Lecture 8: Logistic regression

Estimating probabilities

Estimate the probability of an instance belonging to a particular class.

Can adapt linear regression algorithm for this purpose to perform *logistic regression*.

Sigmoid function

Consider linear weighted sum of inputs $\theta^{\mathrm{T}} x$ again but then apply sigmoid function σ:

$$\hat{p} = h_\theta(x) = \sigma(\theta^{\mathrm{T}} x),$$

where

$$\sigma(t) = \frac{1}{1 + \exp(-t)}.$$

Exercise: what is the domain and range of the sigmoid function?

$$\sigma(t) = \frac{1}{1 + \exp(-t)}$$

Exercise: what is the domain and range of the sigmoid function?

$$\sigma(t) = \frac{1}{1 + \exp(-t)}$$

Domain: $t \in (-\infty, \infty)$.

Range: $\sigma \in (0, 1)$.

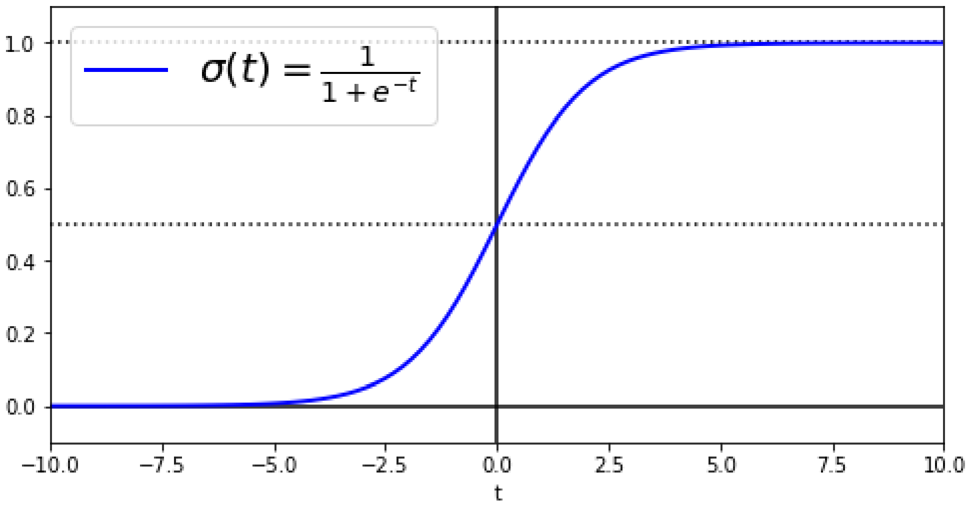
Exercise: plot the sigmoid function.

In [2]:

```
import numpy as np
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt
```

In [3]:

```
t = np.linspace(-10, 10, 100)
sig = 1 / (1 + np.exp(-t))
plt.figure(figsize=(8, 4))
plt.plot([-10, 10], [0, 0], "k-")
plt.plot([-10, 10], [0.5, 0.5], "k:")
plt.plot([-10, 10], [1, 1], "k:")
plt.plot([0, 0], [-1.1, 1.1], "k-")
plt.plot(t, sig, "b-", linewidth=2, label=r"$\sigma(t) = \frac{1}{1 + e^{-t}}$")
plt.xlabel("t")
plt.legend(loc="upper left", fontsize=20)
plt.axis([-10, 10, -0.1, 1.1]);
```



Predictions

Can then make class predictions depending on whether the predicted probability $\hat{p}$ is greater than 0.5, i.e.

$$\hat{y} = \begin{cases} 0, & \text{if } \hat{p} < 0.5 \\ 1, & \text{if } \hat{p} \geq 0.5 \end{cases},$$

where we recall

$$\hat{p} = h_\theta(x) = \sigma(\theta^{\mathrm{T}} x) \quad \text{and} \quad \sigma(t) = \frac{1}{1 + \exp(-t)}.$$

Predictions

Can then make class predictions depending on whether the predicted probability $\hat{p}$ is greater than 0.5, i.e.

$$\hat{y} = \begin{cases} 0, & \text{if } \hat{p} < 0.5, \\ 1, & \text{if } \hat{p} \geq 0.5 \end{cases}$$

where we recall

$$\hat{p} = h_\theta(x) = \sigma(\theta^T x) \quad \text{and} \quad \sigma(t) = \frac{1}{1 + \exp(-t)}.$$

Note that $\sigma(t) < 0.5$ when $t < 0$ and $\sigma(t) \geq 0.5$ when $t \geq 0$.

