Lecture 9: Support vector machines (SVMs)

Large margin classification

Logistic regression with Hinge loss

Recall cost function for logistic regression, with ℓ_2 regularisation, is given by

$$C(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log(\hat{p}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{p}^{(i)}) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2 ,$$

where

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

Logistic regression with Hinge loss

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where

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

Recall, the bias θ_0 is not regularised, i.e. sum over j starts at 1.

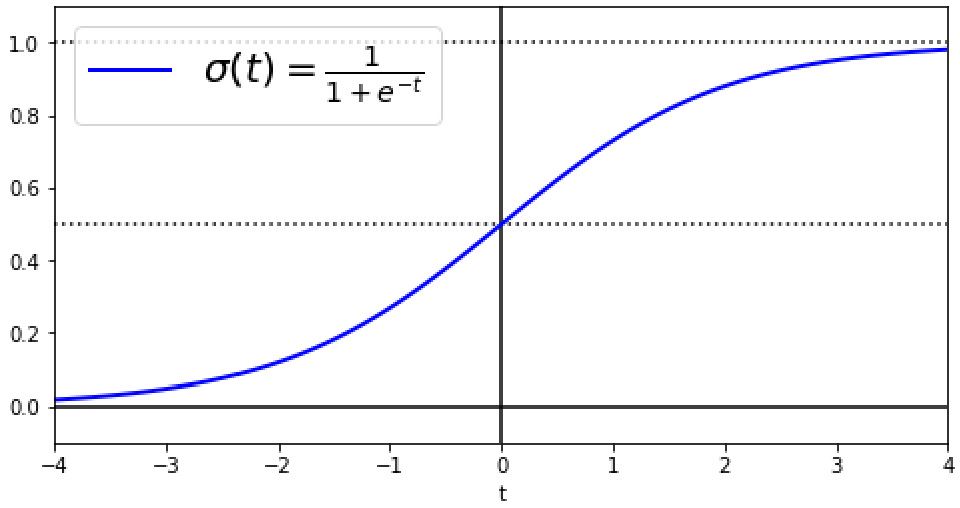
Plot sigmoid

In [2]:

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

In [3]:

```
t = np.linspace(-4, 4, 100)
sig = 1 / (1 + np.exp(-t))
plt.figure(figsize=(8, 4))
plt.plot([-4, 4], [0, 0], "k-")
plt.plot([-4, 4], [0.5, 0.5], "k:")
plt.plot([-4, 4], [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([-4, 4, -0.1, 1.1]);
```



Hinge loss

Logistic regression cost function for reference:

$$C(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(\hat{p}^{(i)}) + (1-y^{(i)})\log(1-\hat{p}^{(i)})\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2 .$$

Hinge loss

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Positive training instances

For $y^{(i)} = 1$, replace cost $-\log(\sigma(\theta^T x))$ with *hinge loss* $\max(1 - \theta^T x, 0)$.

For training, we want not just $\theta^T x \geq 0$ but $\theta^T x \geq 1$.

Exercise: plot cost $-\log(\sigma(\theta^T x))$ and hinge loss $\max(1-\theta^T x, 0)$.

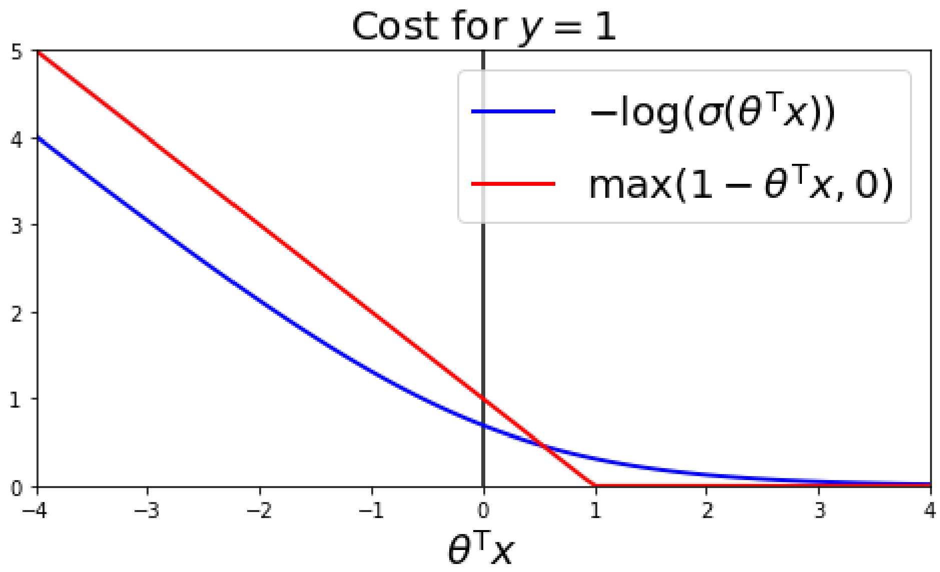
Exercise: plot cost $-\log(\boldsymbol{\sigma}(\boldsymbol{\theta}^T x))$ and hinge loss $\max(1 - \boldsymbol{\theta}^T x, 0)$.

In [4]:

```
cost_one = -np.log(sig)
cost_one_hinge = np.maximum(1 - t, np.zeros(t.size))
```

In [5]:

```
plt.figure(figsize=(8, 4))
plt.plot([0, 0], [0, 5], "k-")
plt.plot(t, cost_one, "b-", linewidth=2, label=r"$-\log{(\sigma(\theta^{\rm T}
 x))}$")
plt.xlabel(r"$\theta^{\rm T} x$", fontsize=20)
plt.axis([-4, 4, 0, 5]);
plt.title('Cost for $y=1$', fontsize=20)
plt.plot(t, cost_one_hinge, "r-", linewidth=2, label=r"$\max(1-\theta^{\rm T} x,
 0)$")
plt.legend(loc="upper right", fontsize=20);
```



Logistic regression cost function for reference:

$$C(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log(\hat{p}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{p}^{(i)}) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2 .$$

Logistic regression cost function for reference:

$$C(\theta) = -\frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(\hat{p}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{p}^{(i)})\right] + \frac{\lambda}{2m}\sum_{j=1}^{n}\theta_j^2.$$

Negative training instances

For $y^{(i)} = 0$, replace $-\log(1 - \sigma(\theta^T x))$ with *hinge loss* $\max(1 + \theta^T x, 0)$.

For training, we want not just $\theta^T x < 0$ but $\theta^T x \leq -1$.

