Methods 3: Multilevel Statistical Modeling and Machine Learning

Week 7: *Logistic regression (machine learning)*

November 16, 2021

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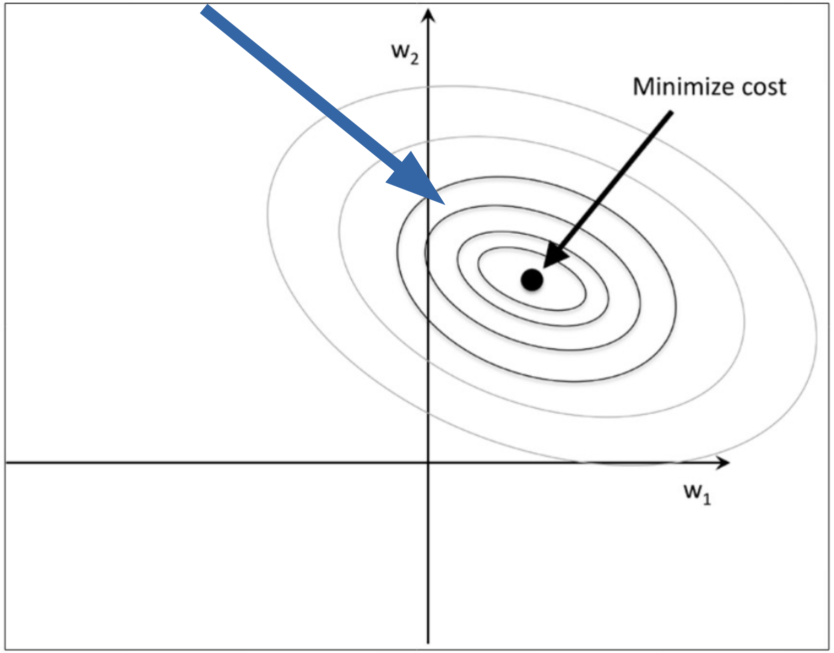
Remember to vote today!

Regularization - recap

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

Solution space is infinite;
$\boldsymbol{w}$ can be any set of values

Solution space



(p. 113: Raschka, 2015)

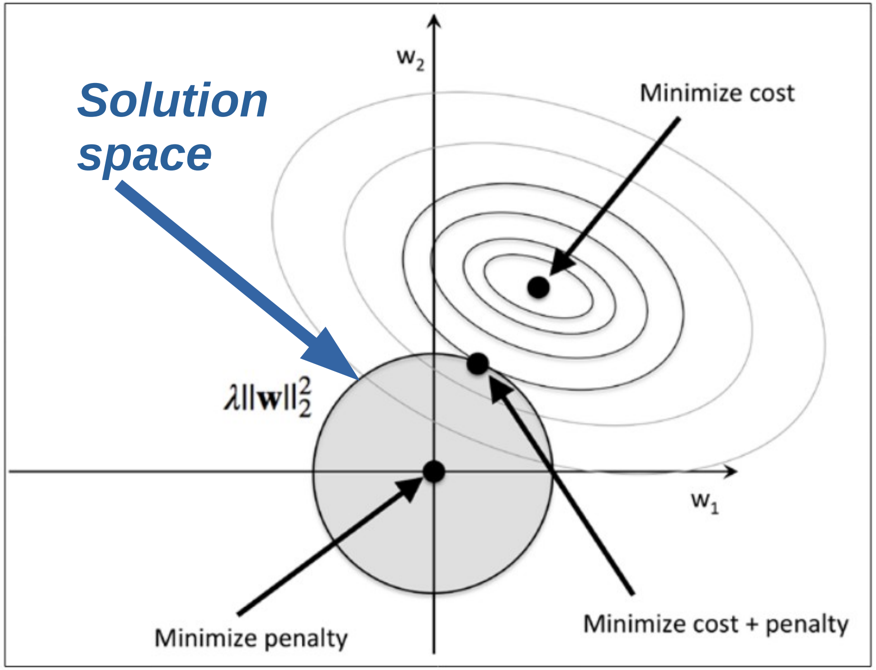
L2 regularization

Why is the *solution space* round?

Compare with a circle centred at (0,0)

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

$$\mathrm{L}_2\,\mathrm{norm}: \|w\|_2 = \sqrt{\left(w_1^2 + w_2^2\right)}$$



(p. 114: Raschka, 2015)

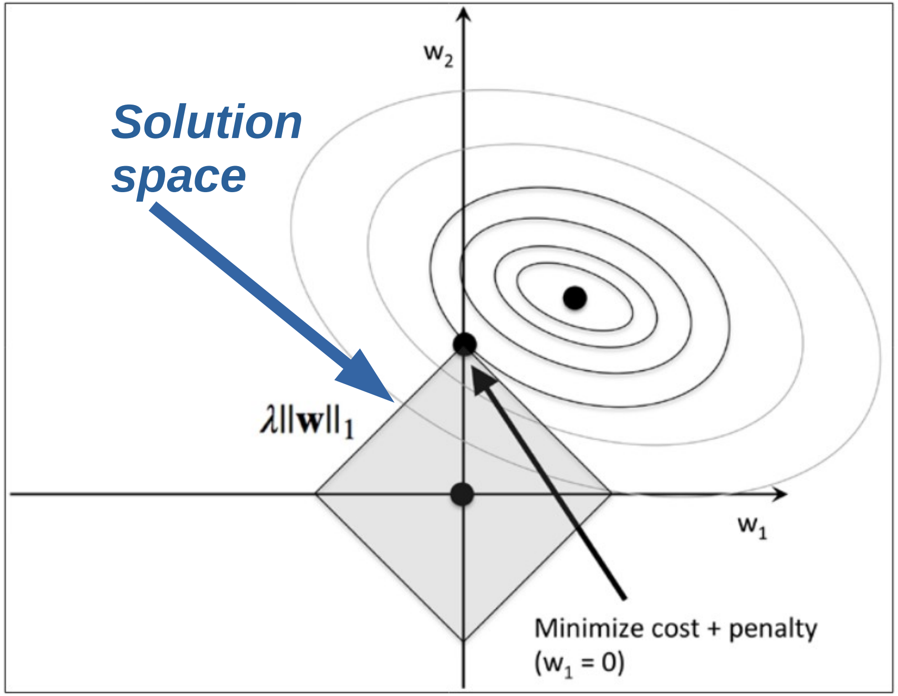
$$J(w)_{Ridge} = \sum_{i=1}^{n} \left(y^{(i)} - \hat{y}^{(i)}\right)^2 + \lambda \| w \|_2^2$$

L1 regularization

Why is the *solution space* square?

$$\mathrm{L}_1\,\mathrm{norm}: \|w\|_1 = |w_1| + |w_2|$$
$$\text{if } w_1 = max(w_1) \text{ then } w_2 = 0$$
$$\text{if } w_2 = max(w_2) \text{ then } w_1 = 0$$

(p. 115: Raschka, 2015)