That is, logistic regression predicts model 1 when $\theta^T x$ is positive, and model 0 when it is negative.

The decision boundary is defined by $\theta^T x = 0$.

Cost functions

Consider the cost function:

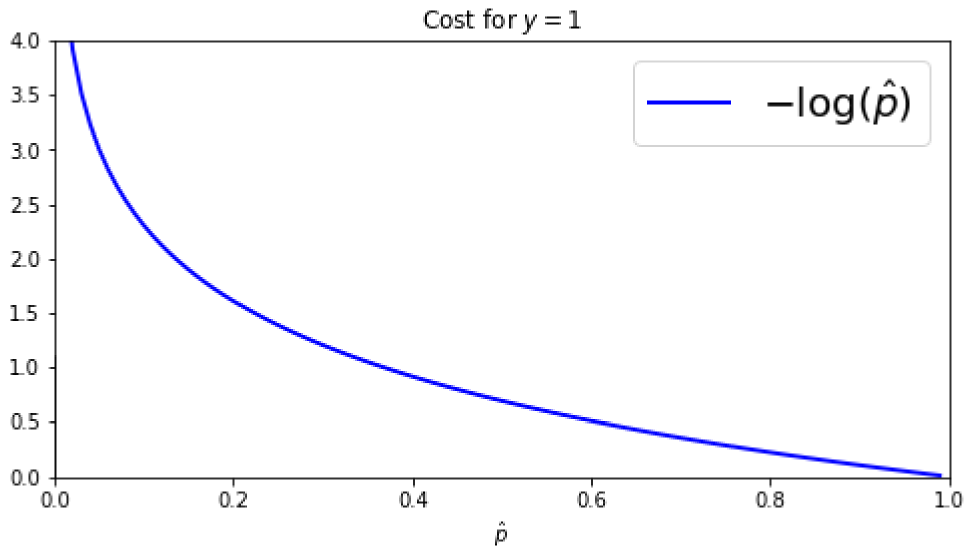
$$C(\theta) = \begin{cases} -\log(\hat{p}), & \text{if } y = 1 \\ -\log(1-\hat{p}), & \text{if } y = 0 \end{cases}.$$

Exercise: plot the cost function for $\mathbf{y} = \mathbf{1}$ as a function of $\hat{\mathbf{p}}$.

Exercise: plot the cost function for y = 1 as a function of p.

In [4]:

```
ph = np.linspace(0.01, 0.99, 100)
cost_one = -np.log(ph)
plt.figure(figsize=(8, 4))
plt.plot([0, 0], [-1.1, 1.1], "k-")
plt.plot(ph, cost_one, "b-", linewidth=2, label=r"$-\log{(\hat{p})}$")
plt.xlabel("$\hat{p}$")
plt.legend(loc="upper right", fontsize=20)
plt.axis([0, 1, 0, 4]);
plt.title('Cost for $y=1$');
```



What can you say intuitively about the cost function?

