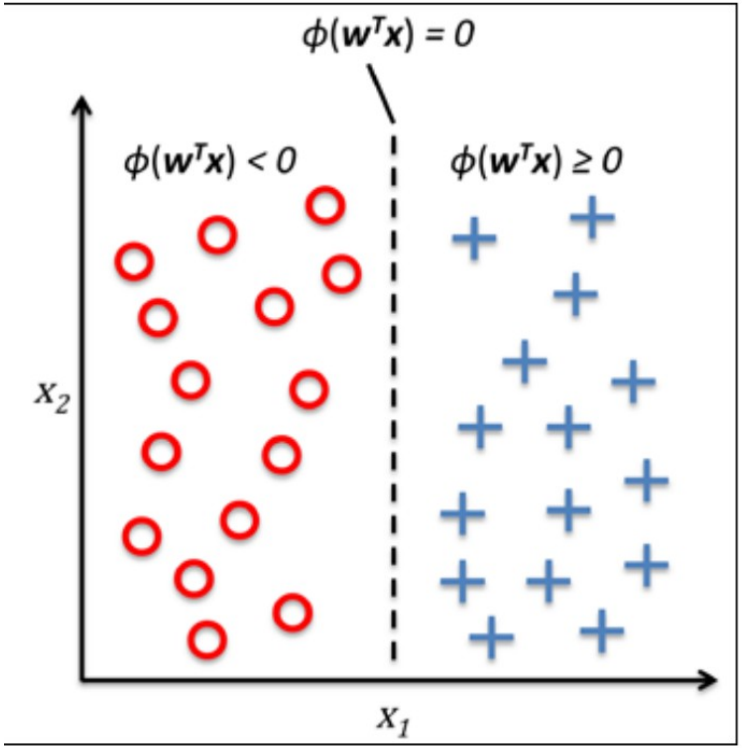
$$f(x) = a + \frac{b-a}{1+e^{\frac{c-x}{d}}}$$

Practical exercise 5...

$a = -1$
$b = 1$
$c = 0$
d going to 0



(p. 21: Raschka, 2015)



We want to find **w**^{T}**x** that achieves this separation

In *Python*

```
class Perceptron(object):
    """ Perceptron classifier

    Parameters
    ------------
    eta : float
        Learning rate (between 0.0 and 1.0)
    n_iter : int
        Passes over the training dataset.

    Attributes
    -----------
    w_ : 1d-array
        Weights after fitting.
    errors_ : list
        Number of misclassifications in every epoch.

    """
```

Special definition that indicates what the object (*Perceptron*) can be initialised with

```
def __init__(self, eta=0.01, n_iter=10):
    self.eta = eta
    self.n_iter = n_iter
```

```
ppn = Perceptron(eta=0.1, n_iter=10)
```

Specifying methods of *Perceptron*

1. Initialize the weights to 0 or small random numbers.
2. For each training sample $\boldsymbol{x}^{(i)}$ perform the following steps:
    1. Compute the output value $\hat{y}$.
    2. Update the weights.

```python
def fit(self, X, y):
    """ Fit training data.

    Parameters
    ----------
    X : {array-like}, shape = [n_samples, n_features]
        Traing vectors, where n_samples
        is the number of samples and
        n_features is the number of features.
    y : array-like, shape = [n_samples]
        Target values.

    Returns
    -------
    self : object

    """
    self.w_ = np.zeros(1 + X.shape[1])
    self.errors_ = []

    for _ in range(self.n_iter):
        errors = 0
        for xi, target in zip(X, y):
            update = self.eta * (target - self.predict(xi))
            self.w_[1:] += update * xi
            self.w_[0] += update
            errors += int(update != 0.0)
        self.errors_.append(errors)
    return self
```

Compute the output value $\hat{y}$

```python
def net_input(self, X):
    """Calculate net input"""
    return np.dot(X, self.w_[1:]) + self.w_[0]

def predict(self, X):
    """Return class label after unit step"""
    return np.where(self.net_input(X) >= 0.0, 1, -1)
```

$$\phi(z) = \begin{cases} 1 \ \ if\ z \geq \theta \\ -1 \ \ otherwise \end{cases}$$

When we are right

real label

$$\Delta w_j = \eta\left(\boxed{-1} - \boxed{-1}\right)x_j^{(i)} = 0$$

predicted label

real label

$$\Delta w_j = \eta\left(\boxed{1} - \boxed{1}\right)x_j^{(i)} = 0$$

predicted label

Δw_j: change in weight

η: learning rate

When we are wrong

real label

$$\Delta w_j = \eta(\boxed{1} - \boxed{-1})x_j^{(i)} = \eta(2)x_j^{(i)}$$

predicted label

real label

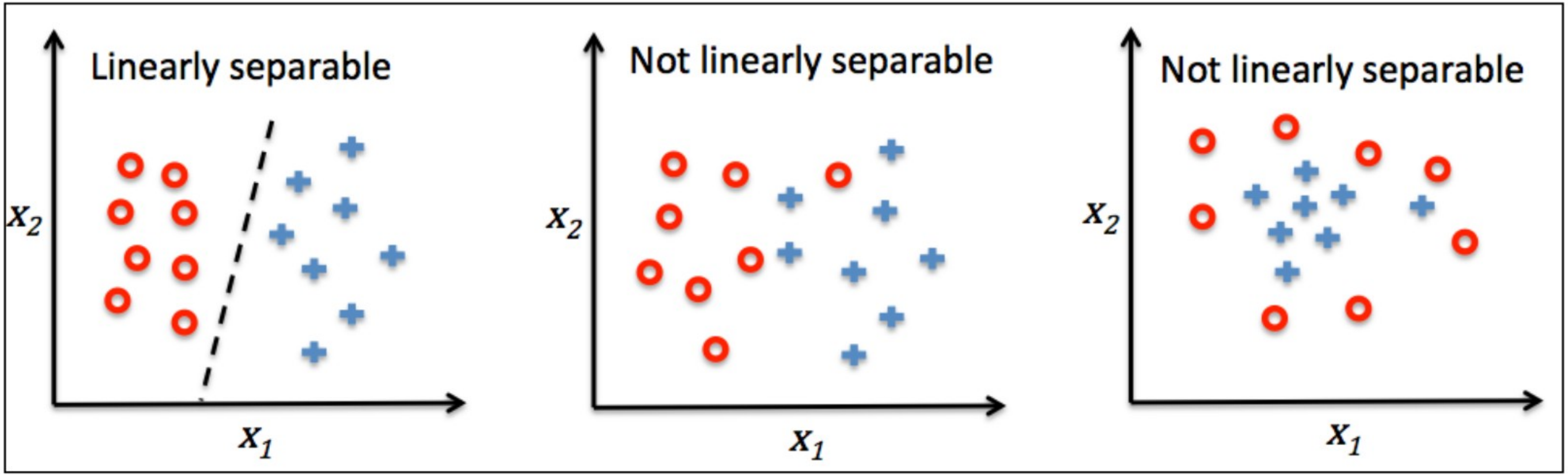
$$\Delta w_j = \eta(\boxed{-1} - \boxed{1})x_j^{(i)} = \eta(-2)x_j^{(i)}$$