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

Learning goals

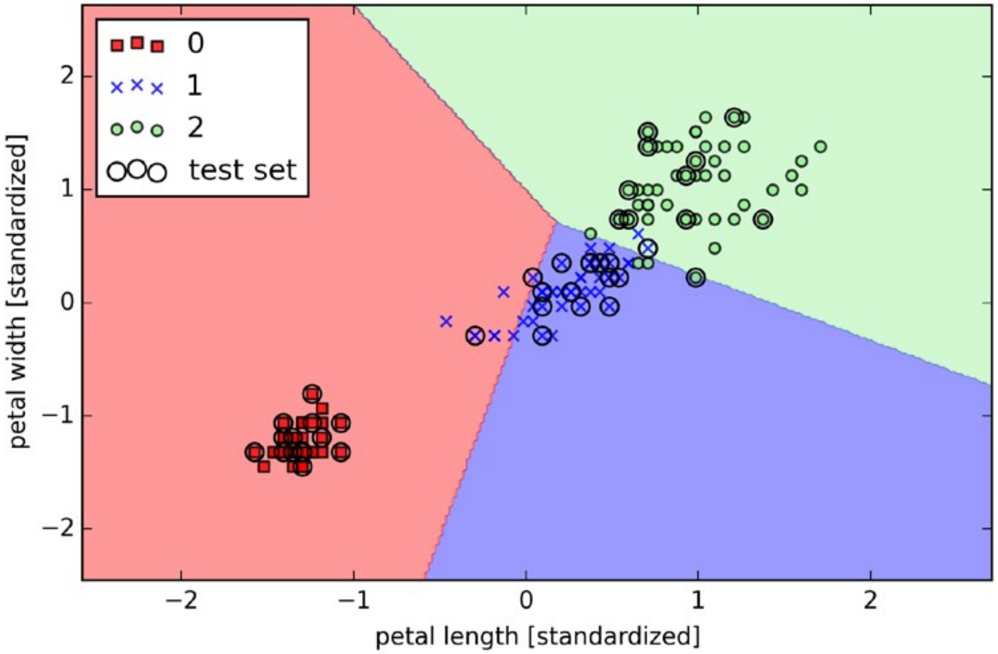
Logistic regression (machine learning)

1) Understanding of how logistic regression can be adapted to a classification framework

2) Understanding the idea of a Support Vector Machine

3) Getting acquainted with how Support Vector Machines can solve non-linear problems

The problem (Perceptron)



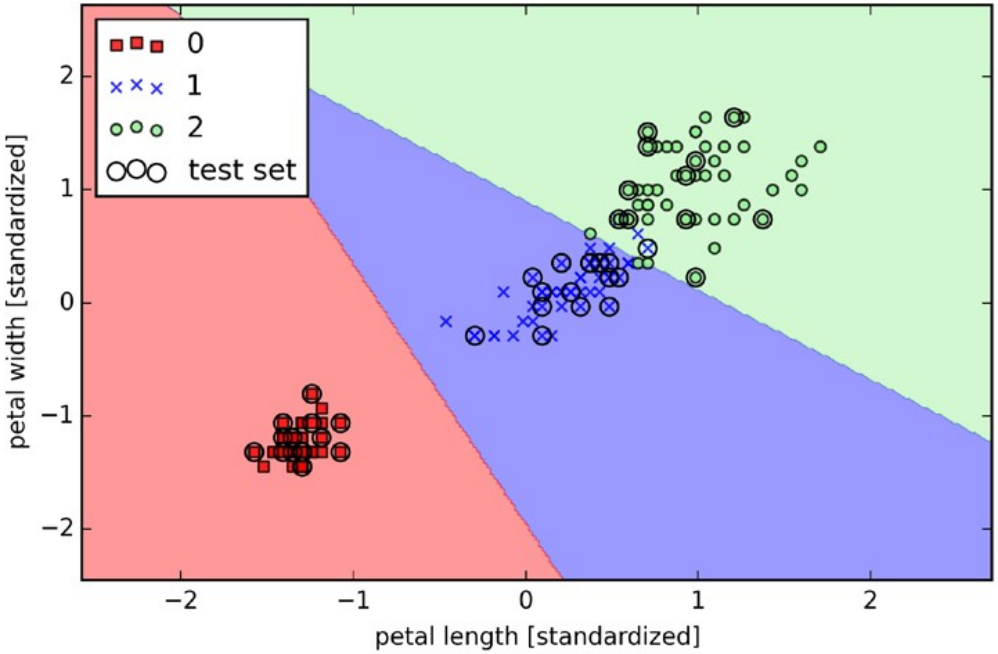
(p. 55: Raschka, 2015)

Not linearly separable ⟶ never converges

WANTED: an algorithm that converges with linearly separable regions that minimise the number of errors made

Something like this

LOGISTIC REGRESSION



(p. 63: Raschka, 2015)

Separates flowers, while keeping errors at a minimum

Odds ratio

$$\text{odds ratio} = \frac{p}{1-p}$$

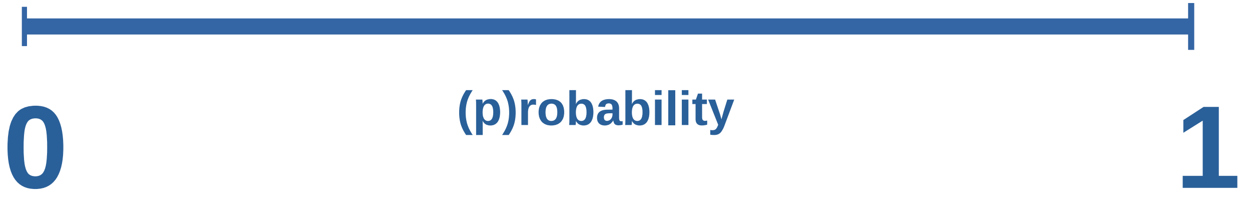
$$\log\text{ odds} = \log\left(\frac{p}{1-p}\right) = logit(p)$$

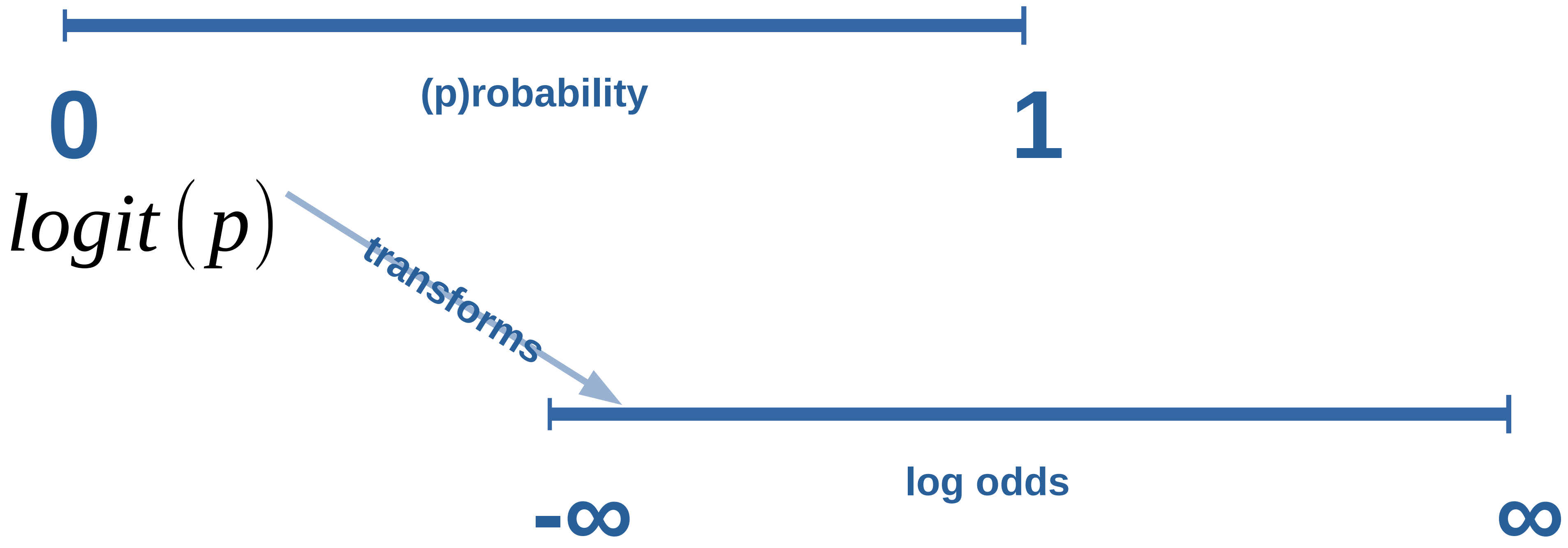
$$logit(p(y=1|\boldsymbol{x})) = w_0 x_0 + w_1 x_1 + \ldots + w_m x_m = \sum_{i=0}^{m} w_i x_i = \boldsymbol{w}^T \boldsymbol{x}$$