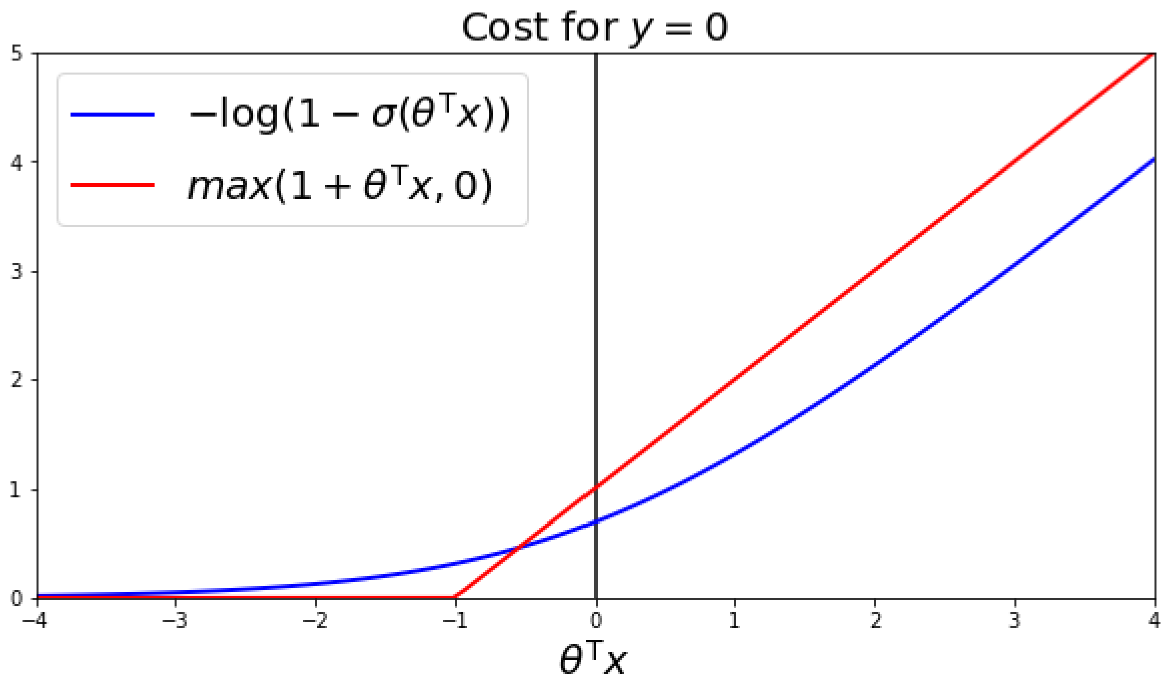
Exercise: plot cost $-\log(1-\sigma(\theta^T x))$ and hinge loss $\max(1+\theta^T x, 0)$.

Exercise: plot cost $-\log(1 - \sigma(\theta^T x))$ and hinge loss $\max(1 + \theta^T x, 0)$.

In [6]:
```
cost_zero = -np.log(1-sig)
cost_zero_hinge = np.maximum(1 + t, np.zeros(t.size))
```

In [7]:

```
plt.figure(figsize=(10, 5))
plt.plot([0, 0], [0, 5], "k-")
plt.plot(t, cost_zero, "b-", linewidth=2, label=r"$-\log{(1-\sigma(\theta^{\rm T}
 x))}$")
plt.xlabel(r"$\theta^{\rm T} x$", fontsize=20)
plt.axis([-4, 4, 0, 5]);
plt.title('Cost for $y=0$', fontsize=20);
plt.plot(t, cost_zero_hinge, "r-", linewidth=2, label=r"$max(1+\theta^{\rm T} x,
 0)$")
plt.legend(loc="upper left", fontsize=20);
```



Replace costs with hinge loss functions

Recall logistic regression with ℓ_2 regularisation cost function is given by

$$C(\theta) = -\frac{1}{m} \sum_{i=1}^{m} \left[y^{(i)} \log(\hat{p}^{(i)}) + (1 - y^{(i)}) \log(1 - \hat{p}^{(i)}) \right] + \frac{\lambda}{2m} \sum_{j=1}^{n} \theta_j^2 .$$

Replace costs for $y^{(i)} = 1$ and $y^{(i)} = 0$ with hinge losses given above:

$$\min_{\theta} \sum_{i=1}^{m} \left[y^{(i)} \max(1 - \theta^{\mathrm{T}} x^{(i)}, 0) + (1 - y^{(i)}) \max(1 + \theta^{\mathrm{T}} x^{(i)}, 0) \right] + \frac{\lambda}{2} \sum_{j=1}^{n} \theta_j^2 .$$

Introduce $k^{(i)} = 1$ for positive instances ($y^{(i)} = 1$) and $k^{(i)} = -1$ for negative instances ($y^{(i)} = 0$):

$$\Rightarrow \min_{\theta} C \sum_{i=1}^{m} \max(1 - k^{(i)}\theta^{\mathrm{T}}x^{(i)}, 0) + \frac{1}{2}\sum_{j=1}^{n}\theta_j^2$$

Introduce $k^{(i)} = 1$ for positive instances ($y^{(i)} = 1$) and $k^{(i)} = -1$ for negative instances ($y^{(i)} = 0$):

$$\Rightarrow \min_{\theta} C \sum_{i=1}^{m} \max\left(1 - k^{(i)}\theta^T x^{(i)}, 0\right) + \frac{1}{2}\sum_{j=1}^{n} \theta_j^2$$

The convention is to weight the fidelity term by C rather than regularisation term by λ (thus C plays the role of 1/λ).

- Large C → little regularisation
- Small C → greater regularisation

Constrained objective problem

So far we considered the *unconstrained* objective problem by adapting the logistic regression cost function:

$$\min_{\theta} C \sum_{i=1}^{m} \max(1 - k^{(i)} \theta^{\mathrm{T}} x^{(i)}, 0) + \frac{1}{2} \sum_{j=1}^{n} \theta_j^2$$

Constrained objective problem

So far we considered the *unconstrained* objective problem by adapting the logistic regression cost function:

$$\min_{\theta} C \sum_{i=1}^{m} \max\left(1 - k^{(i)}\theta^T x^{(i)}, 0\right) + \frac{1}{2}\sum_{j=1}^{n} \theta_j^2$$

We can also consider the *constrained* objective problem:

$$\min_{\theta} \frac{1}{2}\sum_{j=1}^{n} \theta_j^2 \quad \text{subject to} \quad k^{(i)}\theta^T x^{(i)} \geq 1 \text{ for } i = 1, 2, \ldots, m$$

(Follows intuitively by considering large C.)

Intuition for large margin classification

Decision boundary defined by $\theta^{\mathrm{T}} x + b = 0$ (where here θ does *not* include bias and $b = \theta_0$; in notation above θ did include bias, i.e. θ_0 term).

Consequently, θ is orthogonal to decision boundary.

Intuition for large margin classification

Decision boundary defined by $\theta^T x + b = 0$ (where here θ does *not* include bias and $b = \theta_0$; in notation above θ did include bias, i.e. θ_0 term).

Consequently, θ is orthogonal to decision boundary.

Recall constrained objective:

$$\min_{\theta} \frac{1}{2} \sum_{j=1}^{n} \theta_j^2 \quad \text{subject to} \quad k^{(i)} \theta^T x^{(i)} \geq 1 \text{ for } i = 1, 2, \ldots, m$$

Projection

Note that the term $k^{(i)}\theta^{\mathrm{T}}x^{(i)}$ is related to the projection of $x^{(i)}$ onto θ:

$$k^{(i)}\theta^{\mathrm{T}}x^{(i)} = p^{(i)}\|\theta\|,$$

where $p^{(i)}$ is the projection of $x^{(i)}$ onto θ.

Projection

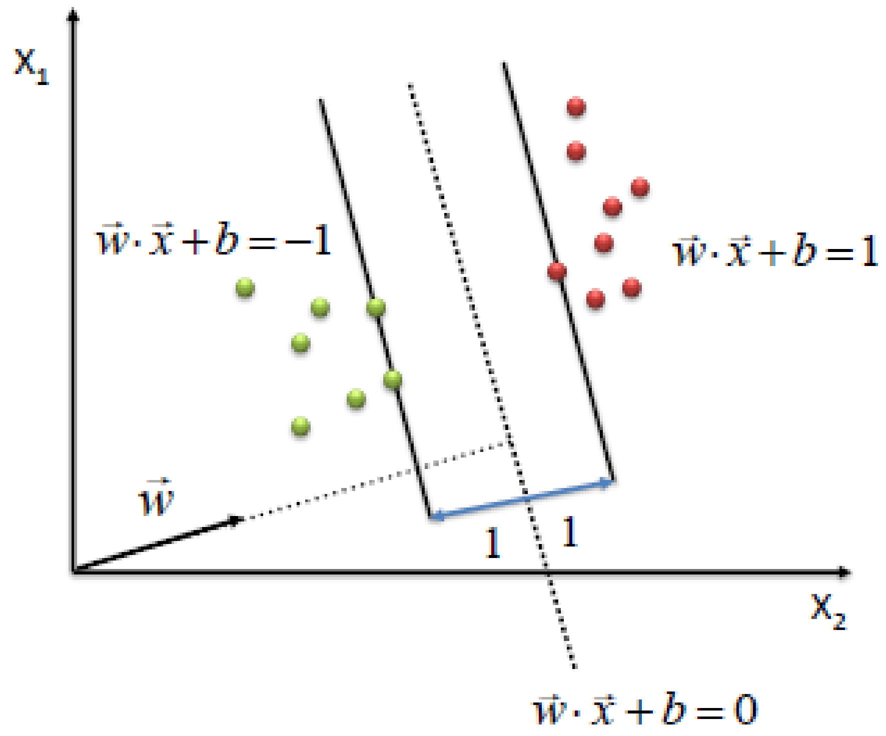
Note that the term $k^{(i)}\theta^T x^{(i)}$ is related to the projection of $x^{(i)}$ onto θ:

$$k^{(i)}\theta^T x^{(i)} = p^{(i)}\|\theta\|,$$

where $p^{(i)}$ is the projection of $x^{(i)}$ onto θ.