predicted label

Δw_j: change in weight

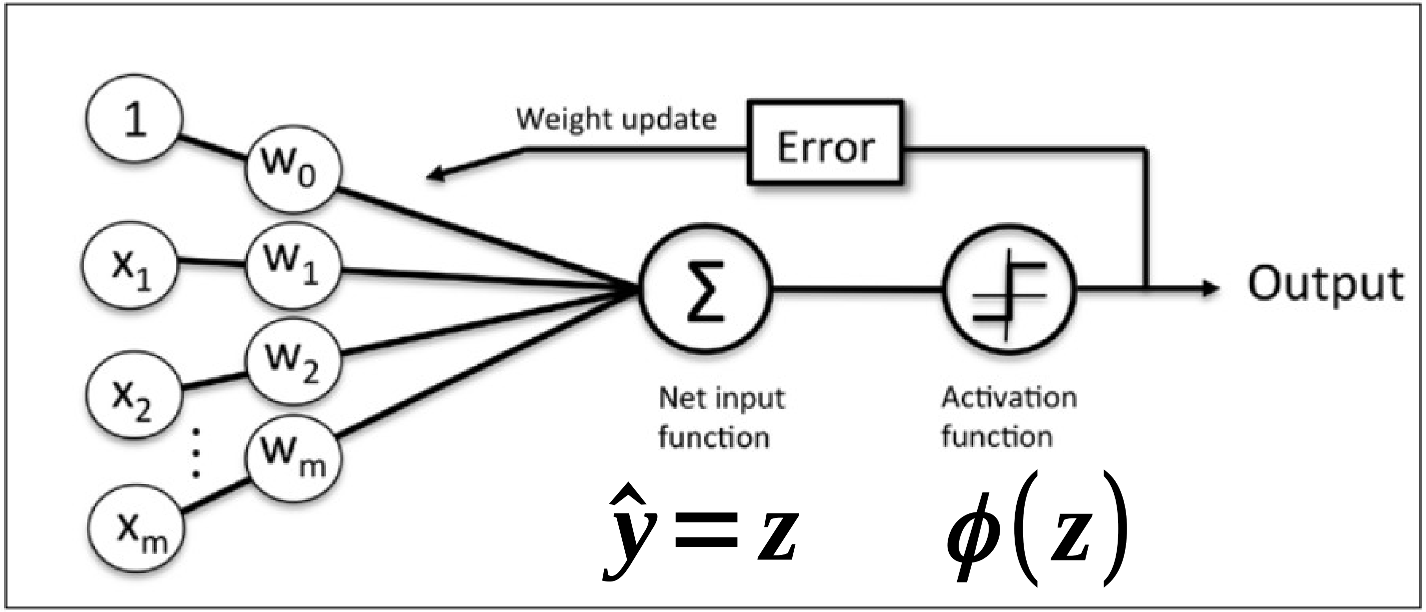
η: learning rate

Convergence only possible when linearly separable



(p. 23: Raschka, 2015)

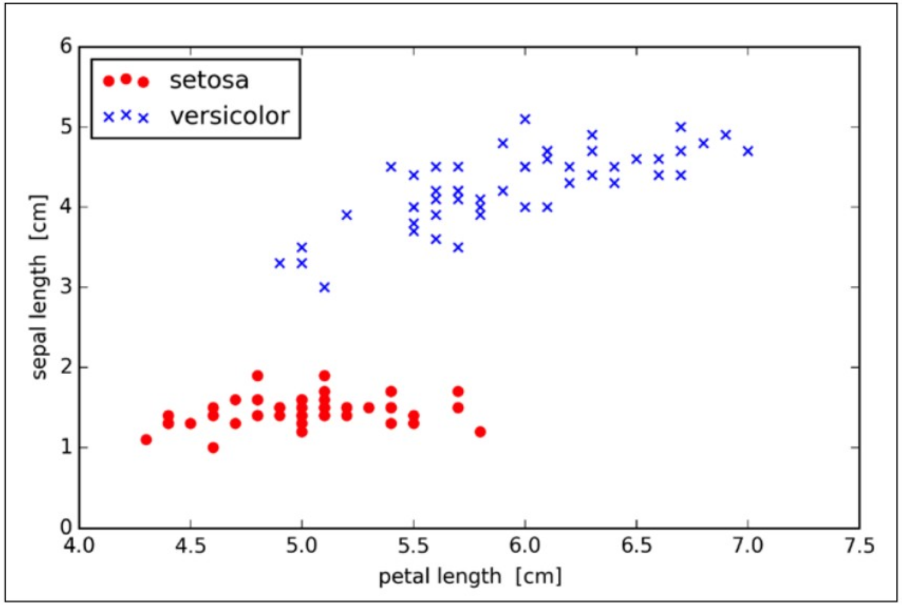
Perceptron: Graphical summary

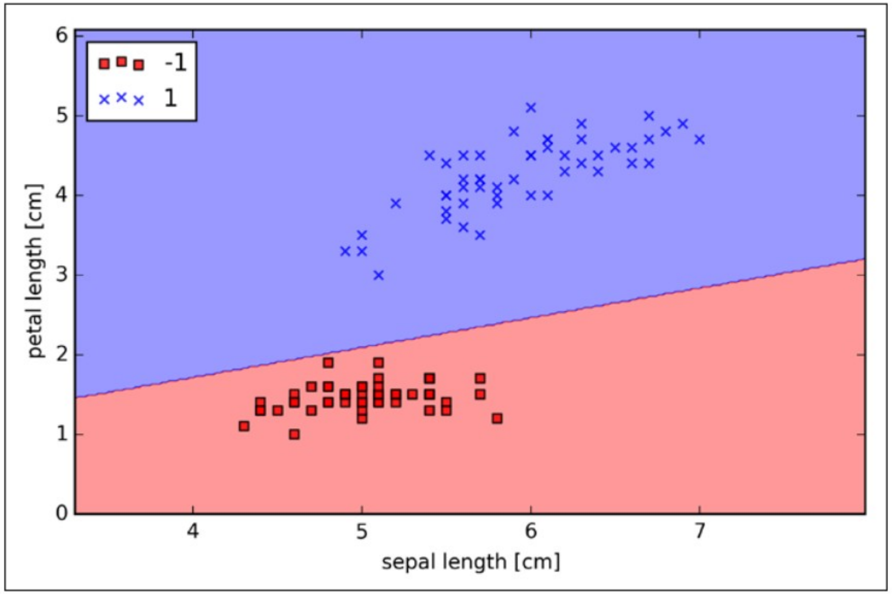


$\hat{y} = z \qquad \phi(z)$

(p. 24: Raschka, 2015)