Example: an odds ratio of 7 to 1 (7:1) means that it is 7 times more likely that something is going to happen than that it is not going to happen

$$logit(p(y=1|\mathbf{x})) = w_0 x_0 + w_1 x_1 + \ldots + w_m x_m = \sum_{i=0}^{m} w_i x_i = \mathbf{w}^T \mathbf{x}$$

$$p(y=1|\mathbf{x}): \text{is the probability that } y=1, \text{ given } \mathbf{x}$$




0
(p)robability
1
$logit(p)$
transforms
log odds
-∞
∞

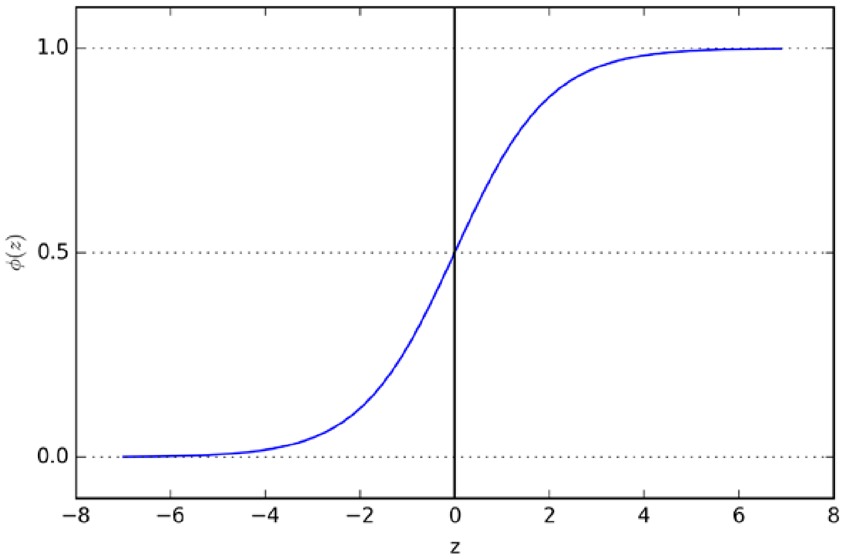
log odds

-∞ **∞**

$$\phi(z) = p$$

$$logit^{-1}(z) = \phi(z) = \frac{1}{1+e^{-z}}$$

$$(\text{sigmoid-shaped})$$



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

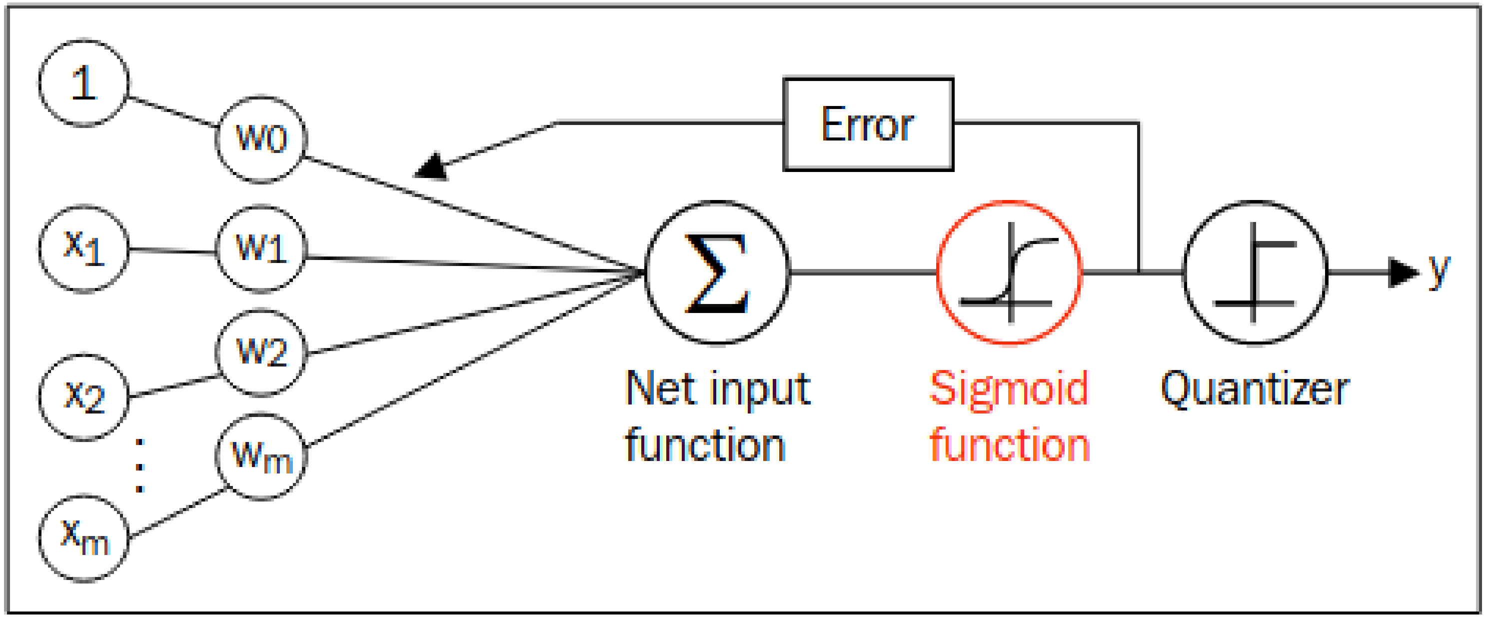
(p. 58: Raschka, 2015)

Quantizer

$$\hat{y} = \left\{ \begin{array}{l} 1 \ \text{if} \ \phi(z) \geq 0.5 \\ 0 \ \text{otherwise} \end{array} \right\}$$

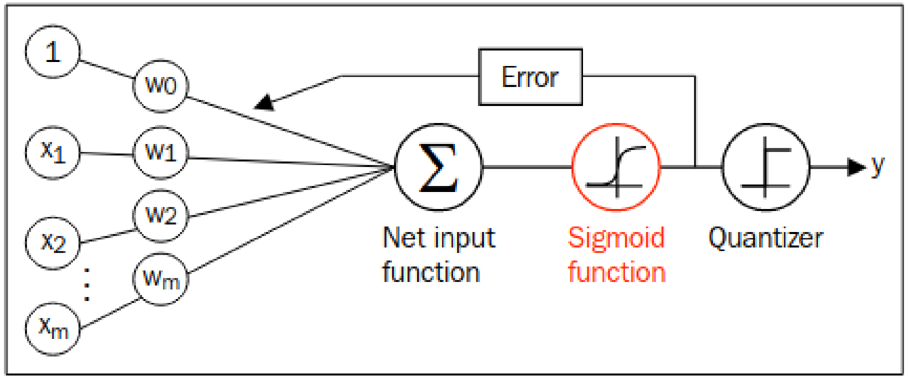
$$\hat{y} = \left\{ \begin{array}{l} 1 \ \text{if} \ z \geq 0.0 \\ 0 \ \text{otherwise} \end{array} \right\}$$

Logistic regression



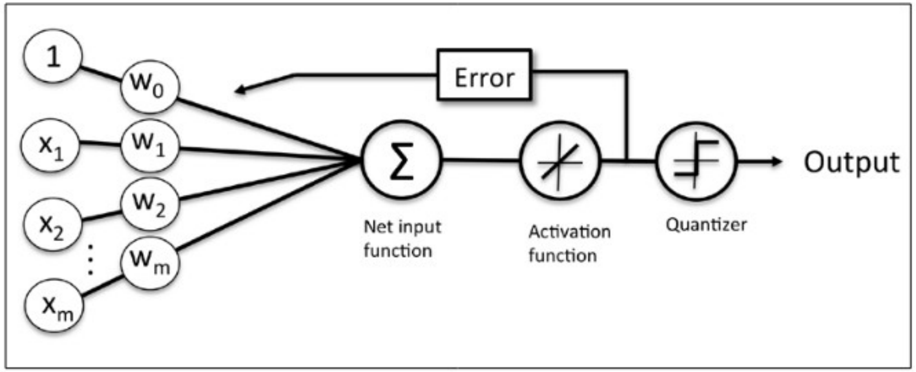
(p. 58: Raschka, 2015)