Attempting to minimise $\|\theta\|$, hence requires $p^{(i)}$ to be large $\Rightarrow$ large margin classification.

Graphical illustration



(Note difference notation used: $w = \theta$ without bias.)

[Image source (http://www.saedsayad.com/support_vector_machine.htm)]

Training SVMs

In [8]:

```
# Common imports
import os
import numpy as np
np.random.seed(42) # To make this notebook's output stable across runs

# To plot pretty figures
%matplotlib inline
import matplotlib
import matplotlib.pyplot as plt
plt.rcParams['axes.labelsize'] = 14
plt.rcParams['xtick.labelsize'] = 12
plt.rcParams['ytick.labelsize'] = 12
```

Load data and train

In [9]:

```
from sklearn.svm import SVC
from sklearn import datasets

iris = datasets.load_iris()
X = iris["data"][:, (2, 3)]  # petal length, petal width
y = iris["target"]

setosa_or_versicolor = (y == 0) | (y == 1)
X = X[setosa_or_versicolor]
y = y[setosa_or_versicolor]

# SVM Classifier model
svm_clf = SVC(kernel="linear", C=float("inf"))
svm_clf.fit(X, y)
```

Out[9]:

```
SVC(C=inf, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape='ovr', degree=3, gamma='auto', kernel='linear',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

Plot decision boundaries

In [10]:

```
# Bad models
x0 = np.linspace(0, 5.5, 200)
#pred_1 = 5*x0 - 20
pred_2 = x0 - 1.8
pred_3 = 0.1 * x0 + 0.5
```

In [11]:

```
def plot_svc_decision_boundary(svm_clf, xmin, xmax):
    w = svm_clf.coef_[0]
    b = svm_clf.intercept_[0]

    # At the decision boundary, w0*x0 + w1*x1 + b = 0
    # => x1 = -w0/w1 * x0 - b/w1
    x0 = np.linspace(xmin, xmax, 200)
    decision_boundary = -w[0]/w[1] * x0 - b/w[1]

    # On the margin, w0*x0 + w1*x1 + b = +/- 1
    margin = 1/w[1]
    gutter_up = decision_boundary + margin
    gutter_down = decision_boundary - margin

    svs = svm_clf.support_vectors_
    plt.scatter(svs[:, 0], svs[:, 1], s=200, facecolors='#FFAAAA')
    plt.plot(x0, decision_boundary, "k-", linewidth=2)
    plt.plot(x0, gutter_up, "k--", linewidth=2)
    plt.plot(x0, gutter_down, "k--", linewidth=2)
```

In [12]:

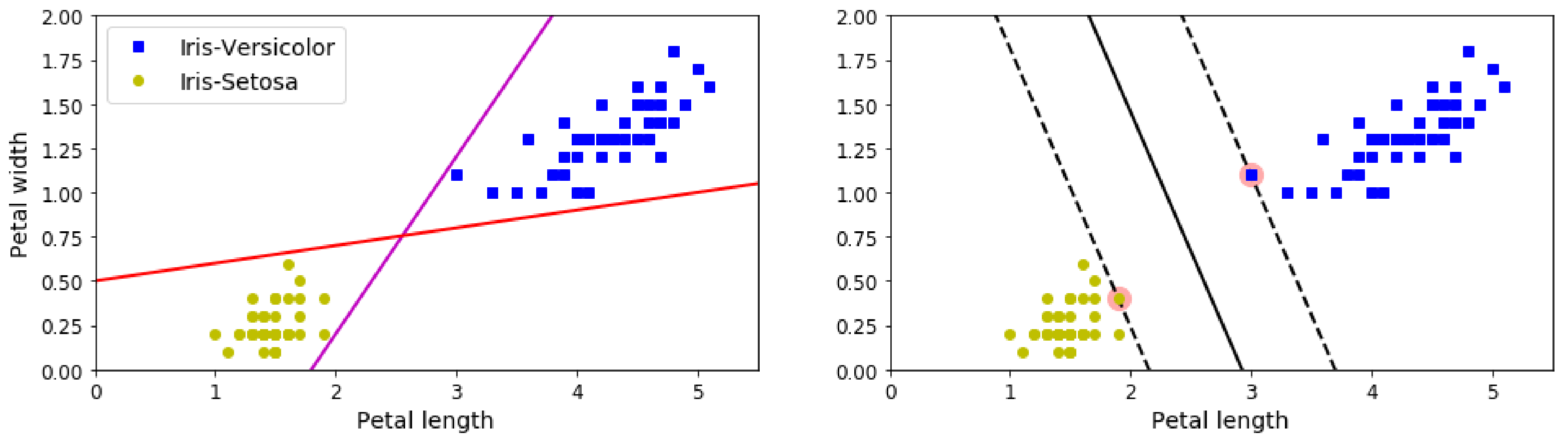
```
plt.figure(figsize=(16,4))

plt.subplot(121)
#plt.plot(x0, pred_1, "g--", linewidth=2)
plt.plot(x0, pred_2, "m-", linewidth=2)
plt.plot(x0, pred_3, "r-", linewidth=2)
plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs", label="Iris-Versicolor")
plt.plot(X[:, 0][y==0], X[:, 1][y==0], "yo", label="Iris-Setosa")
plt.xlabel("Petal length", fontsize=14)
plt.ylabel("Petal width", fontsize=14)
plt.legend(loc="upper left", fontsize=14)
plt.axis([0, 5.5, 0, 2])

plt.subplot(122)
plot_svc_decision_boundary(svm_clf, 0, 5.5)
plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs")
plt.plot(X[:, 0][y==0], X[:, 1][y==0], "yo")
plt.xlabel("Petal length", fontsize=14)
plt.axis([0, 5.5, 0, 2])
```

Out[12]:

```
[0, 5.5, 0, 2]
```



In [12]:

```python
plt.figure(figsize=(16,4))

plt.subplot(121)
#plt.plot(x0, pred_1, "g--", linewidth=2)
plt.plot(x0, pred_2, "m-", linewidth=2)
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plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs", label="Iris-Versicolor")
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plt.legend(loc="upper left", fontsize=14)
plt.axis([0, 5.5, 0, 2])

plt.subplot(122)
plot_svc_decision_boundary(svm_clf, 0, 5.5)
plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs")
plt.plot(X[:, 0][y==0], X[:, 1][y==0], "yo")
plt.xlabel("Petal length", fontsize=14)
plt.axis([0, 5.5, 0, 2])
```
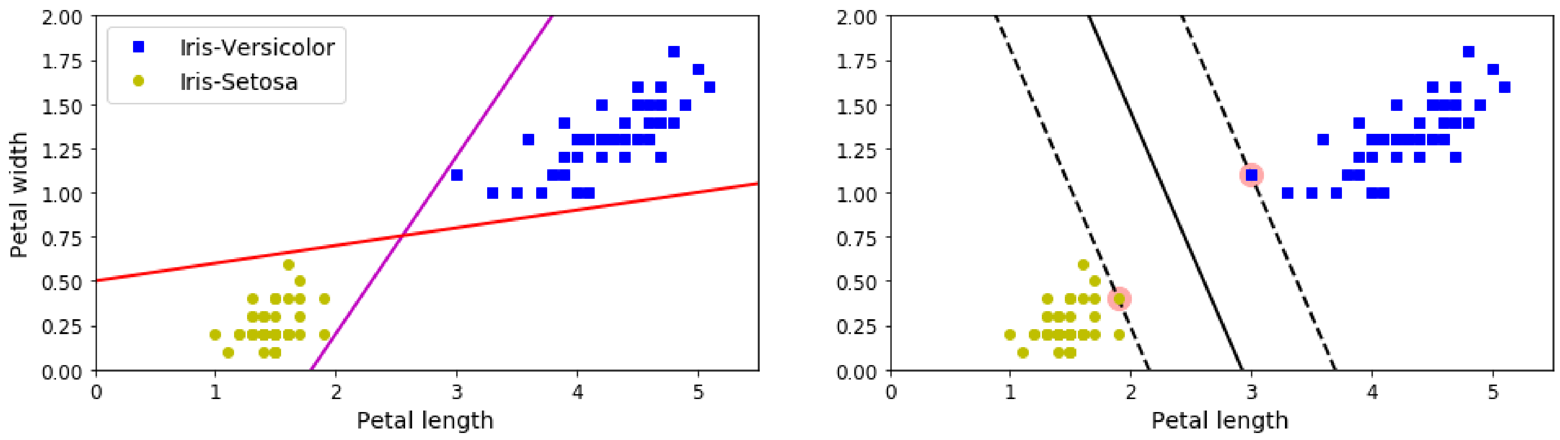

Out[12]:

```
[0, 5.5, 0, 2]
```



Adding training instances outside the margin will not alter the decision boundary.

Boundary is defined by *support vectors* that are located on the edge of the margin.

Exercise: what value would you guess for the weights θ (excluding the bias)?

Exercise: what value would you guess for the weights $\boldsymbol{\theta}$ (excluding the bias)?

From plot appears $w \sim [1, 1]^T$ (or slightly more accurately $w \sim [1.1, 0.9]^T$).

Let's check:

Exercise: what value would you guess for the weights $\boldsymbol{\theta}$ (excluding the bias)?

From plot appears $w \sim [1, 1]^T$ (or slightly more accurately $w \sim [1.1, 0.9]^T$).

Let's check:

In [13]:
```
svm_clf.coef_[0]
```

Out[13]:
```
array([1.29411744, 0.82352928])
```

Feature scaling

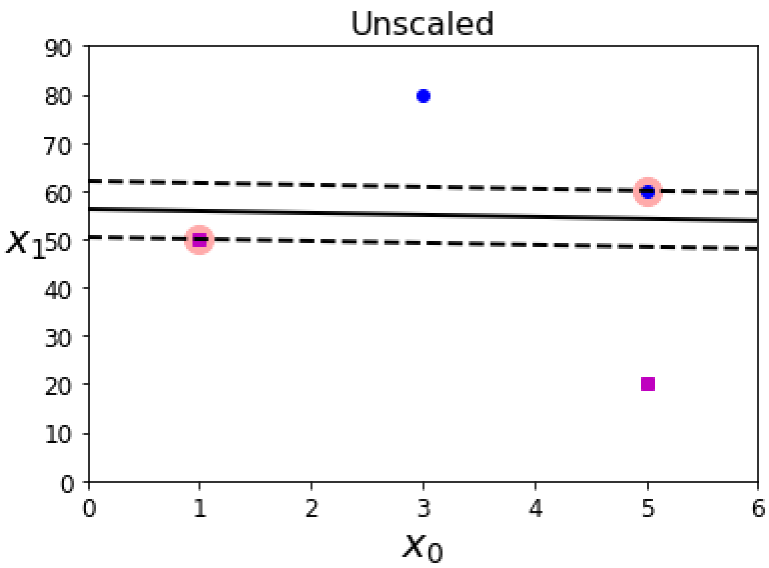
SVMs are sensitive to feature scales, hence feature scaling is important if features not already of similar scale.

In [14]:

```
Xs = np.array([[1, 50], [5, 20], [3, 80], [5, 60]]).astype(np.float64)
ys = np.array([0, 0, 1, 1])
svm_clf = SVC(kernel="linear", C=100)
svm_clf.fit(Xs, ys)

#plt.figure(figsize=(16,4))
#plt.subplot(121)
plt.plot(Xs[:, 0][ys==1], Xs[:, 1][ys==1], "bo")
plt.plot(Xs[:, 0][ys==0], Xs[:, 1][ys==0], "ms")
plot_svc_decision_boundary(svm_clf, 0, 6)
plt.xlabel("$x_0$", fontsize=20)
plt.ylabel("$x_1$  ", fontsize=20, rotation=0)
plt.title("Unscaled", fontsize=16)
plt.axis([0, 6, 0, 90])
```

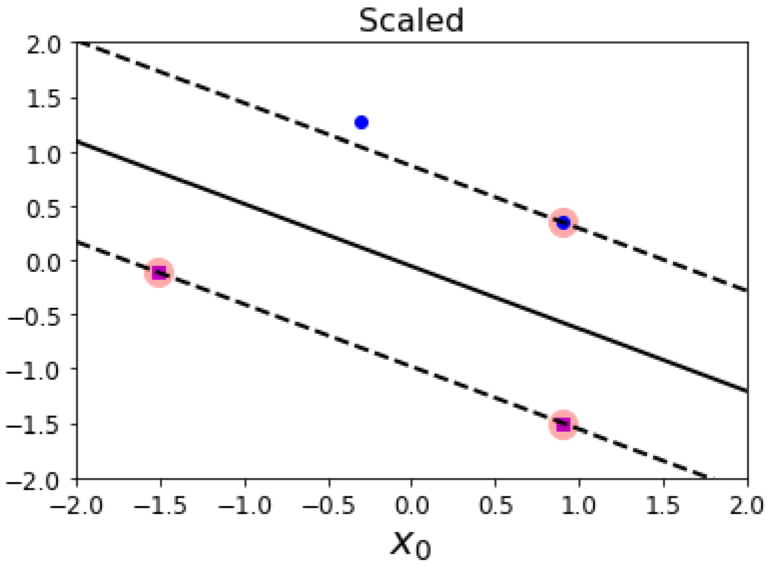
Out[14]:

```
[0, 6, 0, 90]
```



In [15]:
```python
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
X_scaled = scaler.fit_transform(Xs)
svm_clf.fit(X_scaled, ys)

#plt.subplot(122)
plt.plot(X_scaled[:, 0][ys==1], X_scaled[:, 1][ys==1], "bo")
plt.plot(X_scaled[:, 0][ys==0], X_scaled[:, 1][ys==0], "ms")
plot_svc_decision_boundary(svm_clf, -2, 2)
plt.xlabel("$x_0$", fontsize=20)
plt.title("Scaled", fontsize=16)
plt.axis([-2, 2, -2, 2])
```

Out[15]:
```
[-2, 2, -2, 2]
```



Hard margin classification

Hard margin classification corresponds to strictly imposing all training instances correctly classfied.

Problems with hard margin classification

- Can fail if data not linearly separable.
- Sensitive to outliers.

In [16]:

```
X_outliers = np.array([[3.4, 1.3], [3.2, 0.8]])
y_outliers = np.array([0, 0])
Xo1 = np.concatenate([X, X_outliers[:1]], axis=0)
yo1 = np.concatenate([y, y_outliers[:1]], axis=0)
Xo2 = np.concatenate([X, X_outliers[1:]], axis=0)
yo2 = np.concatenate([y, y_outliers[1:]], axis=0)

svm_clf2 = SVC(kernel="linear", C=10**9)
svm_clf2.fit(Xo2, yo2)
```

Out[16]:

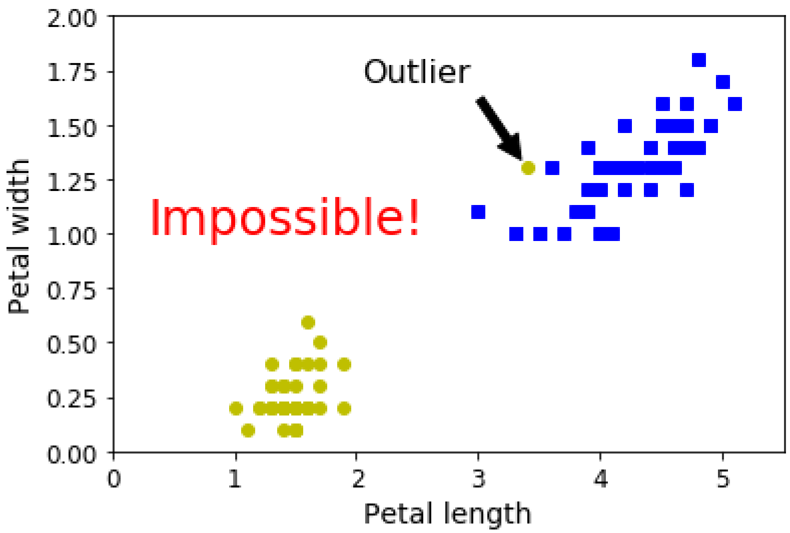
```
SVC(C=1000000000, cache_size=200, class_weight=None, coef0=0.0,
  decision_function_shape='ovr', degree=3, gamma='auto', kernel='linear',
  max_iter=-1, probability=False, random_state=None, shrinking=True,
  tol=0.001, verbose=False)
```

In [17]:

```
# plt.figure(figsize=(16,5))
# plt.subplot(121)
plt.plot(Xo1[:, 0][yo1==1], Xo1[:, 1][yo1==1], "bs")
plt.plot(Xo1[:, 0][yo1==0], Xo1[:, 1][yo1==0], "yo")
plt.text(0.3, 1.0, "Impossible!", fontsize=24, color="red")
plt.xlabel("Petal length", fontsize=14)
plt.ylabel("Petal width", fontsize=14)
plt.annotate("Outlier",
             xy=(X_outliers[0][0], X_outliers[0][1]),
             xytext=(2.5, 1.7),
             ha="center",
             arrowprops=dict(facecolor='black', shrink=0.1),
             fontsize=16,
            )
plt.axis([0, 5.5, 0, 2])
```

Out[17]:

```
[0, 5.5, 0, 2]
```

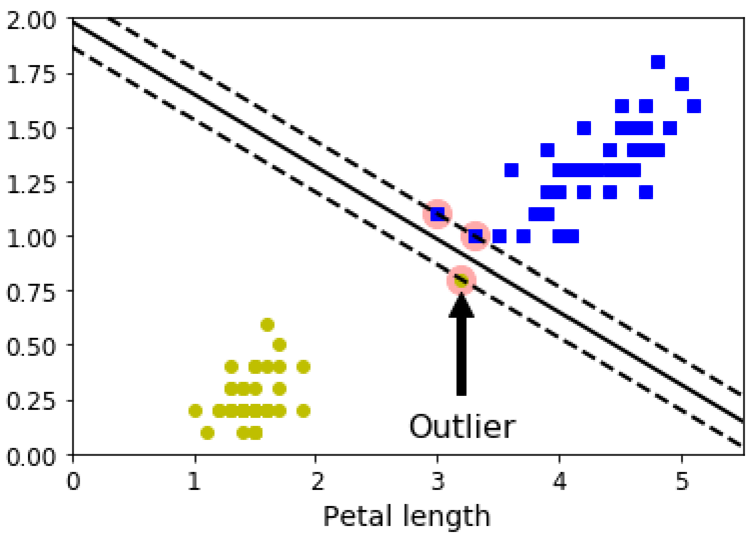


In [18]:

```
# plt.subplot(122)
plt.plot(Xo2[:, 0][yo2==1], Xo2[:, 1][yo2==1], "bs")
plt.plot(Xo2[:, 0][yo2==0], Xo2[:, 1][yo2==0], "yo")
plot_svc_decision_boundary(svm_clf2, 0, 5.5)
plt.xlabel("Petal length", fontsize=14)
plt.annotate("Outlier",
             xy=(X_outliers[1][0], X_outliers[1][1]),
             xytext=(3.2, 0.08),
             ha="center",
             arrowprops=dict(facecolor='black', shrink=0.1),
             fontsize=16,
            )
plt.axis([0, 5.5, 0, 2])
```

Out[18]:

```
[0, 5.5, 0, 2]
```



Soft margin classification

Allow some margin violations by varying hyperparameter C.

Recall, large C corresponds to small regularisation and thus few margin violoations. Small C corresponds to greater regularisation and thus more margin violations.

Load data

In [19]:
```
import numpy as np
from sklearn import datasets
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
from sklearn.svm import LinearSVC

iris = datasets.load_iris()
X = iris["data"][:, (2, 3)]  # petal length, petal width
y = (iris["target"] == 2).astype(np.float64)  # Iris-Virginica
```

Train SVMs

In [20]:

```
scaler = StandardScaler()
svm_clf1 = LinearSVC(C=1, loss="hinge", random_state=42)
svm_clf2 = LinearSVC(C=100, loss="hinge", random_state=42)

scaled_svm_clf1 = Pipeline((
        ("scaler", scaler),
        ("linear_svc", svm_clf1),
    ))
scaled_svm_clf2 = Pipeline((
        ("scaler", scaler),
        ("linear_svc", svm_clf2),
    ))

scaled_svm_clf1.fit(X, y)
scaled_svm_clf2.fit(X, y)
```

Out[20]:

```
Pipeline(memory=None,
     steps=[('scaler', StandardScaler(copy=True, with_mean=True, with_std=Tru
e)), ('linear_svc', LinearSVC(C=100, class_weight=None, dual=True, fit_interce
pt=True,
     intercept_scaling=1, loss='hinge', max_iter=1000, multi_class='ovr',
     penalty='l2', random_state=42, tol=0.0001, verbose=0))])
```

Compute support vectors

In [21]:

```
# Convert to unscaled parameters
b1 = svm_clf1.decision_function([-scaler.mean_ / scaler.scale_])
b2 = svm_clf2.decision_function([-scaler.mean_ / scaler.scale_])
w1 = svm_clf1.coef_[0] / scaler.scale_
w2 = svm_clf2.coef_[0] / scaler.scale_
svm_clf1.intercept_ = np.array([b1])
svm_clf2.intercept_ = np.array([b2])
svm_clf1.coef_ = np.array([w1])
svm_clf2.coef_ = np.array([w2])