An example






```
In [4]: ppn.w_
Out[4]: array([-0.4 , -0.68,  1.82])
```

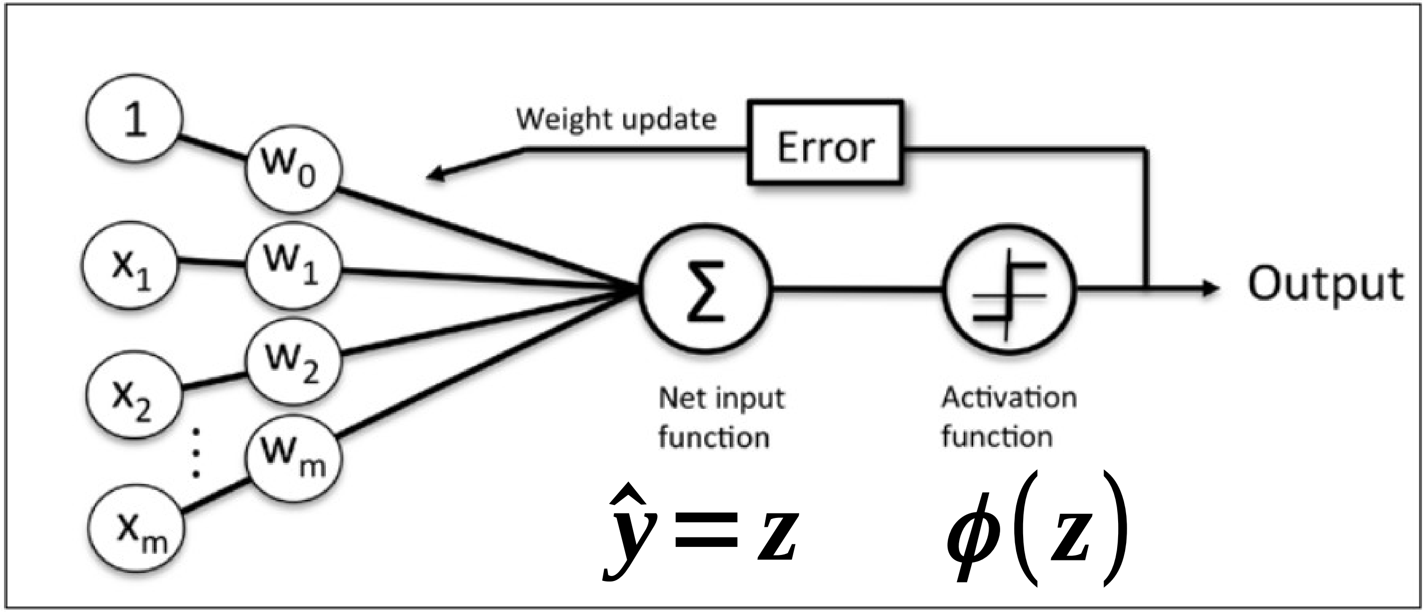
```
In [12]: X[1, :]
Out[12]: array([4.9, 1.4])
```

$$\hat{y} = -0.4 - 0.68 \cdot 4.9 + 1.82 \cdot 1.4 = -1.184$$

```
In [11]: ppn.net_input(X[1, :])
Out[11]: -1.1839999999999975
```

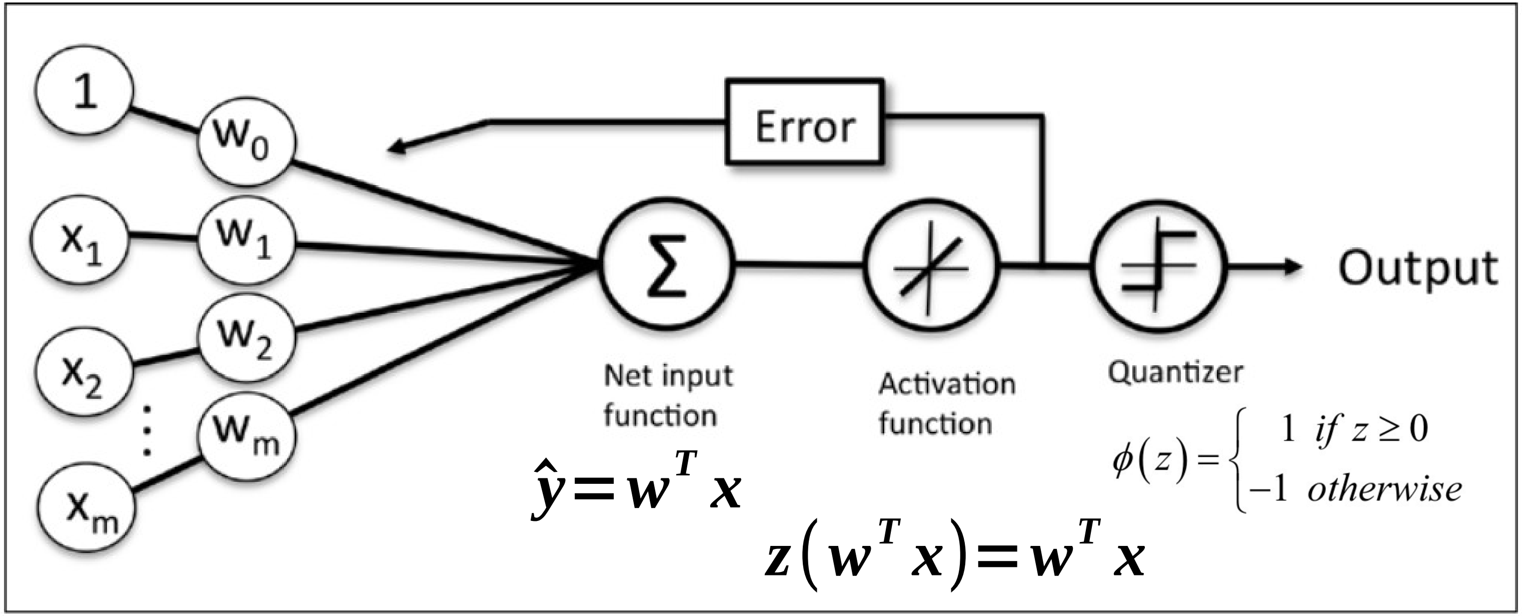
(p. 29 & p. 32: Raschka, 2015)

Perceptron: Graphical summary



(p. 24: Raschka, 2015)

ADAptive LInear NEuron (ADALINE)



$$\hat{\boldsymbol{y}} = \boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x}$$

$$\boldsymbol{z}(\boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x}) = \boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x}$$

$$\boldsymbol{w}^{\boldsymbol{T}} \boldsymbol{x} = w_0 x_0 + w_1 x_1 + \ldots + w_{m-1} x_{m-1} + w_m x_m$$

(p. 33: Raschka, 2015)

ADALINE Gradient descent

```
def __init__(self, eta=0.01, n_iter=50):
    self.eta = eta
    self.n_iter = n_iter
```

```
class AdalineGD(object):
    """ ADAptive LInear NEuron classifier

    Parameters
    ------------
    eta : float
        Learning rate (between 0.0 and 1.0)
    n_iter : int
        Passes over the training dataset.

    Attributes
    -----------
    w_ : 1d-array
        Weights after fitting.
    errors_ : list
        Number of misclassifications in every epoch.

    """
```

Methods

$$\hat{y} = \boldsymbol{w}^T \boldsymbol{x}$$

$$z(\boldsymbol{w}^T \boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x}$$

$$\phi(z) = \begin{cases} 1 & if\ z \geq 0 \\ -1 & otherwise \end{cases}$$

```python
def net_input(self, X):
    """Calculate net input"""
    return np.dot(X, self.w_[1:]) + self.w_[0]

def activation(self, X):
    """Computer linear activation"""
    return self.net_input(X)

def predict(self, X):
    """Return class label after unit step"""
    return np.where(self.activation(X) >= 0.0, 1, -1)
```