Comparison with ADALINE



(p. 58: Raschka, 2015)

$$\phi(z)=\frac{1}{1+e^{-z}}$$

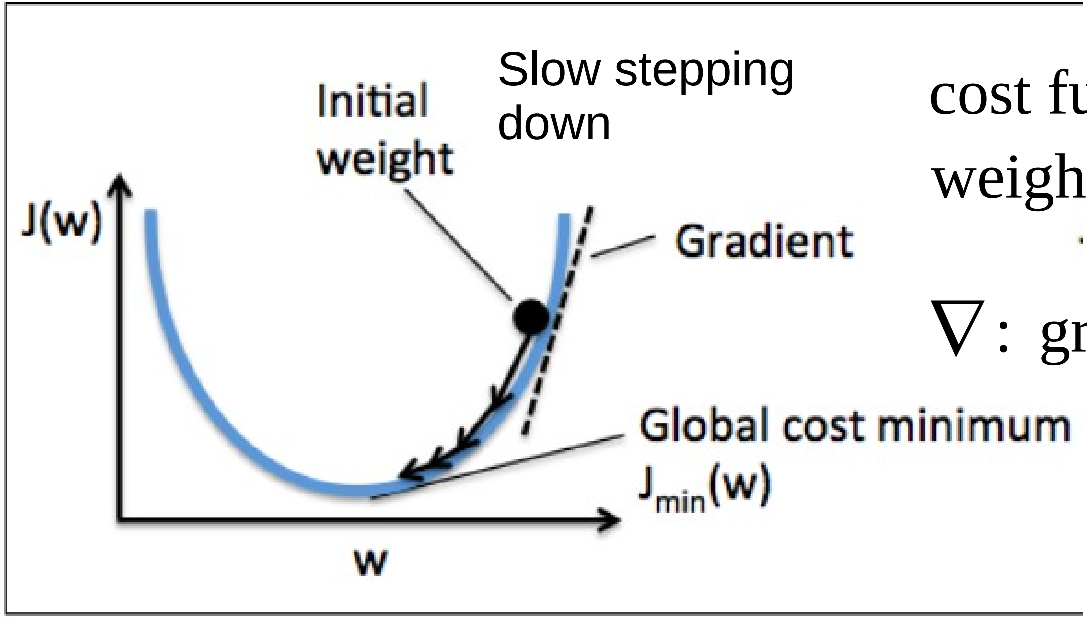


(p. 33: Raschka, 2015)

$$\phi(z)=z$$

Still updating with **Gradient Descent**

Gradient descent $\phi(z) = z$



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

weight change: $\Delta \boldsymbol{w} = -\eta \nabla J(\boldsymbol{w})$

∇: gradient (rate of change)

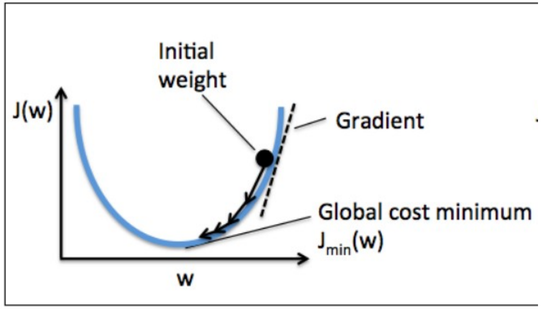
(p. 40: Raschka, 2015)

Gradient descent $\phi(z)=\frac{1}{1+e^{-z}}$

cost function: $J(w)=-\boxed{\sum_{i}^{n} y^{(i)}\log\left(\phi\left(z^{i}\right)\right)+\left(1-y^{(i)}\right)\log\left(1-\phi\left(z^{(i)}\right)\right)}$

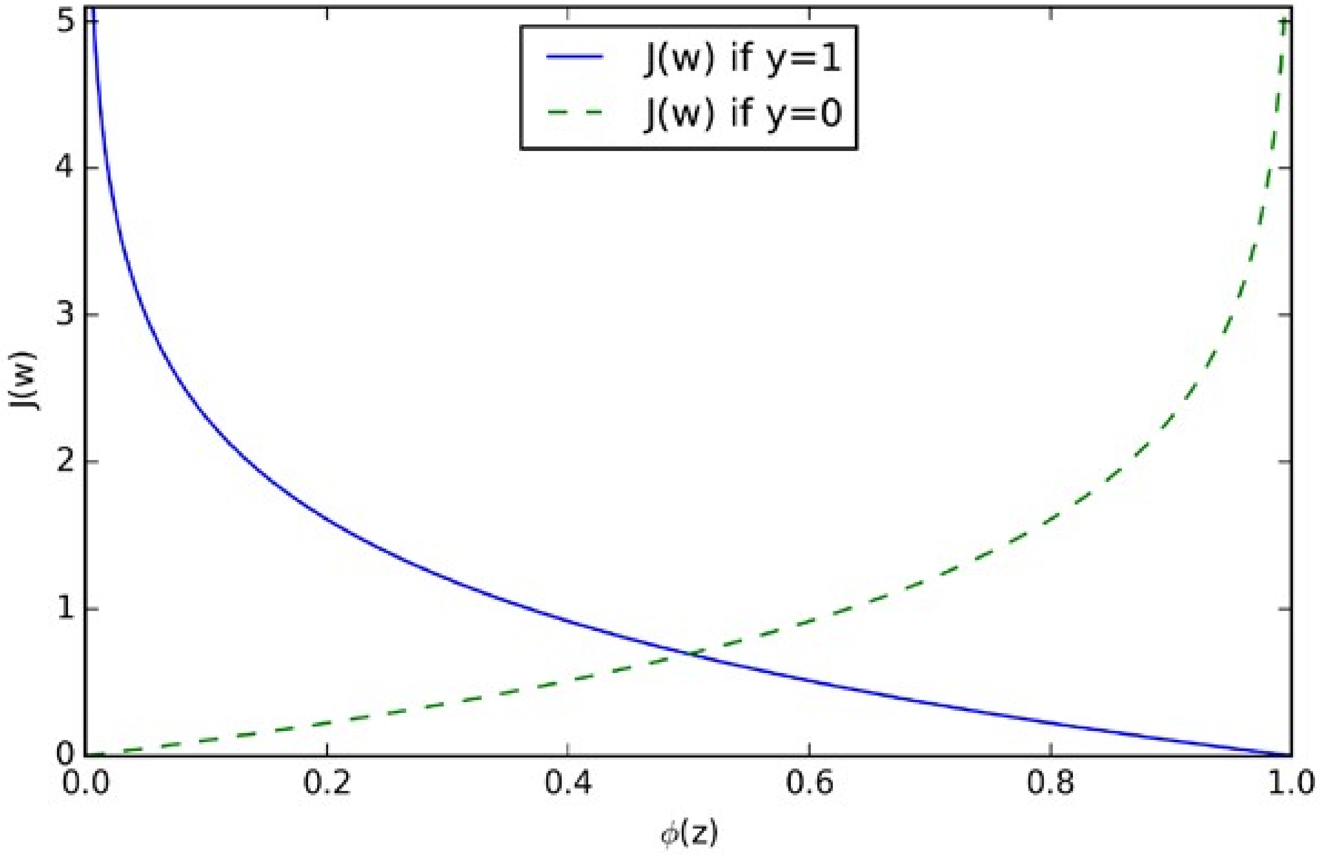
weight change: $\Delta w=-\eta\nabla J(w)$

What’s this part equal to?