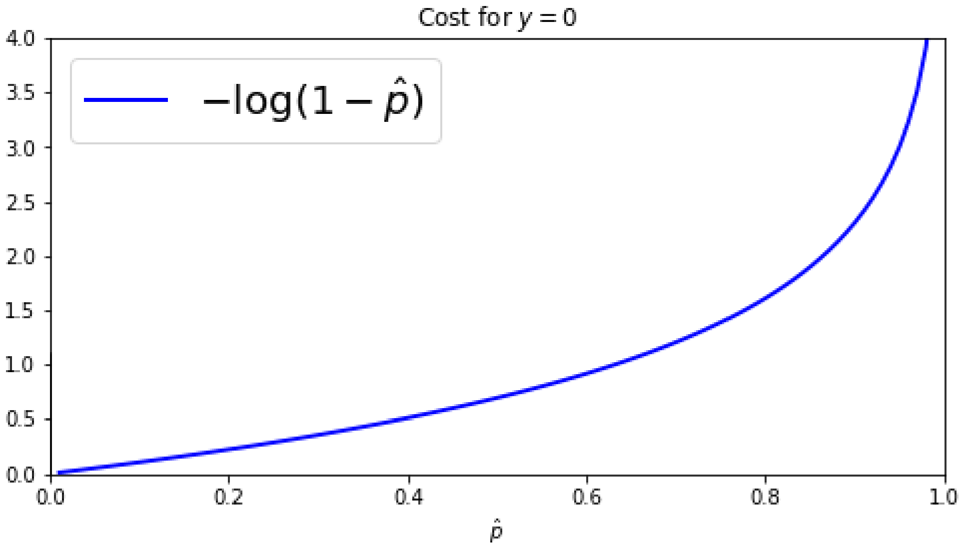
What can you say intuitively about the cost function?

- For $\hat{p} = 1, C(\hat{p}) = 0$.
- For $\hat{p} = 0, C(\hat{p}) \to \infty$.

Exercise: plot the cost function for $\mathbf{y} = \mathbf{0}$ as a function of $\hat{\mathbf{p}}$.

Exercise: plot the cost function for y = 0 as a function of p.

In [5]:
```
cost_zero = -np.log(1-ph)
plt.figure(figsize=(8, 4))
plt.plot([0, 0], [-1.1, 1.1], "k-")
plt.plot(ph, cost_zero, "b-", linewidth=2, label=r"$-\log{(1-\hat{p})}$")
plt.xlabel("$\hat{p}$")
plt.legend(loc="upper left", fontsize=20)
plt.axis([0, 1, 0, 4]);
plt.title('Cost for $y=0$');
```



What can you say intuitively about the cost function?

What can you say intuitively about the cost function?

- For $\hat{p} = 0$, $C(\hat{p}) = 0$.
- For $\hat{p} = 1$, $C(\hat{p}) \to \infty$.

Log-loss function for logistic regression

Cost function can be written by the single expression

$$C(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(\hat{p}^{(i)}) + (1-y^{(i)})\log(1-\hat{p}^{(i)})\right],$$

since $y^{(i)}$ is always 0 or 1 and we thus recover the separate cases considered above.

Log-loss function for logistic regression

Cost function can be written by the single expression

$$C(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(\hat{p}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{p}^{(i)})\right],$$

since $y^{(i)}$ is always 0 or 1 and we thus recover the separate cases considered above.

Aside: statistical interpretation

Interpret p as probability of target y:

$$P(y \mid p) = p^{y}(1 - p)^{1-y}\log P(y \mid p, x) = y\log(p) + (1 - y)\log(1 - p)$$

See [MacKay (http://www.inference.org.uk/itila/book.html)](http://www.inference.org.uk/itila/book.html) [Chapter 41] for further details.

Minimising the cost function

No closed form solution like linear regression.

But since the cost function is convex guaranteed to find global minimum by gradient descent.

Derivative of the cost function

$$
\begin{aligned}
\frac{\partial C}{\partial \theta} &= \frac{1}{m} \sum_{i=1}^{m} \left[\sigma\left(\theta^{\mathrm{T}} x^{(i)}\right) - y^{(i)}\right] x^{(i)} \\
&= \frac{1}{m} X^{\mathrm{T}} \left[\sigma\left(X\theta\right) - y\right] \\
&= \frac{1}{m} X^{\mathrm{T}} \left[h_{\theta}\left(X\right) - y\right]
\end{aligned}
$$

Similarity with linear regression

Identical to linear regression (up to factor of 2 depending on conventions adopted) but with a different prediction function:

$$h_\theta(x) = \sigma(\theta^{\mathrm{T}} x),$$

instead of

$$h_\theta(x) = \theta^{\mathrm{T}} x.$$

Example of logistic regression

Consider [Iris flower data (https://en.wikipedia.org/wiki/Iris_flower_data_set)](https://en.wikipedia.org/wiki/Iris_flower_data_set) again.