# Find support vectors (LinearSVC does not do this automatically)
t = y * 2 - 1 # t = +/-1
support_vectors_idx1 = (t * (X.dot(w1) + b1) < 1).ravel()
support_vectors_idx2 = (t * (X.dot(w2) + b2) < 1).ravel()
svm_clf1.support_vectors_ = X[support_vectors_idx1]
svm_clf2.support_vectors_ = X[support_vectors_idx2]
```

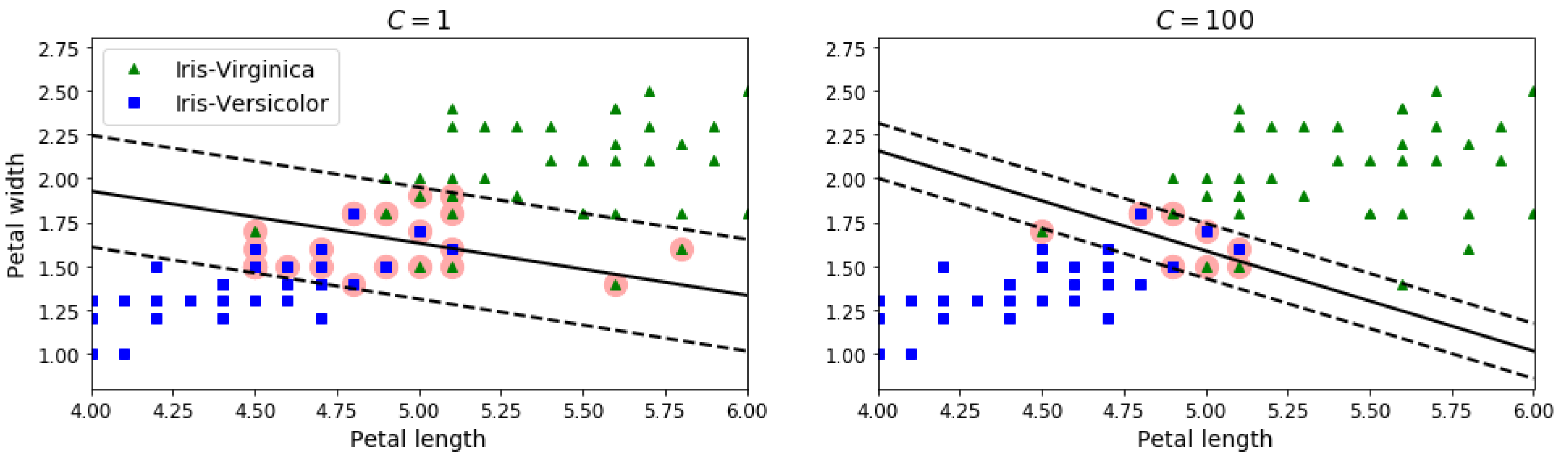
Plot

In [22]:

```
plt.figure(figsize=(16,4))
plt.subplot(121)
plt.plot(X[:, 0][y==1], X[:, 1][y==1], "g^", label="Iris-Virginica")
plt.plot(X[:, 0][y==0], X[:, 1][y==0], "bs", label="Iris-Versicolor")
plot_svc_decision_boundary(svm_clf1, 4, 6)
plt.xlabel("Petal length", fontsize=14)
plt.ylabel("Petal width", fontsize=14)
plt.legend(loc="upper left", fontsize=14)
plt.title("$C = {}$".format(svm_clf1.C), fontsize=16)
plt.axis([4, 6, 0.8, 2.8])

plt.subplot(122)
plt.plot(X[:, 0][y==1], X[:, 1][y==1], "g^")
plt.plot(X[:, 0][y==0], X[:, 1][y==0], "bs")
plot_svc_decision_boundary(svm_clf2, 4, 6)
plt.xlabel("Petal length", fontsize=14)
plt.title("$C = {}$".format(svm_clf2.C), fontsize=16)
plt.axis([4, 6, 0.8, 2.8])
```

Out[22]:

```
[4, 6, 0.8, 2.8]
```



Non-linear classification with polynomial features

So far we have considered linear classification only.

Most data-sets are not linearly separable.

1D example

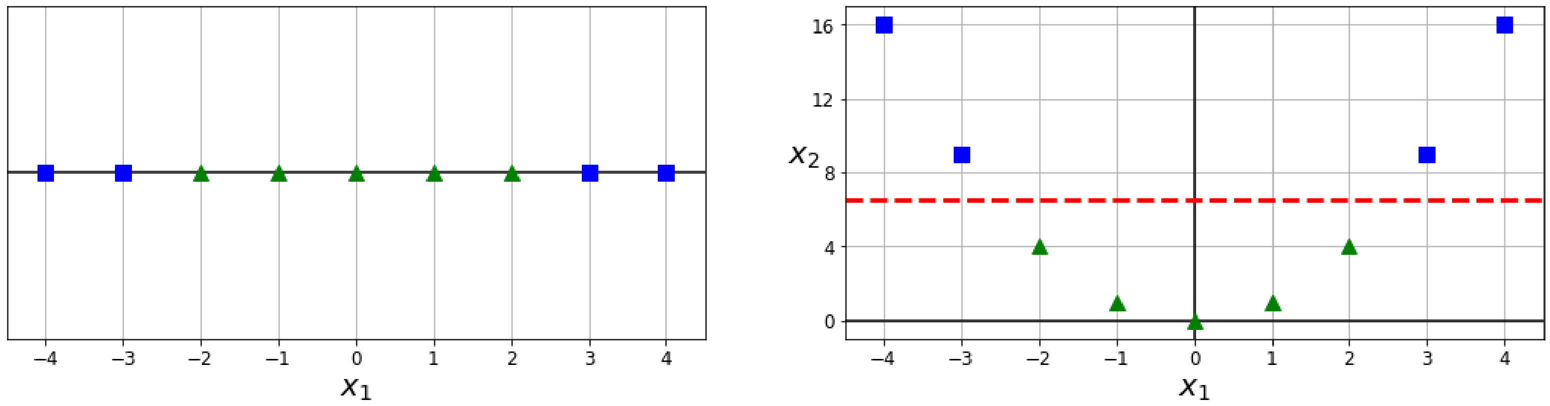
Consider 1D feature space with x_1, which is clearly not linearly separable.

However, if augment feature space with $x_2 = (x_1)^2$ we see that the resulting 2D feature space is linearly separable.

In [23]:
```
X1D = np.linspace(-4, 4, 9).reshape(-1, 1)
X2D = np.c_[X1D, X1D**2]
y = np.array([0, 0, 1, 1, 1, 1, 1, 0, 0])
```

In [24]:

```python
plt.figure(figsize=(16, 4))
plt.subplot(121)
plt.grid(True, which='both')
plt.axhline(y=0, color='k')
plt.plot(X1D[:, 0][y==0], np.zeros(4), "bs", markersize=10)
plt.plot(X1D[:, 0][y==1], np.zeros(5), "g^", markersize=10)
plt.gca().get_yaxis().set_ticks([])
plt.xlabel(r"$x_1$", fontsize=20)
plt.axis([-4.5, 4.5, -0.2, 0.2])

plt.subplot(122)
plt.grid(True, which='both')
plt.axhline(y=0, color='k')
plt.axvline(x=0, color='k')
plt.plot(X2D[:, 0][y==0], X2D[:, 1][y==0], "bs", markersize=10)
plt.plot(X2D[:, 0][y==1], X2D[:, 1][y==1], "g^", markersize=10)
plt.xlabel(r"$x_1$", fontsize=20)
plt.ylabel(r"$x_2$", fontsize=20, rotation=0)
plt.gca().get_yaxis().set_ticks([0, 4, 8, 12, 16])
plt.plot([-4.5, 4.5], [6.5, 6.5], "r--", linewidth=3)
plt.axis([-4.5, 4.5, -1, 17])