The *fit* method

```
def fit(self, X, y):
    """ Fit training data.

    Parameters
    ----------
    X : {array-like}, shape = [n_samples, n_features]
        Traing vectors, where n_samples
        is the number of samples and
        n_features is the number of features.
    y : array-like, shape = [n_samples]
        Target values.

    Returns
    -------
    self : object

    """
    self.w_ = np.zeros(1 + X.shape[1])
    self.cost_ = []

    for i in range(self.n_iter):
        output = self.net_input(X)
        errors = (y - output)
        self.w_[1:] += self.eta * X.T.dot(errors)
        self.w_[0] += self.eta * errors.sum()
        cost = (errors**2).sum() / 2.0
        self.cost_.append(cost)
    return self
```

eta: learning rate (a constant)

output: $X\beta = \hat{y}$

errors: $y - \hat{y}$

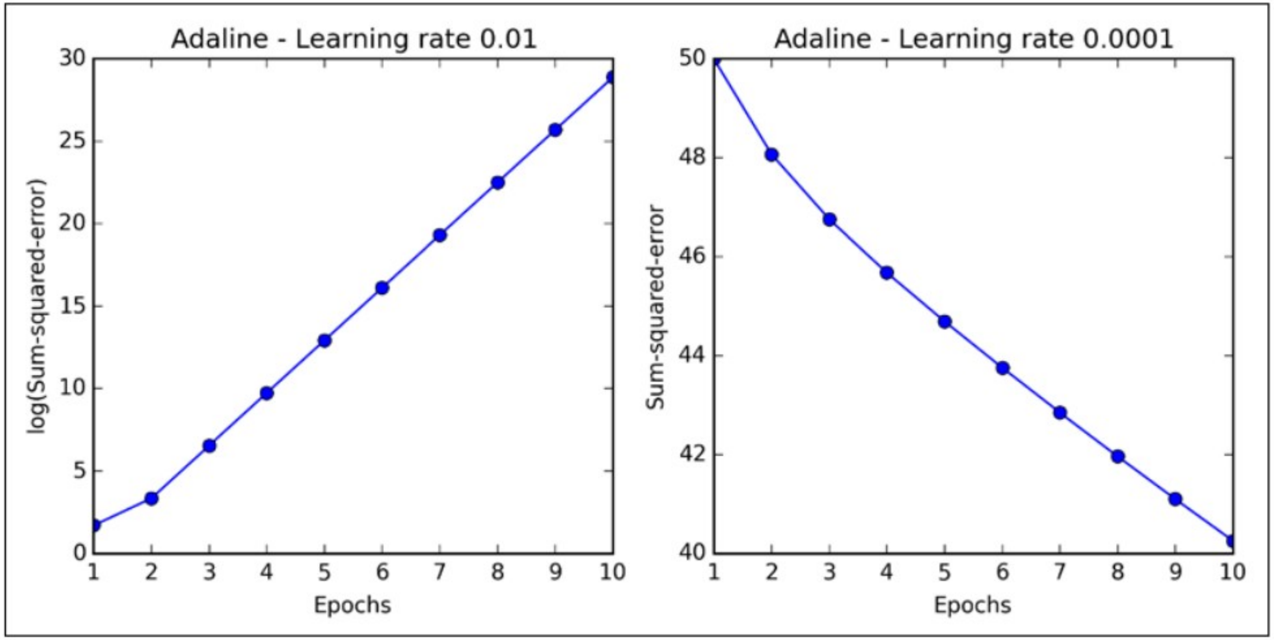
X.T.dot(errors): $X^T \cdot (y - \hat{y})$

$$X^T \cdot (y - \hat{y}) = \Delta w_1 + \Delta w_2 + \ldots + \Delta w_{m-1} + \Delta w_m$$

cost function: $\left(\sum (y - \hat{y})^2\right)/2$

Learning rate

Overshooting the global minimum

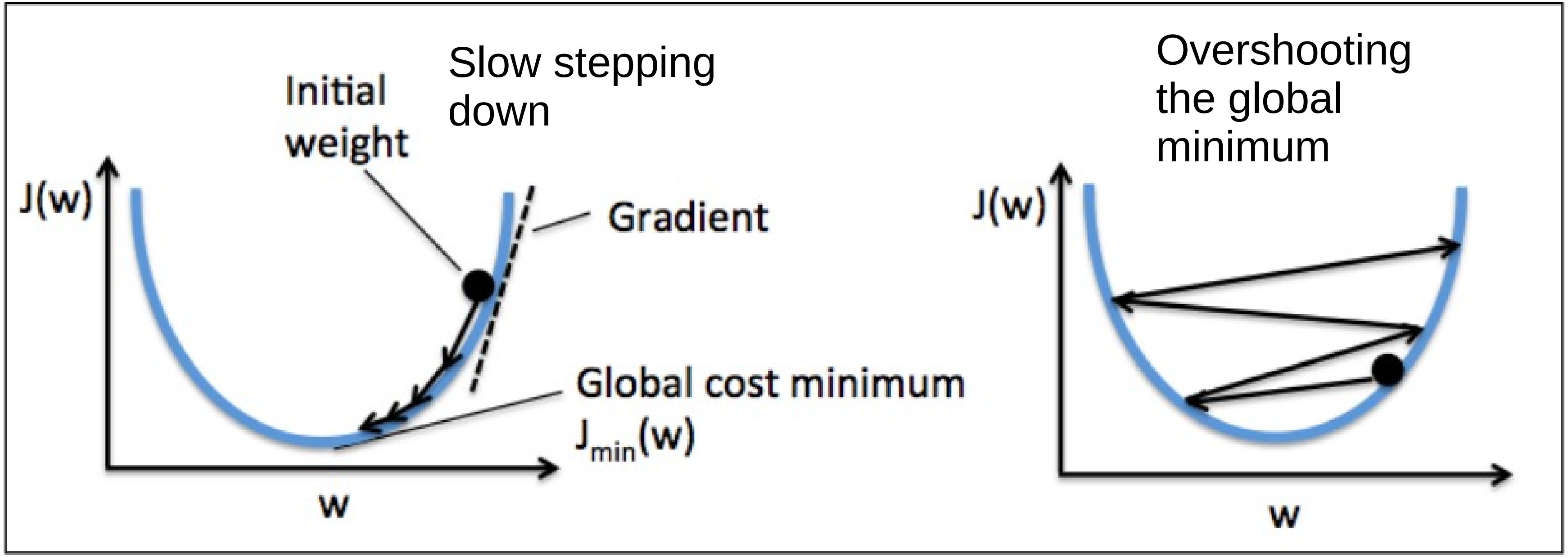


Slow stepping down

Always check whether it converges

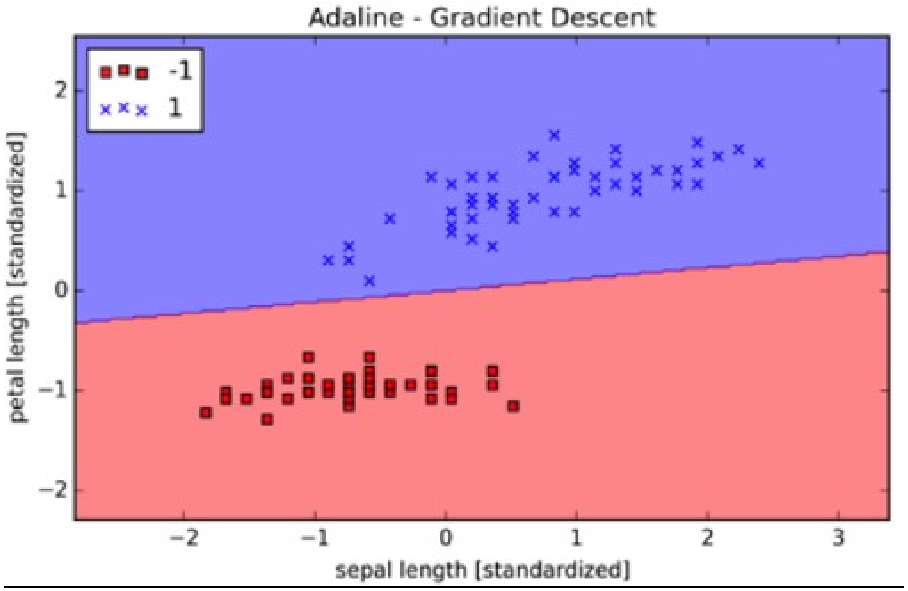
(p. 40: Raschka, 2015)