In [6]:
```
from sklearn import datasets
iris = datasets.load_iris()
list(iris.keys())
```

Out[6]:
```
['DESCR', 'target_names', 'data', 'target', 'feature_names']
```

Train model

Use petal width to classify whether Virginica or not.

In [7]:
```
# Set up training data
X_1d = iris["data"][:, 3:]  # petal width
y = (iris["target"] == 2).astype(np.int)  # 1 if Iris-Virginica, else 0
```

In [8]:
```
from sklearn.linear_model import LogisticRegression
log_reg = LogisticRegression(random_state=42)
log_reg.fit(X_1d, y)
```

Out[8]:
```
LogisticRegression(C=1.0, class_weight=None, dual=False, fit_intercept=True,
          intercept_scaling=1, max_iter=100, multi_class='ovr', n_jobs=1,
          penalty='l2', random_state=42, solver='liblinear', tol=0.0001,
          verbose=0, warm_start=False)
```

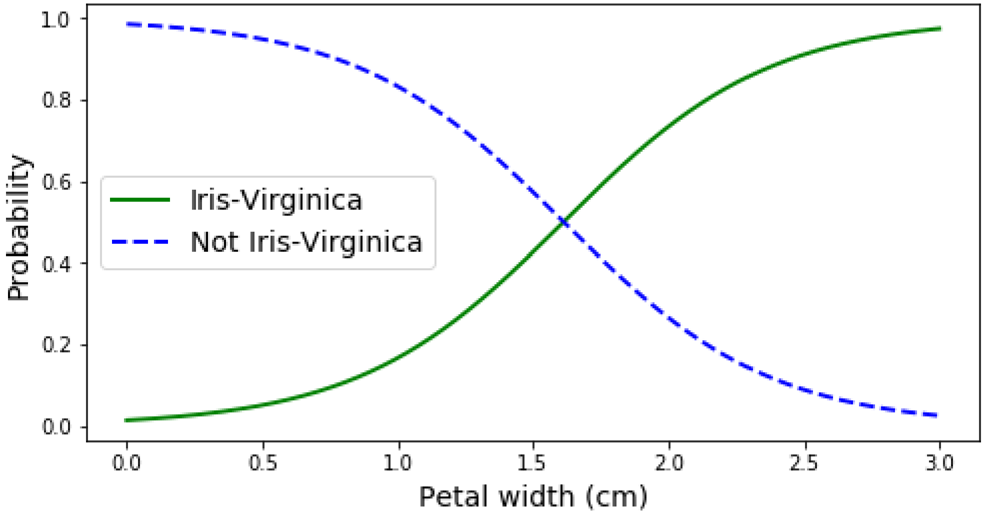
Note that Scikit-Learn automatically adds ℓ_2 regularizer to cost function.

Prediction

In [9]:
```
X_1d_new = np.linspace(0, 3, 1000).reshape(-1, 1)
y_1d_proba = log_reg.predict_proba(X_1d_new)

plt.figure(figsize=(8,4))
plt.plot(X_1d_new, y_1d_proba[:, 1], "g-", linewidth=2, label="Iris-Virginica")
plt.plot(X_1d_new, y_1d_proba[:, 0], "b--", linewidth=2, label="Not Iris-Virginic
a")
plt.xlabel("Petal width (cm)", fontsize=14)
plt.ylabel("Probability", fontsize=14)
plt.legend(loc="center left", fontsize=14)
```