(p. 40: Raschka, 2015)

A closer look at the cost function



(p. 61: Raschka, 2015)

A closer look at the updating of weights

$\Delta \boldsymbol{w} = -\eta \nabla J(\boldsymbol{w})$ This is common between ADALINE and Linear and Logistic Regression

but $J(\boldsymbol{w})$ is not the same across these different methods?!

A general formulation: $\Delta w_j = \eta \sum_{i}^{n} \left(y^{(i)} - \phi\left(z^{(i)}\right) \right) x_j^{(i)}$

It can be shown that: $\frac{\delta}{\delta w_j} l(\boldsymbol{w}) = \left(y - \phi(z) \right) x_j$

$\frac{\delta}{\delta w_j} l(\boldsymbol{w})$: (partial) derivative of log-likelihood function (proof on p. 64)

A clarification on ADALINE

$$\Delta w_j = \eta \sum_i^n \left(y^{(i)} - \phi\left(z^{(i)}\right)\right) x_j^{(i)}$$

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

```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.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
```

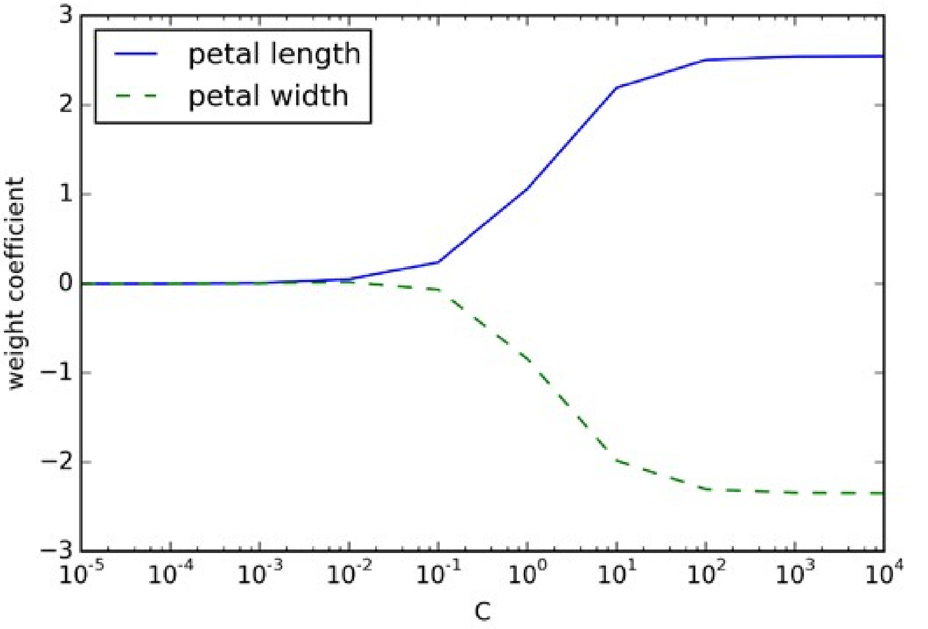
With regularisation

$$J(\boldsymbol{w}) = -\sum_{i}^{n} y^{(i)} \log\left(\phi\left(z^{(i)}\right)\right) + \left(1 - y^{(i)}\right) \log\left(1 - \phi\left(z^{(i)}\right)\right) + \frac{\lambda}{2} \|\boldsymbol{w}\|_2^2$$

NB! Regularisation in *sklearn.linear_model.LogisticRegression* is controlled by *C*

$$C = \frac{1}{\lambda}$$

Effect of *C* parameter



Now for the **classification**

score(*X*, *y*, *sample_weight=None*) [source]

Return the mean accuracy on the given test data and labels.

In multi-label classification, this is the subset accuracy which is a harsh metric since you require for each sample that each label set be correctly predicted.

Parameters:	**X** : ***array-like of shape (n_samples, n_features)*** Test samples. **y** : ***array-like of shape (n_samples,) or (n_samples, n_outputs)*** True labels for `X`. **sample_weight** : ***array-like of shape (n_samples,), default=None*** Sample weights.
Returns:	**score** : ***float*** Mean accuracy of `self.predict(X)` wrt. `y`.

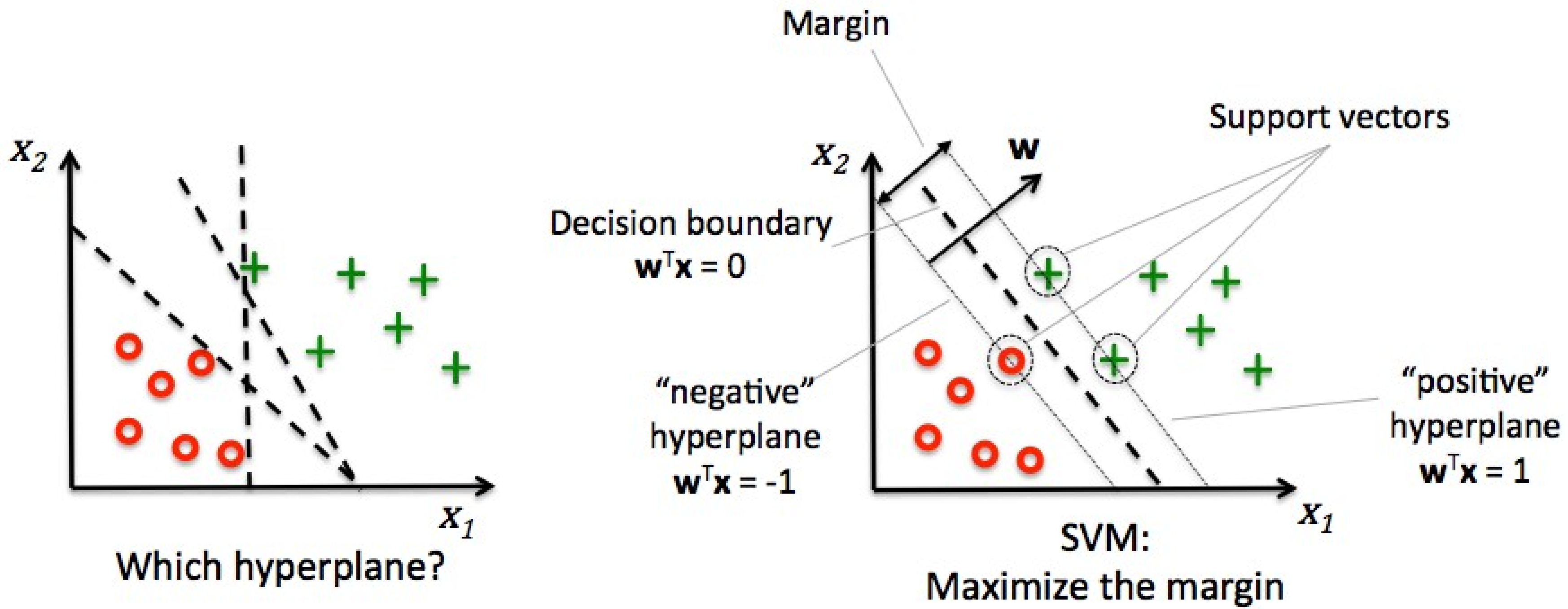
```
#%% LOGISTIC REGRESSION

from sklearn.linear_model import LogisticRegression
logR = LogisticRegression(penalty='none') # no regularisation
logR.fit(X_train_std, y_train)
print(logR.score(X_test_std, y_test))
```

Live coding

EXAMPLE_00

SUPPORT VECTOR MACHINES



(p. 69: Raschka, 2015)