Gradient descent



$$J(w) = \left(\sum (y - \hat{y})^2\right)/2$$

(p. 40: Raschka, 2015)



(p. 42: Raschka, 2015)

```
In [50]: X_std[1, :]
Out[50]: array([-0.89430898, -1.01435952])
```

```
In [38]: ada.w_
Out[38]: array([ 1.59872116e-16, -1.26256159e-01,  1.10479201e+00])
```

$$\hat{y} \approx 0 - 0.127 \cdot (-0.894) + 1.10 \cdot (-1.014) = -1.01$$

```
In [49]: ada.net_input(X_std[1, :])
Out[49]: -1.0077442758158444
```

How does this relate to linear regression?

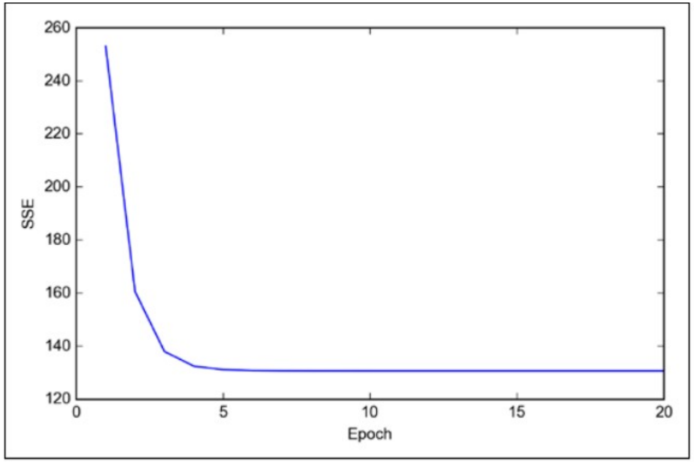
From ADALINE

$$\boldsymbol{w}^T \boldsymbol{x} = w_0 x_0 + w_1 x_1 + \ldots + w_{m-1} x_{m-1} + w_m x_m$$

Very similar to ADALINE
and when converged will be virtually identical to the ordinary least squares solution

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

Convergence

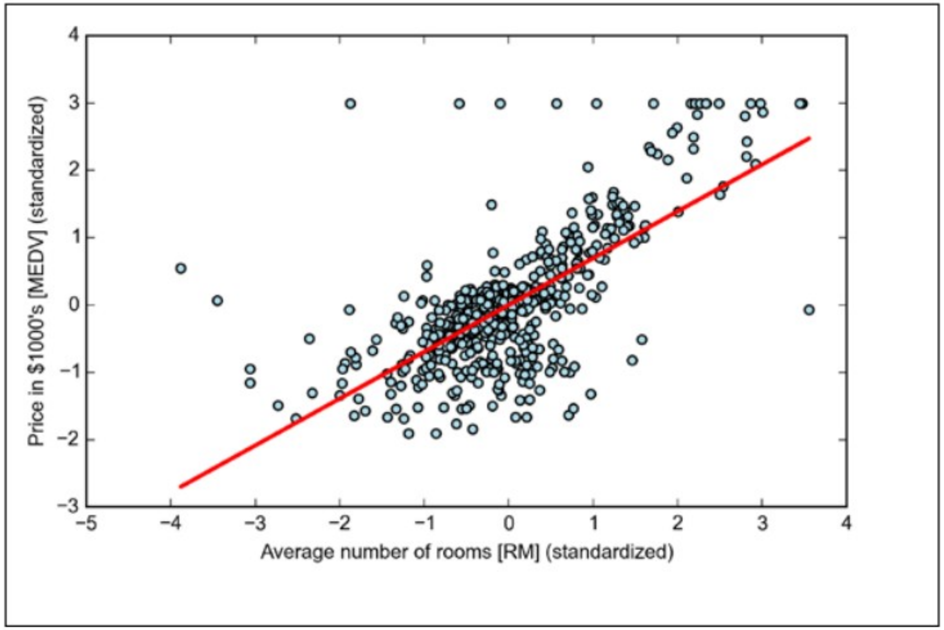



```python
class LinearRegressionGD(object):

    def __init__(self, eta=0.001, n_iter=20):
        self.eta = eta
        self.n_iter = n_iter

    def fit(self, X, y):
        self.w_ = np.zeros(1 + X.shape[1])
        self.cost_ = []

        for i in range(self.n_iter):
            output = self.net_input(X)
            errors = (y - output)
            self.w_[1:] += self.eta * X.T.dot(errors)
            self.w_[0] += self.eta * errors.sum()
            cost = (errors**2).sum() / 2.0
            self.cost_.append(cost)
        return self

    def net_input(self, X):
        return np.dot(X, self.w_[1:]) + self.w_[0]

    def predict(self, X):
        return self.net_input(X)
```

What we have seen before

```
lr = LinearRegressionGD()
lr.fit(X_std, y_std)
```

(p. 288: Raschka, 2015)




```
In [8]: lr.w_
Out[8]: array([-4.68958206e-16,  6.95359426e-01])
```

Intercept and slope

Olivier Grisel
@ogrisel

In scikit-learn 1.0, we decided to deprecate the sklearn.datasets.load_boston function because the design of this dataset casually assumes that people prefer to buy housing in racially segregated neighborhoods.