Out[9]:
```
<matplotlib.legend.Legend at 0x1a184e3cf8>
```



Decision boundary

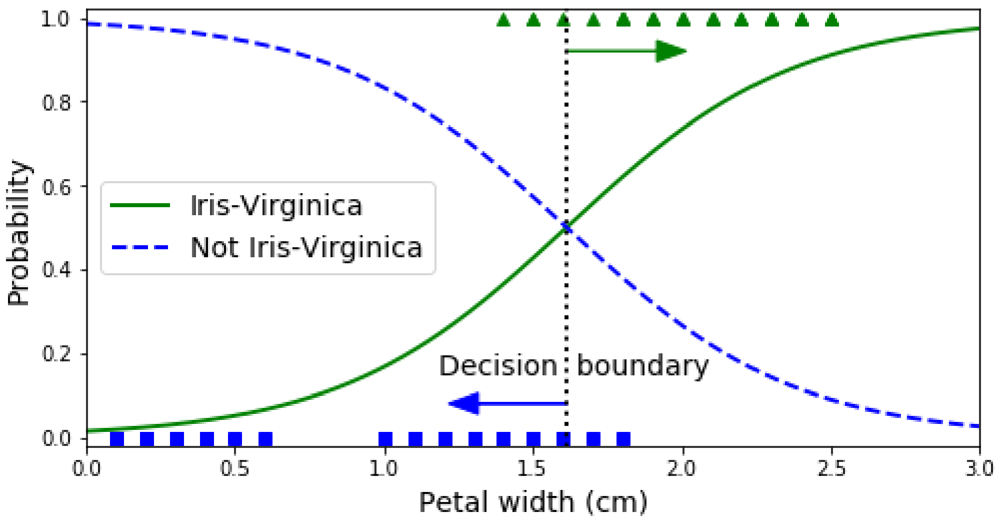
Recall the decision boundary is given by $\hat{p} = 0.5$ or, equivalently, $\theta^\mathrm{T} x = 0$.

In [10]:
```
decision_boundary = X_1d_new[y_1d_proba[:, 1] >= 0.5][0]
decision_boundary
```

Out[10]:
```
array([1.61561562])
```

Updating plot with decision boundary and training data

In [11]:
```
plt.figure(figsize=(8, 4))
plt.plot(X_1d[y==0], y[y==0], "bs")
plt.plot(X_1d[y==1], y[y==1], "g^")
plt.plot([decision_boundary, decision_boundary], [-1, 2], "k:", linewidth=2)
plt.plot(X_1d_new, y_1d_proba[:, 1], "g-", linewidth=2, label="Iris-Virginica")
plt.plot(X_1d_new, y_1d_proba[:, 0], "b--", linewidth=2, label="Not Iris-Virginic
a")
plt.text(decision_boundary+0.02, 0.15, "Decision  boundary", fontsize=14, color=
"k", ha="center")
plt.arrow(decision_boundary, 0.08, -0.3, 0, head_width=0.05, head_length=0.1, fc=
'b', ec='b')
plt.arrow(decision_boundary, 0.92, 0.3, 0, head_width=0.05, head_length=0.1, fc=
'g', ec='g')
plt.xlabel("Petal width (cm)", fontsize=14)
plt.ylabel("Probability", fontsize=14)
plt.legend(loc="center left", fontsize=14)
plt.axis([0, 3, -0.02, 1.02]);
```



Predictions depend on what side of decision boundary fall.

In [12]:

```
log_reg.predict([[1.7], [1.5]])
```

Out[12]:

```
array([1, 0])
```

Extending to two features

In [13]:

```
from sklearn.linear_model import LogisticRegression

X = iris["data"][:, (2, 3)]  # petal length, petal width
y = (iris["target"] == 2).astype(np.int)  # 1 if Iris-Virginica, else 0

C = 1000 # inverse regularization (smaller values correspond to stronger regulariz
ation)
log_reg = LogisticRegression(C=C, random_state=42)
log_reg.fit(X, y)

x0, x1 = np.meshgrid(
        np.linspace(2.9, 7, 500).reshape(-1, 1),
        np.linspace(0.8, 2.7, 200).reshape(-1, 1),
    )
X_new = np.c_[x0.ravel(), x1.ravel()]

y_proba = log_reg.predict_proba(X_new)
```