plt.subplots_adjust(right=1)
```

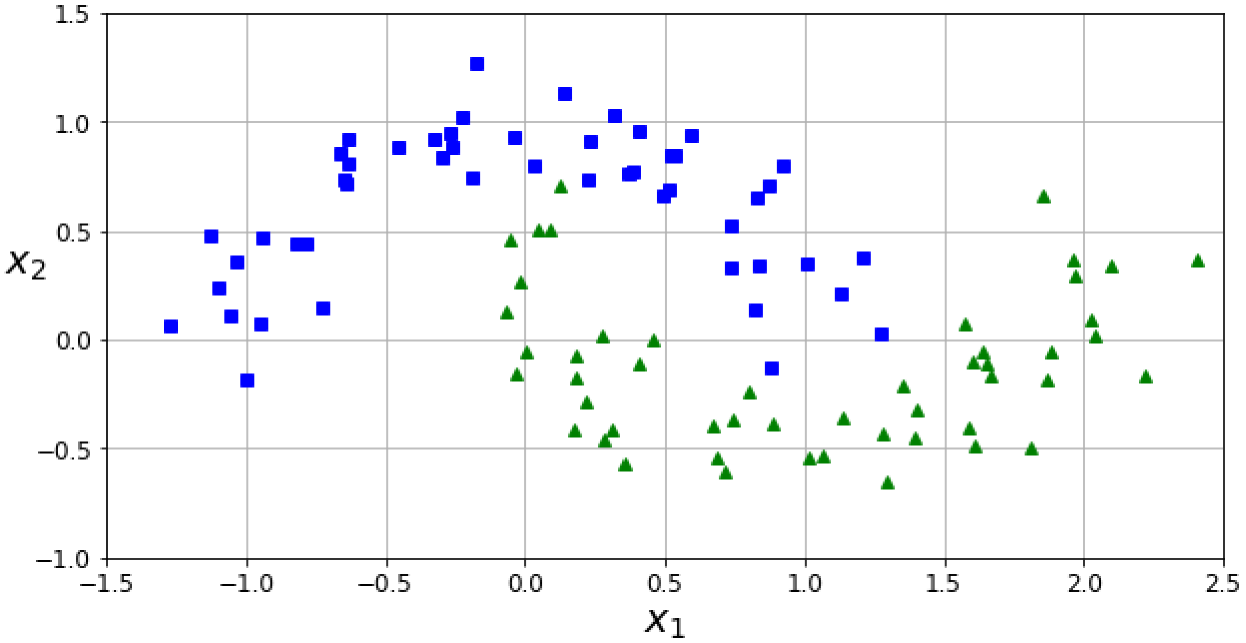


−4
−3
−2
−1
0
1
2
3
4
x_1
16
12
8
4
0
x_2
−4
−3
−2
−1
0
1
2
3
4
x_1

2D example

In [25]:

```python
from sklearn.datasets import make_moons
X, y = make_moons(n_samples=100, noise=0.15, random_state=42)

def plot_dataset(X, y, axes):
    plt.plot(X[:, 0][y==0], X[:, 1][y==0], "bs")
    plt.plot(X[:, 0][y==1], X[:, 1][y==1], "g^")
    plt.axis(axes)
    plt.grid(True, which='both')
    plt.xlabel(r"$x_1$", fontsize=20)
    plt.ylabel(r"$x_2$", fontsize=20, rotation=0)

plt.figure(figsize=(10, 5))
plot_dataset(X, y, [-1.5, 2.5, -1, 1.5])
plt.show()
```



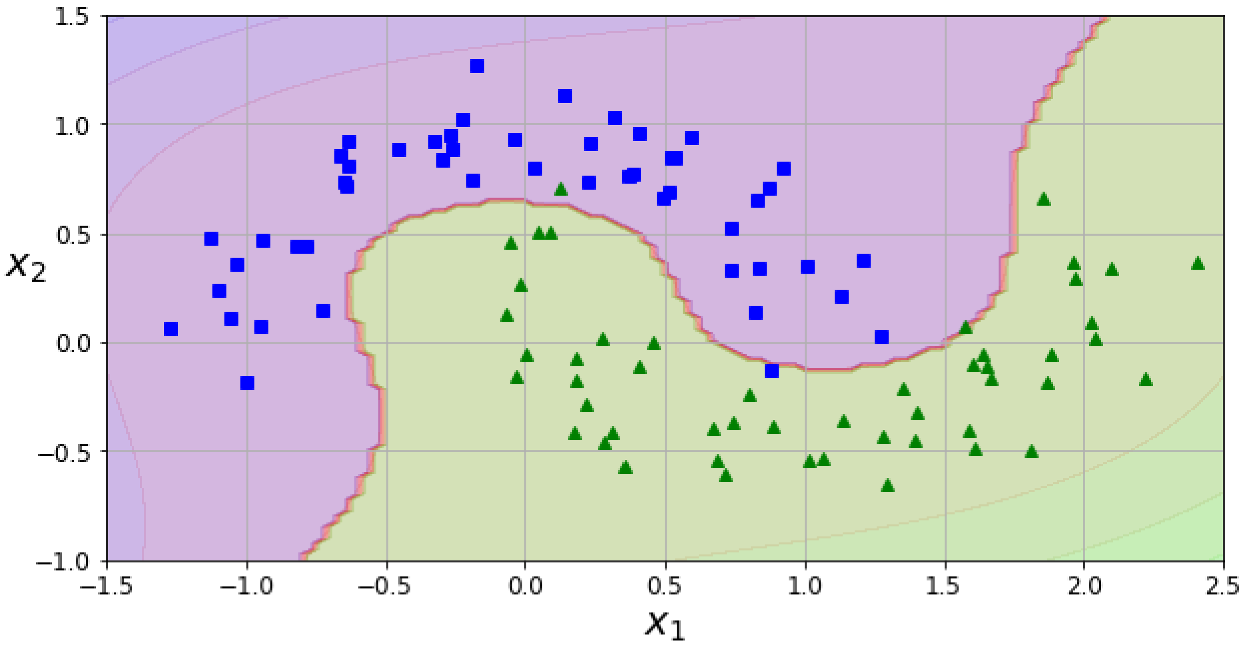
In [26]:

```python
from sklearn.datasets import make_moons
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures

polynomial_svm_clf = Pipeline((
        ("poly_features", PolynomialFeatures(degree=3)),
        ("scaler", StandardScaler()),
        ("svm_clf", LinearSVC(C=10, loss="hinge", random_state=42))
    ))

polynomial_svm_clf.fit(X, y)
```

Out[26]:

```
Pipeline(memory=None,
     steps=[('poly_features', PolynomialFeatures(degree=3, include_bias=True,
interaction_only=False)), ('scaler', StandardScaler(copy=True, with_mean=True,
with_std=True)), ('svm_clf', LinearSVC(C=10, class_weight=None, dual=True, fit
_intercept=True,
     intercept_scaling=1, loss='hinge', max_iter=1000, multi_class='ovr',
     penalty='l2', random_state=42, tol=0.0001, verbose=0))])
```

In [27]:
```
def plot_predictions(clf, axes):
    x0s = np.linspace(axes[0], axes[1], 100)
    x1s = np.linspace(axes[2], axes[3], 100)
    x0, x1 = np.meshgrid(x0s, x1s)
    X = np.c_[x0.ravel(), x1.ravel()]
    y_pred = clf.predict(X).reshape(x0.shape)
    y_decision = clf.decision_function(X).reshape(x0.shape)
    plt.contourf(x0, x1, y_pred, cmap=plt.cm.brg, alpha=0.2)
    plt.contourf(x0, x1, y_decision, cmap=plt.cm.brg, alpha=0.1)