(p. 229: Raschka, 2015)

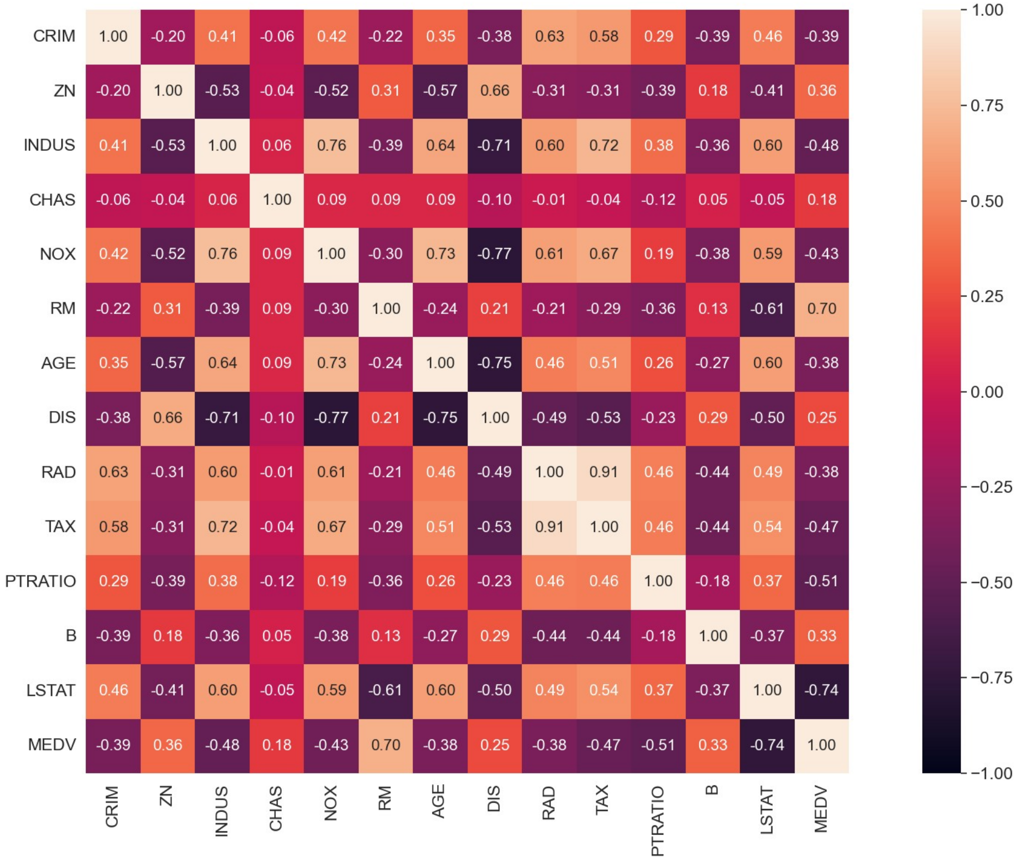
The features of the 506 samples may be summarized as shown in the excerpt of the dataset description:

- **CRIM**: This is the per capita crime rate by town
- **ZN**: This is the proportion of residential land zoned for lots larger than 25,000 sq.ft.
- **INDUS**: This is the proportion of non-retail business acres per town
- **CHAS**: This is the Charles River dummy variable (this is equal to 1 if tract bounds river; 0 otherwise)
- **NOX**: This is the nitric oxides concentration (parts per 10 million)
- **RM**: This is the average number of rooms per dwelling
- **AGE**: This is the proportion of owner-occupied units built prior to 1940
- **DIS**: This is the weighted distances to five Boston employment centers
- **RAD**: This is the index of accessibility to radial highways
- **TAX**: This is the full-value property-tax rate per $10,000
- **PTRATIO**: This is the pupil-teacher ratio by town
- **B**: This is calculated as *1000(Bk - 0.63)^2*, where Bk is the proportion of people of African American descent by town
- **LSTAT**: This is the percentage lower status of the population
- **MEDV**: This is the median value of owner-occupied homes in $1000s

Multiple linear regression

$$\hat{MEDV} = w_0 x_0 + w_1 CRIM + w_2 ZN + w_3 INDUS + w_4 CHAS$$
$$+ w_5 NOX + w_6 RM + w_7 AGE + w_8 DIS$$
$$+ w_9 RAD + w_{10} TAX + w_{11} PTRATIO + w_{12} B + w_{13} LSTAT + \epsilon$$

Collinearity – correlation matrix



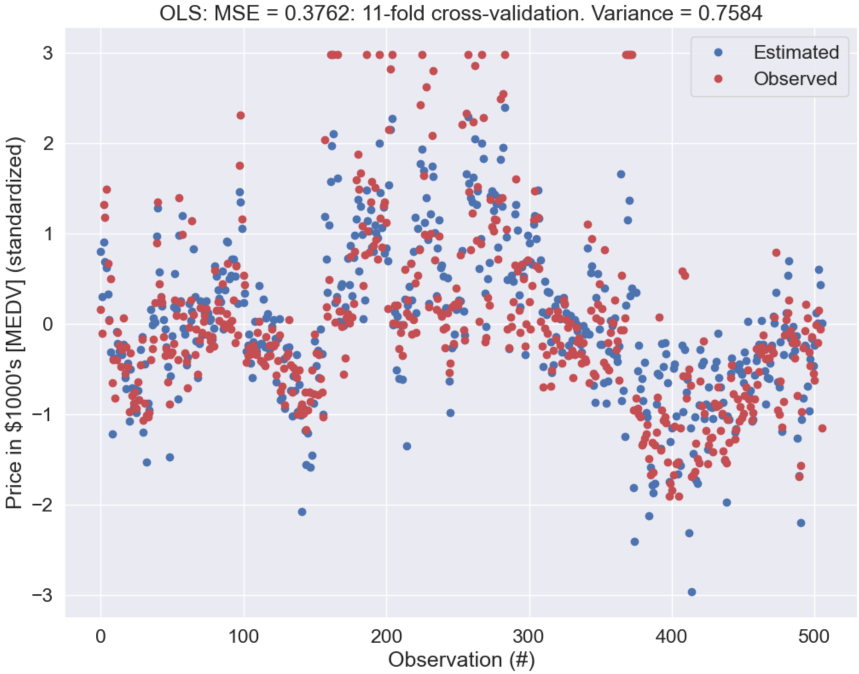
Because of the collinearity, we know we are prone to overfitting, so we do **out-of-sample** prediction instead of validating our model with traditional measures like R^2 and maximum likelihood

How to choose the **out-of-sample** dataset?

Cross-validation

(p. 176: Raschka, 2015)

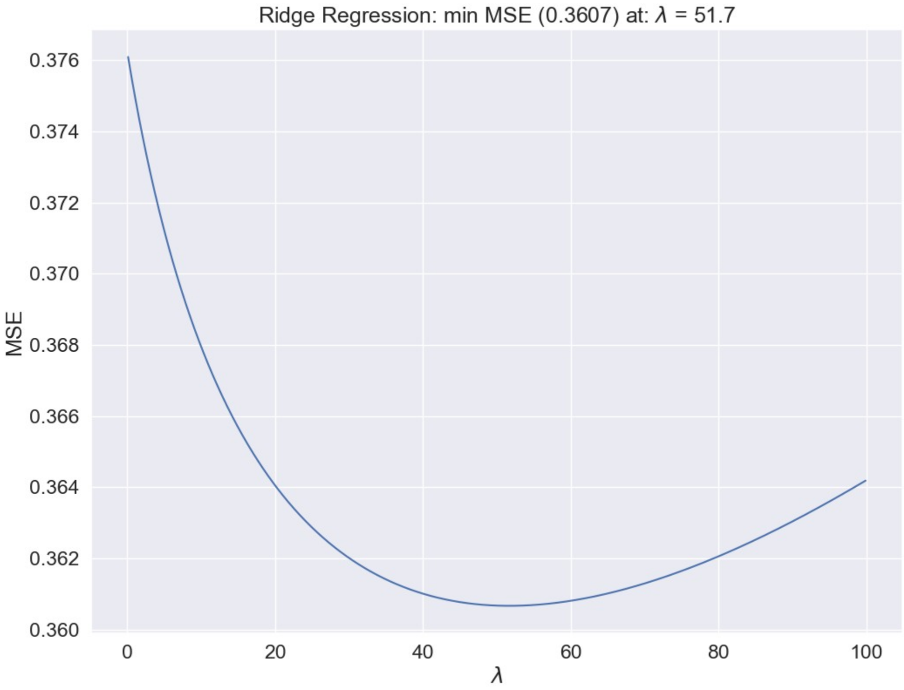
```python
OLS = LinearRegression()
OLS.fit(X_std, y_std)

MSE = np.mean(cross_validate(OLS, X_std, y_std, k=11))
```