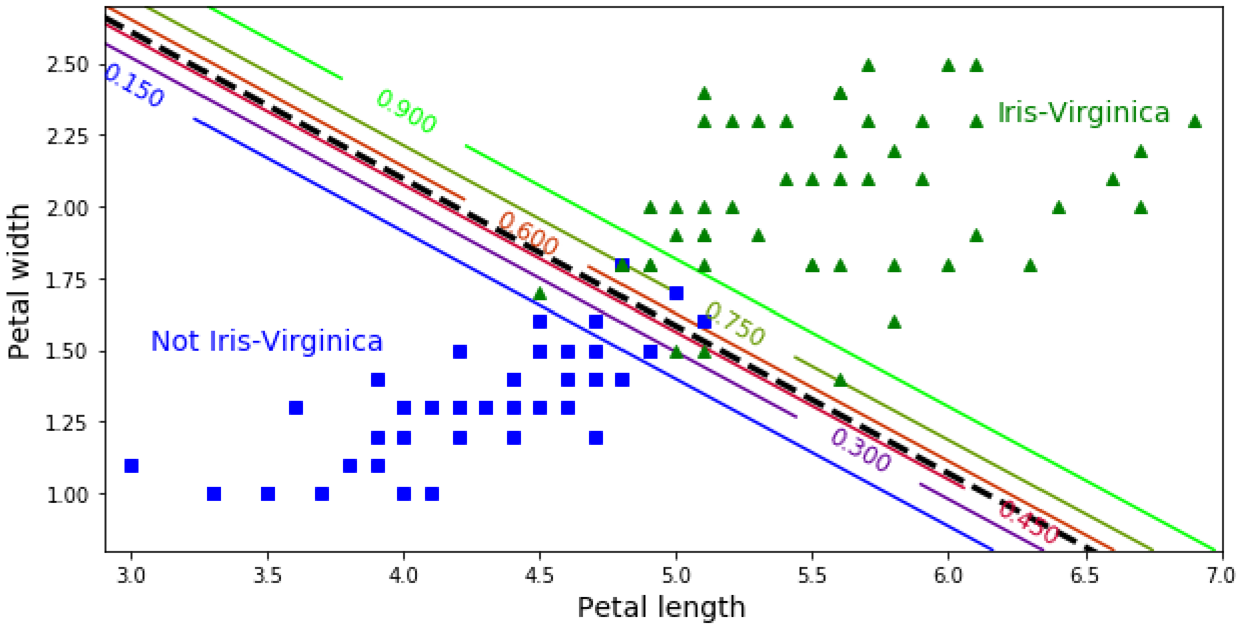
In [14]:

```
plt.figure(figsize=(10, 5))
plt.plot(X[y==0, 0], X[y==0, 1], "bs")
plt.plot(X[y==1, 0], X[y==1, 1], "g^")

zz = y_proba[:, 1].reshape(x0.shape)
contour = plt.contour(x0, x1, zz, cmap=plt.cm.brg)

# Solve theta^T x = 0 to determine boundary
left_right = np.array([2.9, 7])
boundary = -(log_reg.coef_[0][0] * left_right + log_reg.intercept_[0]) / log_reg.c
oef_[0][1]

plt.clabel(contour, inline=1, fontsize=12)
plt.plot(left_right, boundary, "k--", linewidth=3)
plt.text(3.5, 1.5, "Not Iris-Virginica", fontsize=14, color="b", ha="center")
plt.text(6.5, 2.3, "Iris-Virginica", fontsize=14, color="g", ha="center")
plt.xlabel("Petal length", fontsize=14)
plt.ylabel("Petal width", fontsize=14)
plt.axis([2.9, 7, 0.8, 2.7]);
```



Petal width
Petal length
Iris-Virginica
Not Iris-Virginica
0.150
0.300
0.450
0.600
0.750
0.900
2.50
2.25
2.00
1.75
1.50
1.25
1.00
3.0
3.5
4.0
4.5
5.0
5.5
6.0
6.5
7.0

Softmax regression

Can generalise logistic regression to classify multiple classes.

Softmax score

Consider the softmax score function for class k:

$$s_k(x) = \left(\theta^{(k)}\right)^{\mathrm{T}} x.$$

Softmax score

Consider the softmax score function for class k:

$$s_k(x) = \left(\theta^{(k)}\right)^T x.$$

Important note: each class k has its own score and set of parameters $\theta^{(k)}$, for K classes (i.e. $k = 1, \ldots, K$).

Define:

- Parameter matrix: $\Theta_{K \times n} = [\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(K)}]^T$.