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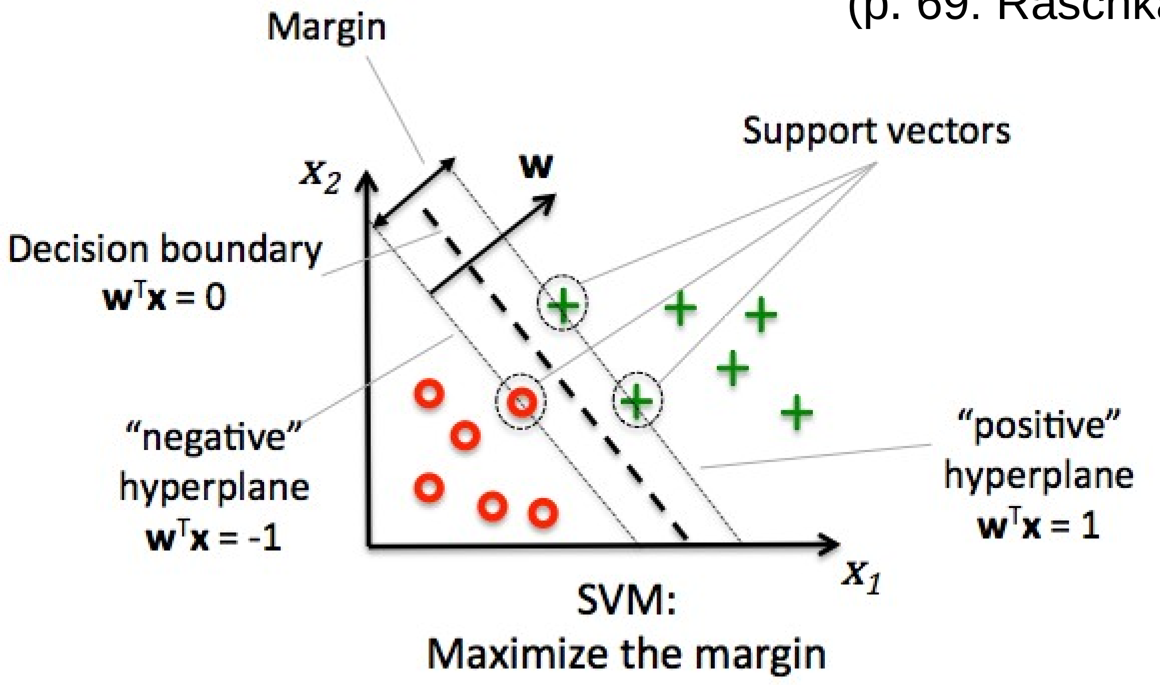


$$w_0 + \boldsymbol{w}^T \boldsymbol{x}_{\mathbf{pos}} = 1 \qquad (1)$$
$$w_0 + \boldsymbol{w}^T \boldsymbol{x}_{\mathbf{neg}} = -1 \qquad (2)$$

QUESTION: What is the subtraction of equation (2) from equation (1) equal to on the figure?

Subtraction

$$\boldsymbol{w}^T(\boldsymbol{x}_{\mathbf{pos}} - \boldsymbol{x}_{\mathbf{neg}}) = 2$$

normalizing by w's length: $\|\boldsymbol{w}\| = \sqrt{(\sum_{j=1}^{m} w_j^2)}$

... we get: $\boldsymbol{w}^T \frac{(\boldsymbol{x}_{\mathbf{pos}} - \boldsymbol{x}_{\mathbf{neg}})}{\|\boldsymbol{w}\|} = \frac{2}{\|\boldsymbol{w}\|}$

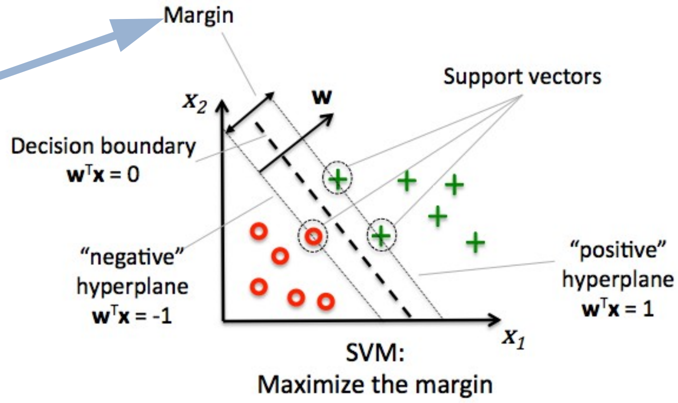
This will optimise the width of the margin

So we want to maximize: $\dfrac{2}{\|\boldsymbol{w}\|}$

under the constraints:

$$w_0 + \boldsymbol{w}^T \boldsymbol{x}^{(i)} \geq 1 \; if \; y^{(i)} = 1$$

$$w_0 + \boldsymbol{w}^T \boldsymbol{x}^{(i)} < -1 \; if \; y^{(i)} = -1$$



(p. 69: Raschka, 2015)

In practice, the following is minimized: $\dfrac{1}{2}\|\boldsymbol{w}\|^2$

This faces a problem that the **Perceptron** also faces

Which?

SOLUTION: introducing a *slack* variable ξ (xi)

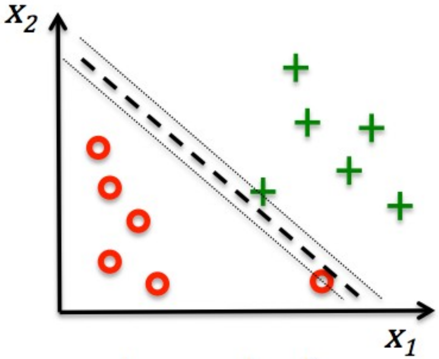
Introducing ξ

$$w_0 + \boldsymbol{w}^T \boldsymbol{x}_{\mathbf{pos}} = 1 - \xi^{(i)}$$
$$w_0 + \boldsymbol{w}^T \boldsymbol{x}_{\mathbf{neg}} = -1 + \xi^{(i)}$$

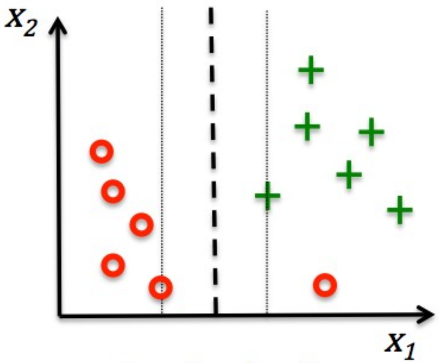
now we need to minimize: $\frac{1}{2}\|\boldsymbol{w}\|^2 + C\left(\sum_{i}^{n} \xi^{(i)}\right)$ (p. 72: Raschka, 2015)

to maximise the margin

Large *C*: narrow margin – penalises errors harshly
Small *C*: wide margin – penalises errors mildly