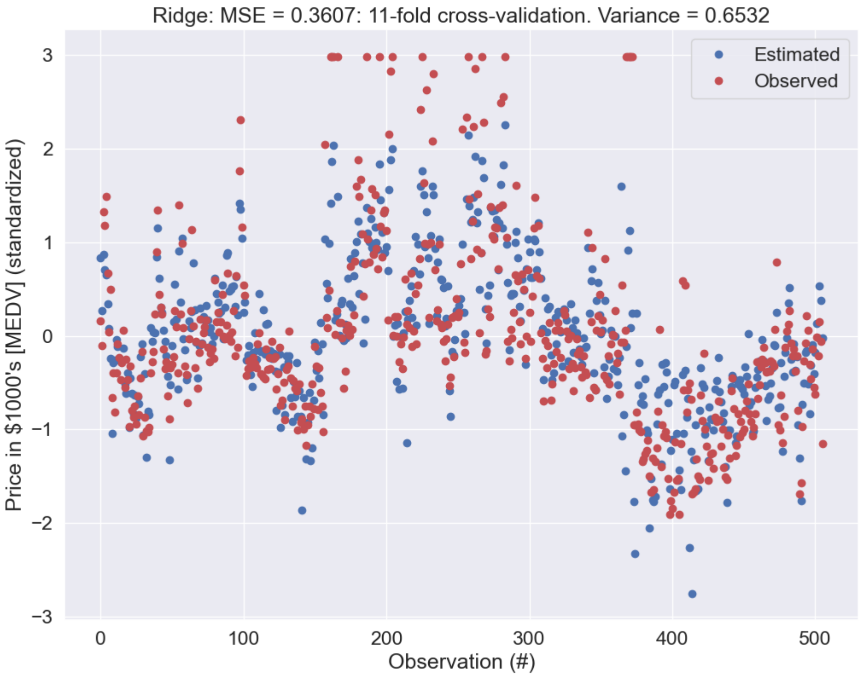


We can impose penalties

(but not on the intercept)

$$J(w)_{Ridge} = \sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda \| w \|_2^2$$

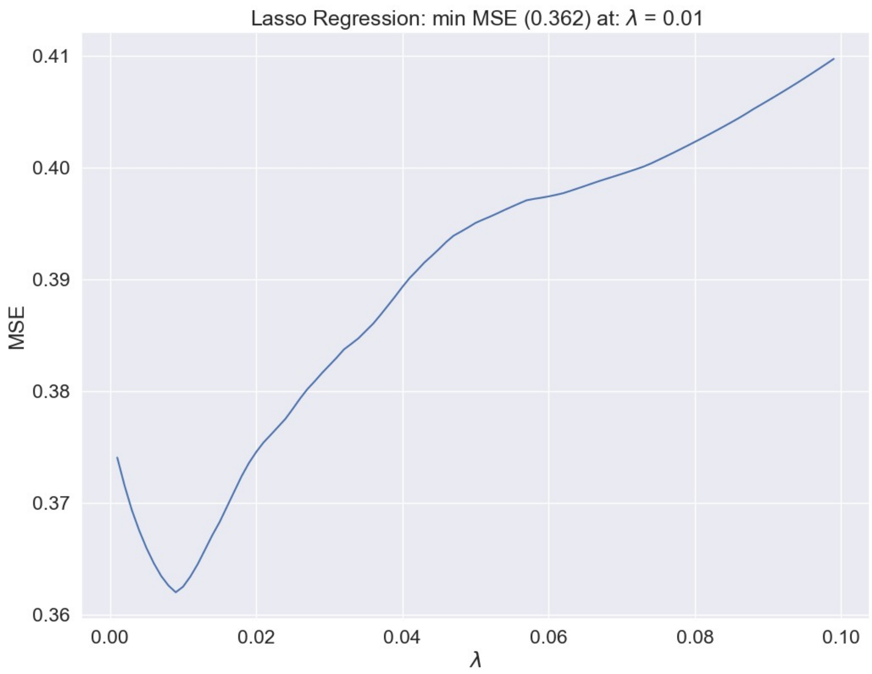


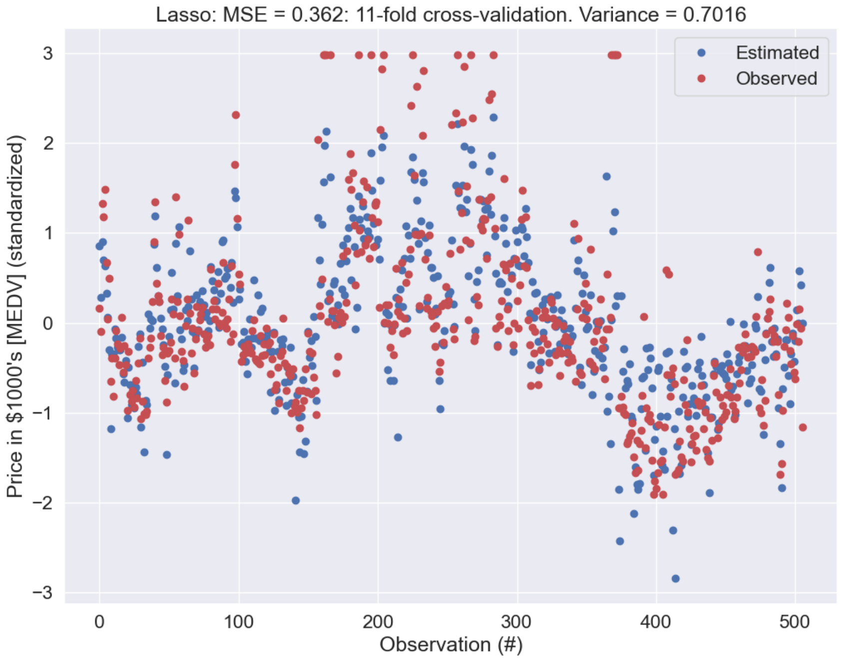


We can impose penalties

(but not on the intercept)

$$J(w)_{LASSO} = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)} \right)^2 + \lambda \| w \|_1$$





Coefficients are shrunk

```
In [131]: OLS.coef_
Out[131]:
array([-0.09874812,  0.12473758,  0.02386168,  0.06945318, -0.22231612,
        0.2911837 ,  0.0325356 , -0.32907266,  0.34212986, -0.28361575,
       -0.21482076,  0.09763631, -0.43131412])

In [132]: RR.coef_
Out[132]:
array([-0.07536542,  0.08180161, -0.03182673,  0.07855868, -0.13185121,
        0.31082552,  0.00548938, -0.23491485,  0.11242408, -0.0959682 ,
       -0.18436614,  0.09154233, -0.36579723])

In [133]: lasso.coef_
Out[133]:
array([-0.07348948,  0.09107936, -0.        ,  0.07003181, -0.17110318,
        0.30950805,  0.        , -0.29010247,  0.16456993, -0.1319311 ,
       -0.19668957,  0.09063304, -0.41664587])
```