Softmax function

Predictions are then given by the softmax function $\sigma_k(s(x))$ for each k:

$$\hat{p}_k = \sigma_k(s(x)) = \frac{\exp(s_k(x))}{\sum_{k'=1}^{K} \exp\left(s_{k'}(x)\right)}.$$

Softmax function

Predictions are then given by the softmax function $\sigma_k(s(x))$ for each k:

$$\hat{p}_k = \sigma_k(s(x)) = \frac{\exp\left(s_k(x)\right)}{\sum_{k'=1}^{K'} \exp\left(s_k{}'(x)\right)}.$$

Normalised such that

- $\sum_k \hat{p}_k = 1$
- $0 \leq \hat{p}_k \leq 1$

Predictions

Can then make class predictions based on which class has the highest predicted probability, i.e.

$$\hat{y} = \arg\max_k \hat{p}_k = \arg\max_k s_k(x) = \arg\max_k \left(\theta^{(k)}\right)^{\mathrm{T}} x,$$

where we recall

$$\hat{p}_k = \sigma_k(s(x)) = \frac{\exp(s_k(x))}{\sum_{k'=1}^{K} \exp\left(s_{k'}(x)\right)} \quad \text{and} \quad s_k(x) = \left(\theta^{(k)}\right)^{\mathrm{T}} x.$$

Cost function

Generalization of the logistic regression cost function is given by the *cross-entropy* (measure of similarity of probability distributions):

$$C(\Theta) = -\frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{K} y_k^{(i)} \log\left(\hat{p}_k^{(i)}\right).$$

Cost function

Generalization of the logistic regression cost function is given by the *cross-entropy* (measure of similarity of probability distributions):

$$C(\Theta) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{K} y_k^{(i)}\log\left(\hat{p}_k^{(i)}\right).$$

For the case $K = 2$, the cost functions reduces to the standard cost function for logistic regression.

Minimising the cost function

Can solve by gradient descent.

Derivative of cost function given by

$$\frac{\partial C}{\partial \theta^{(k)}} = \frac{1}{m} \sum_{i=1}^{m} \left(\hat{p}_k^{(i)} - y_k^{(i)} \right) x^{(i)}.$$

Example of softmax regression

In [15]:
```
X = iris["data"][:, (2, 3)]  # petal length, petal width
y = iris["target"] # consider all three target classes

C = 10
softmax_reg = LogisticRegression(multi_class="multinomial", solver="lbfgs", C=C, r
andom_state=42)
softmax_reg.fit(X, y)
```

Out[15]:
```
LogisticRegression(C=10, class_weight=None, dual=False, fit_intercept=True,
          intercept_scaling=1, max_iter=100, multi_class='multinomial',
          n_jobs=1, penalty='l2', random_state=42, solver='lbfgs',
          tol=0.0001, verbose=0, warm_start=False)
```

In [16]:

```
x0, x1 = np.meshgrid(
        np.linspace(0, 8, 500).reshape(-1, 1),
        np.linspace(0, 3.5, 200).reshape(-1, 1),
    )
X_new = np.c_[x0.ravel(), x1.ravel()]

y_proba = softmax_reg.predict_proba(X_new)
y_predict = softmax_reg.predict(X_new)

# Select contours to plot
# zz1 = y_proba[:, 0].reshape(x0.shape)
zz1 = y_proba[:, 1].reshape(x0.shape)
# zz1 = y_proba[:, 2].reshape(x0.shape)
zz = y_predict.reshape(x0.shape)
```

In [17]:

```
plt.figure(figsize=(10, 5))
plt.plot(X[y==2, 0], X[y==2, 1], "g^", label="Iris-Virginica")
plt.plot(X[y==1, 0], X[y==1, 1], "bs", label="Iris-Versicolor")
plt.plot(X[y==0, 0], X[y==0, 1], "yo", label="Iris-Setosa")

from matplotlib.colors import ListedColormap
custom_cmap = ListedColormap(['#fafab0','#9898ff','#a0faa0'])

plt.contourf(x0, x1, zz, cmap=custom_cmap)
contour = plt.contour(x0, x1, zz1, cmap=plt.cm.brg)
plt.clabel(contour, inline=1, fontsize=12)
plt.xlabel("Petal length", fontsize=14)
plt.ylabel("Petal width", fontsize=14)
plt.legend(loc="center left", fontsize=14)
plt.axis([0, 7, 0, 3.5]);
```