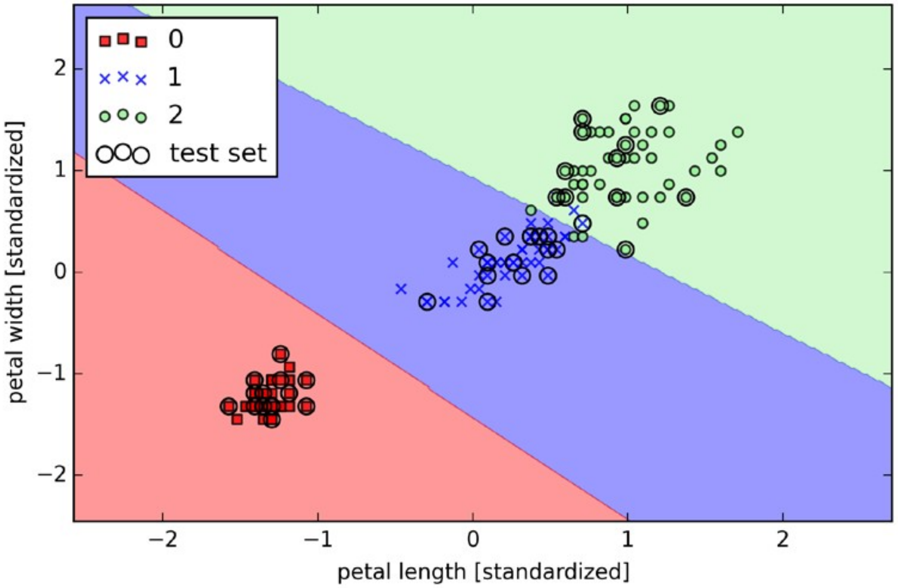


Large value for parameter *C*

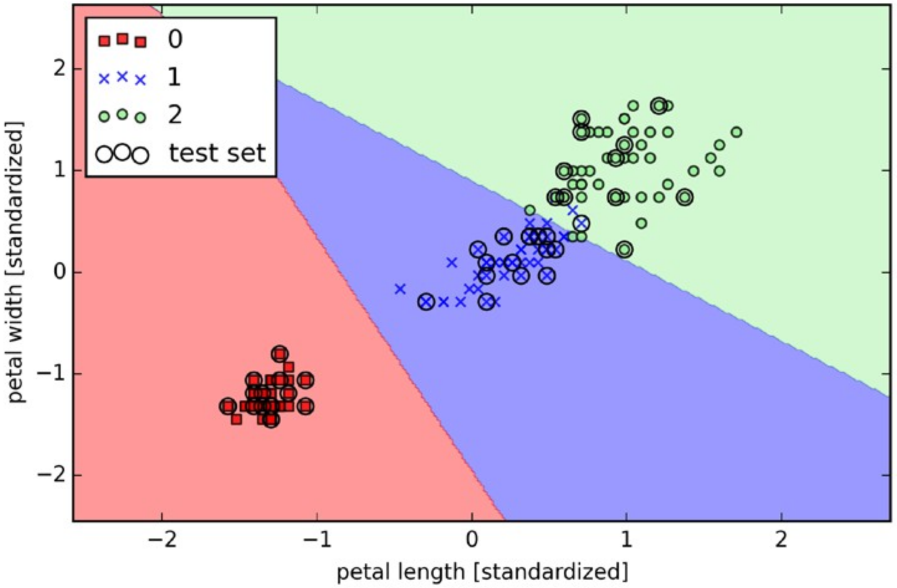


Small value for parameter *C*

Comparison to logistic regression



Support Vector Machine (p.763, Raschka 2015)



Logistic regression (p. 63, Raschka 2015)

Logistic regression versus SVM

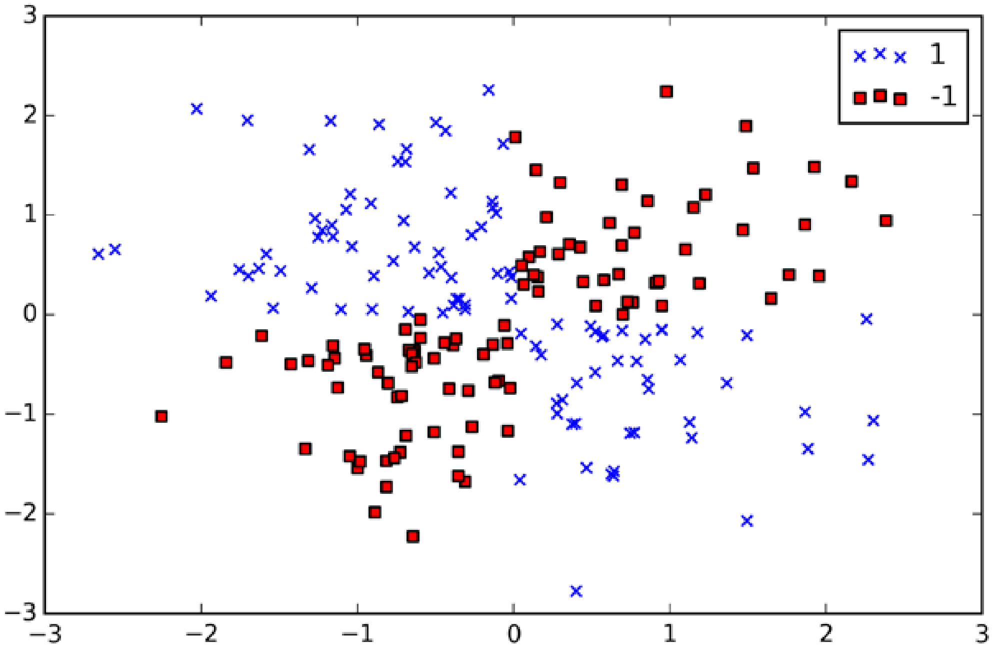
In practical classification tasks, linear logistic regression and linear SVMs often yield very similar results. Logistic regression tries to maximize the conditional likelihoods of the training data, which makes it more prone to outliers than SVMs. The SVMs mostly care about the points that are closest to the decision boundary (support vectors). On the other hand, logistic regression has the advantage that it is a simpler model that can be implemented more easily. Furthermore, logistic regression models can be easily updated, which is attractive when working with streaming data.

(p. 74: Raschka, 2015)

Live coding

EXAMPLE_00

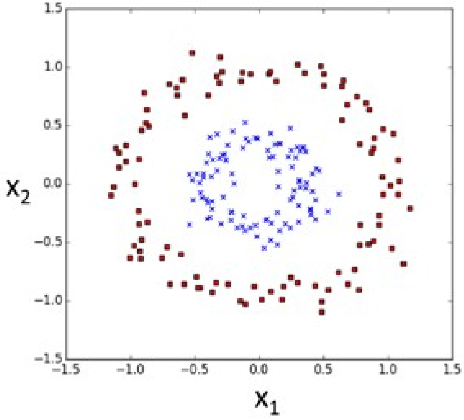
A brief look at a non-linear problem

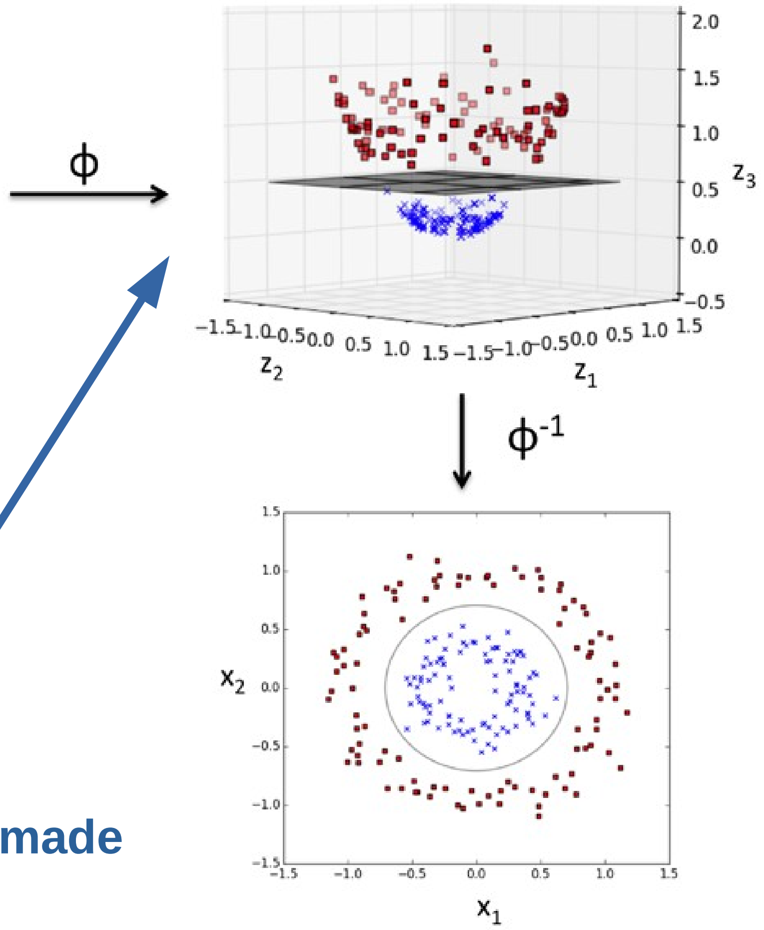


(p. 75: Raschka, 2015)