We can impose penalties

(but not on the intercept)

$$J(w)_{ElasticNet} = \sum_{i=1}^{n}\left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda_1 \sum_{j=1}^{m} w_j^{\ 2} + \lambda_2 \sum_{j=1}^{m} \left|w_j\right|$$

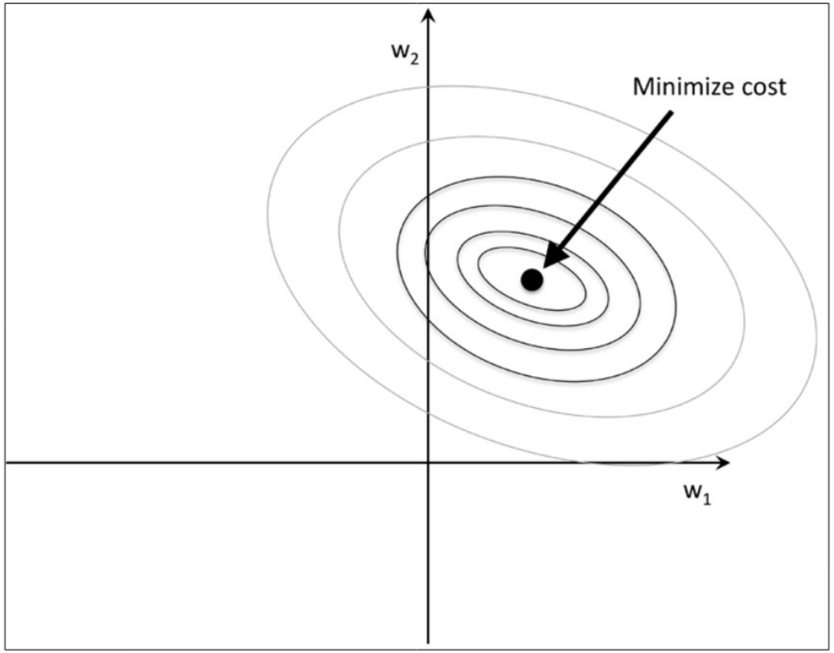
Did you learn?

Linear regression revisited (machine learning)

1) Learning some early classification methods
2) Learning how linear regression (with biasing penalties) can be constructed and cross-validated
3) Understanding that biasing in-sample solutions can improve out-of-sample predictions

Extra slides on regularization

$$J(w) = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$



(p. 113: Raschka, 2015)

L2 regularization

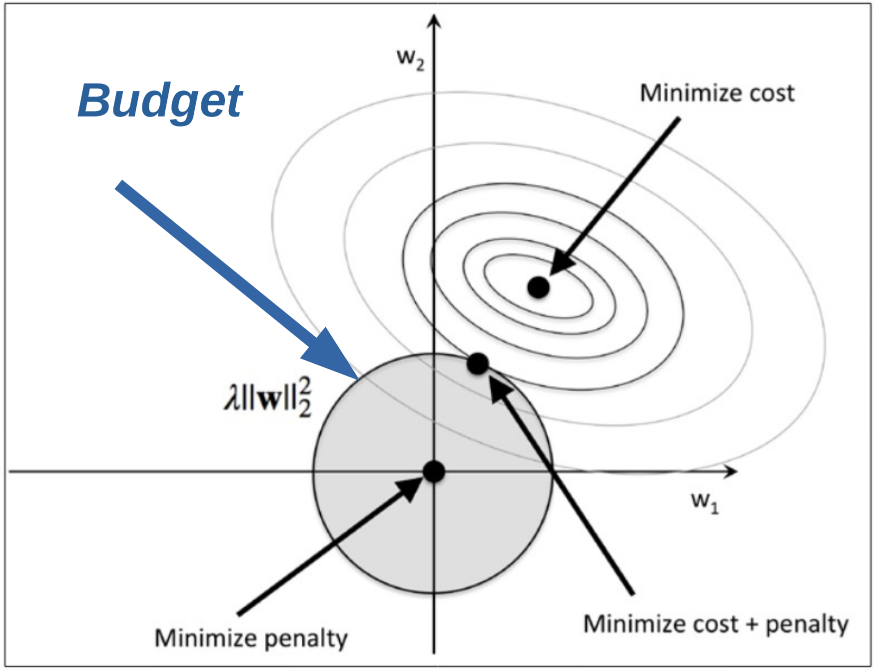
Why is the *budget* round?

Compare with a circle centred at (0,0)

$$x^2 + y^2 = r^2$$

$$w_1^2 + w_2^2 = r^2$$

$$\|w\|_2 = \sqrt{(w_1^2 + w_2^2)}$$



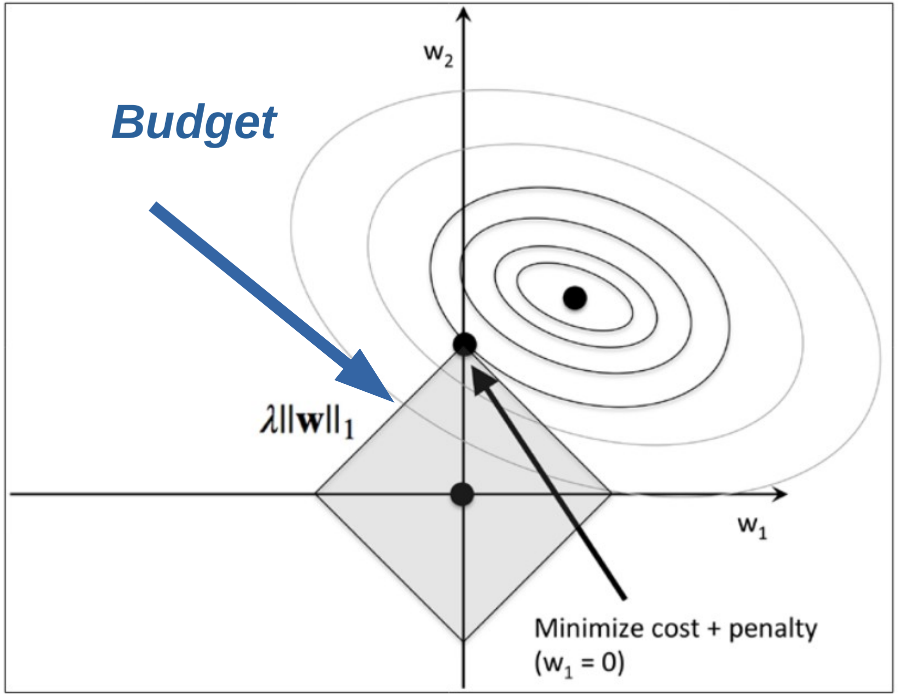
(p. 114: Raschka, 2015)

$$J(w)_{Ridge} = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda \| w \|_2^2$$

L1 regularization

Why is the *budget* square?

$$\|w\|_1 = |w_1| + |w_2|$$
$$\text{if } w_1 = max(w_1) \text{ then } w_2 = 0$$
$$\text{if } w_2 = max(w_2) \text{ then } w_1 = 0$$



$$J(w)_{LASSO} = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)} \right)^2 + \lambda \| w \|_1$$

References

- Raschka, S., 2015. Python Machine Learning. Packt Publishing Ltd.