Map onto higher-dimensional space

$$\phi(\cdot)$$





$$\phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1, x_2, x_1^2 + x_2^2)$$

Note that a linear solution is made

$$\phi(x_1, x_2) = (z_1, z_2, z_3) = (x_1, x_2, \boxed{x_1^2 + x_2^2})$$

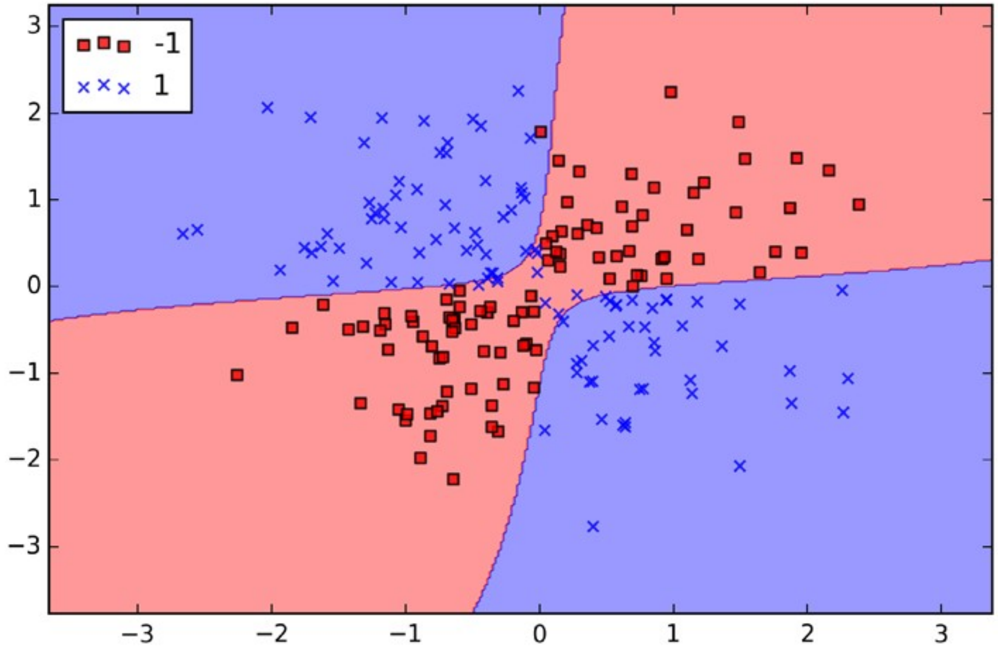
Creating the higher dimensions can be computationally expensive

$$k(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) = \phi(\boldsymbol{x}^{(i)})^T \phi(\boldsymbol{x}^{(j)})$$

$$k(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)}) = e^{\left(-\gamma \left\| \boldsymbol{x}^{(i)} - \boldsymbol{x}^{(j)} \right\|^2\right)}$$

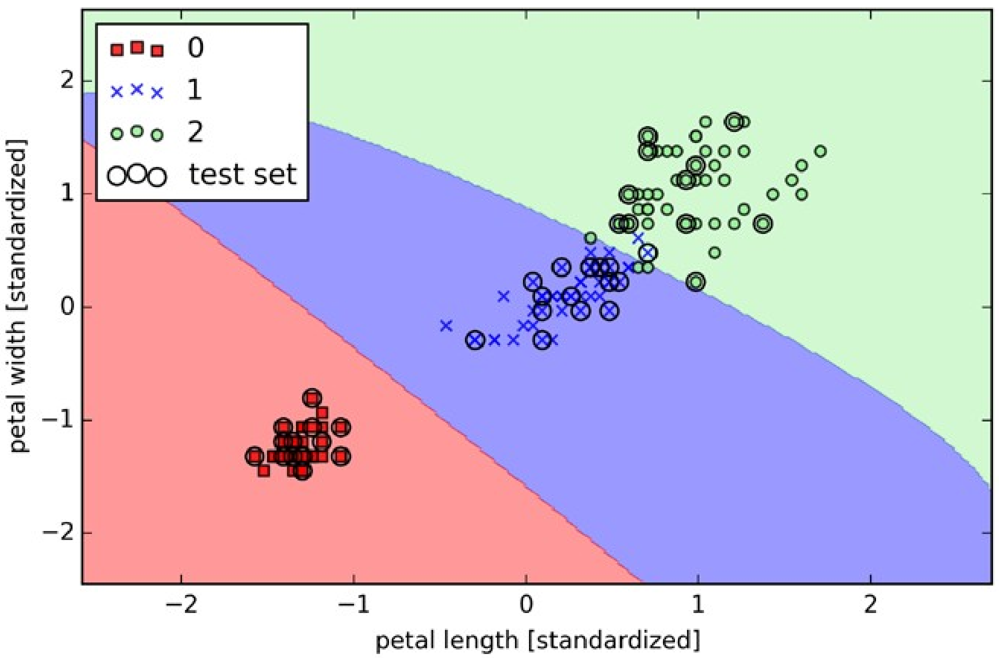
$$\left(\gamma = \frac{1}{2\sigma^2},\ \text{also called the precision}\right)$$

Non-linear decision boundaries



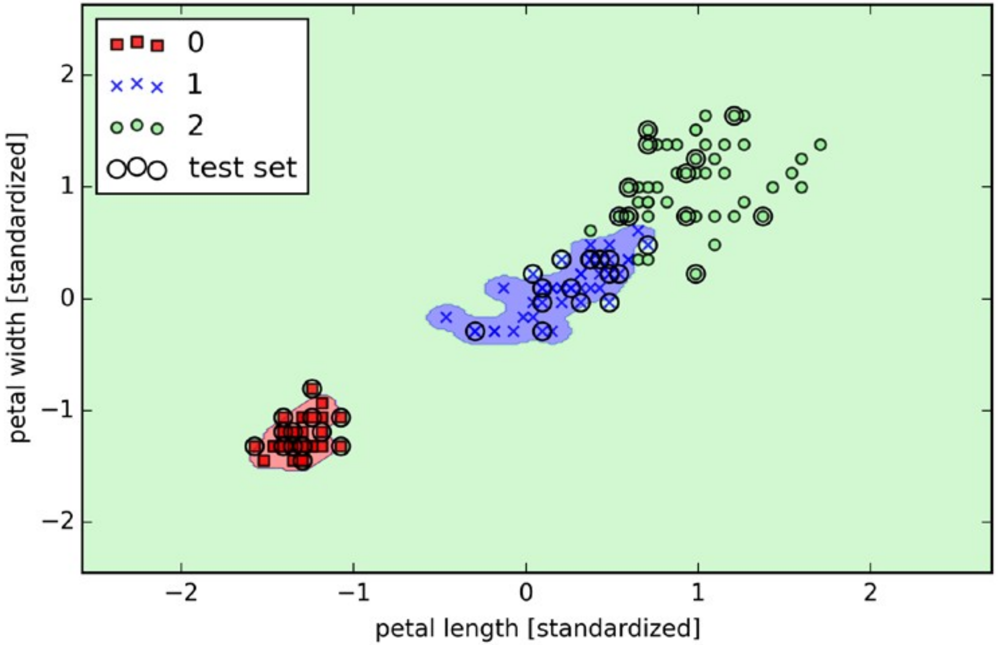
(p. 78: Raschka, 2015)

Low γ - soft boundary



(p. 79: Raschka, 2015)

High γ - tight boundary



(p. 80: Raschka, 2015)

Live coding

EXAMPLE_00

Did you learn?

Logistic regression (machine learning)

1) Understanding of how logistic regression can be adapted to a classification framework
2) Understanding the idea of a Support Vector Machine
3) Getting acquainted with how Support Vector Machines can solve non-linear problems

References

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