plt.figure(figsize=(10,5))
plot_predictions(polynomial_svm_clf, [-1.5, 2.5, -1, 1.5])
plot_dataset(X, y, [-1.5, 2.5, -1, 1.5])
```



Adding polynomial features leads to a combinatorial increase in the dimensionality of the feature space and thus is computationally costly.

Adding polynomial features leads to a combinatorial increase in the dimensionality of the feature space and thus is computationally costly.

There are much better ways to perform non-linear classification with SVMs, where computational tricks can be exploited...

Non-linear classification with kernels

Similarity features and landmarks

Compute new features based on proximity to landmarks.

Consider landmarks $l^{(1)}, l^{(2)}, \ldots$

Then for each training instance x, compute features $f_j = \mathrm{sim}(x, l^{(j)})$, where $\mathrm{sim}(.,.)$ defines a *similarity* function.

Similarity functions

The Gaussian radial basis function (RBF) is a common *similarity function*:

$$\phi_\gamma(x, l) = exp(-\gamma \|x - l\|^2),$$

where γ controls the width of the kernel.

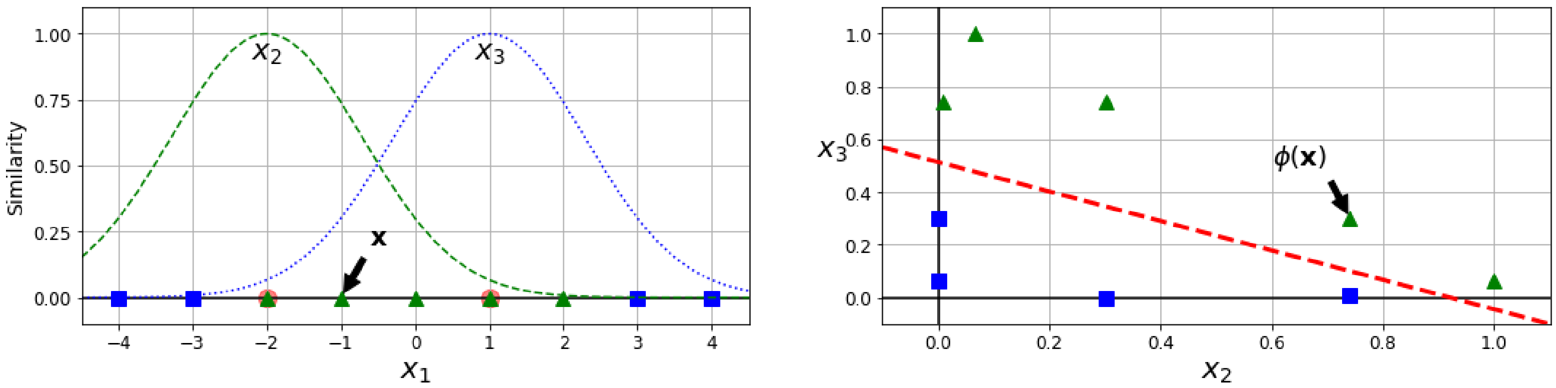
1D example (from above)

Consider landmarks at $x_1 = -2$ and $x_1 = 1$.

In [28]:
```
def gaussian_rbf(x, landmark, gamma):
    return np.exp(-gamma * np.linalg.norm(x - landmark, axis=1)**2)

gamma = 0.3

x1s = np.linspace(-4.5, 4.5, 200).reshape(-1, 1)
x2s = gaussian_rbf(x1s, -2, gamma)
x3s = gaussian_rbf(x1s, 1, gamma)

XK = np.c_[gaussian_rbf(X1D, -2, gamma), gaussian_rbf(X1D, 1, gamma)]
yk = np.array([0, 0, 1, 1, 1, 1, 1, 0, 0])
```

In [29]:
```
plt.figure(figsize=(16, 4))
plt.subplot(121)
plt.grid(True, which='both')
plt.axhline(y=0, color='k')
plt.scatter(x=[-2, 1], y=[0, 0], s=150, alpha=0.5, c="red")
plt.plot(X1D[:, 0][yk==0], np.zeros(4), "bs", markersize=10)
plt.plot(X1D[:, 0][yk==1], np.zeros(5), "g^", markersize=10)
plt.plot(x1s, x2s, "g--")
plt.plot(x1s, x3s, "b:")
plt.gca().get_yaxis().set_ticks([0, 0.25, 0.5, 0.75, 1])
plt.xlabel(r"$x_1$", fontsize=20)
plt.ylabel(r"Similarity", fontsize=14)
plt.annotate(r'$\mathbf{x}$',
             xy=(X1D[3, 0], 0),
             xytext=(-0.5, 0.20),
             ha="center",
             arrowprops=dict(facecolor='black', shrink=0.1),
             fontsize=18,
            )
plt.text(-2, 0.9, "$x_2$", ha="center", fontsize=20)
plt.text(1, 0.9, "$x_3$", ha="center", fontsize=20)
plt.axis([-4.5, 4.5, -0.1, 1.1])

plt.subplot(122)
plt.grid(True, which='both')
plt.axhline(y=0, color='k')
plt.axvline(x=0, color='k')
plt.plot(XK[:, 0][yk==0], XK[:, 1][yk==0], "bs", markersize=10)
plt.plot(XK[:, 0][yk==1], XK[:, 1][yk==1], "g^", markersize=10)
plt.xlabel(r"$x_2$", fontsize=20)
plt.ylabel(r"$x_3$  ", fontsize=20, rotation=0)
plt.annotate(r'$\phi\left(\mathbf{x}\right)$',
             xy=(XK[3, 0], XK[3, 1]),
             xytext=(0.65, 0.50),
             ha="center",
             arrowprops=dict(facecolor='black', shrink=0.1),
```

```
                fontsize=18,
               )
plt.plot([-0.1, 1.1], [0.57, -0.1], "r--", linewidth=3)
plt.axis([-0.1, 1.1, -0.1, 1.1])

plt.subplots_adjust(right=1)
```



Training data *are* linearly separable in new feature space.

Exercise: What are new feature values corresponding to the instance at $\mathbf{x_1} = -1$ ($\gamma = 0.3$)?

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$$x_2 = \exp(-0.3 \times (1)^2) = 0.74$$

$$x_3 = \exp(-0.3 \times (2)^2) = 0.30$$

Let's check:

Exercise: What are new feature values corresponding to the instance at $x_1 = -1$ ($\gamma = 0.3$)?

$$x_2 = \exp(-0.3 \times (1)^2) = 0.74$$

$$x_3 = \exp(-0.3 \times (2)^2) = 0.30$$

Let's check:

In [30]:

```
x1_example = X1D[3, 0]
for landmark in (-2, 1):
    k = gaussian_rbf(np.array([[x1_example]]), np.array([[landmark]]), gamma)
    print("Phi({}, {}) = {}".format(x1_example, landmark, k))
```

```
Phi(-1.0, -2) = [0.74081822]
Phi(-1.0, 1) = [0.30119421]
```

How set landmarks?

How set landmarks?

Common approach is to set a landmark at the location of each instance in the training dataset.

Kernel trick

For SVMs it is not necessary to actually compute new features for each kernel.

Instead, can be done implicitly, providing *considerable* computational saving.

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SVM are well suited for small to medium sized data-sets, with complex structure.

The kernel trick is based on Mercer's theorem.

Mercer's theorem

For (feature) mapping function $\phi(x)$, the inner product of two transformed vectors can be computed implicitly by the evaluation of the kernel function K by

$$K(x, z) = \langle \phi(x), \phi(z) \rangle.$$

There is therefore no need to explicitly compute $\phi(x)$.

Moreoever, it is not necessary to even know the explicit form of the (feature) mapping function $\phi(x)$.

Mercer’s theorem

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Moreoever, it is not necessary to even know the explicit form of the (feature) mapping function $\phi(x)$.

(We will not cover the kernel trick and Mercer's theorem in any further detail.)

Common kernels

Some common similarity function, or *kernel*, include the following.

1. Gaussian radial basis function (RBF):
$$K_\gamma(x, l) = exp(-\gamma \|x - l\|^2),$$
where γ controls the width of the kernel.

2. Polynomial kernel:
$$K_{c,d}(x, l) = (x^{\mathrm{T}} l + c)^d,$$
for constant offset c and degree d.

3. Linear kernel, i.e. linear SVM:
$$K(x, l) = x^{\mathrm{T}} l.$$

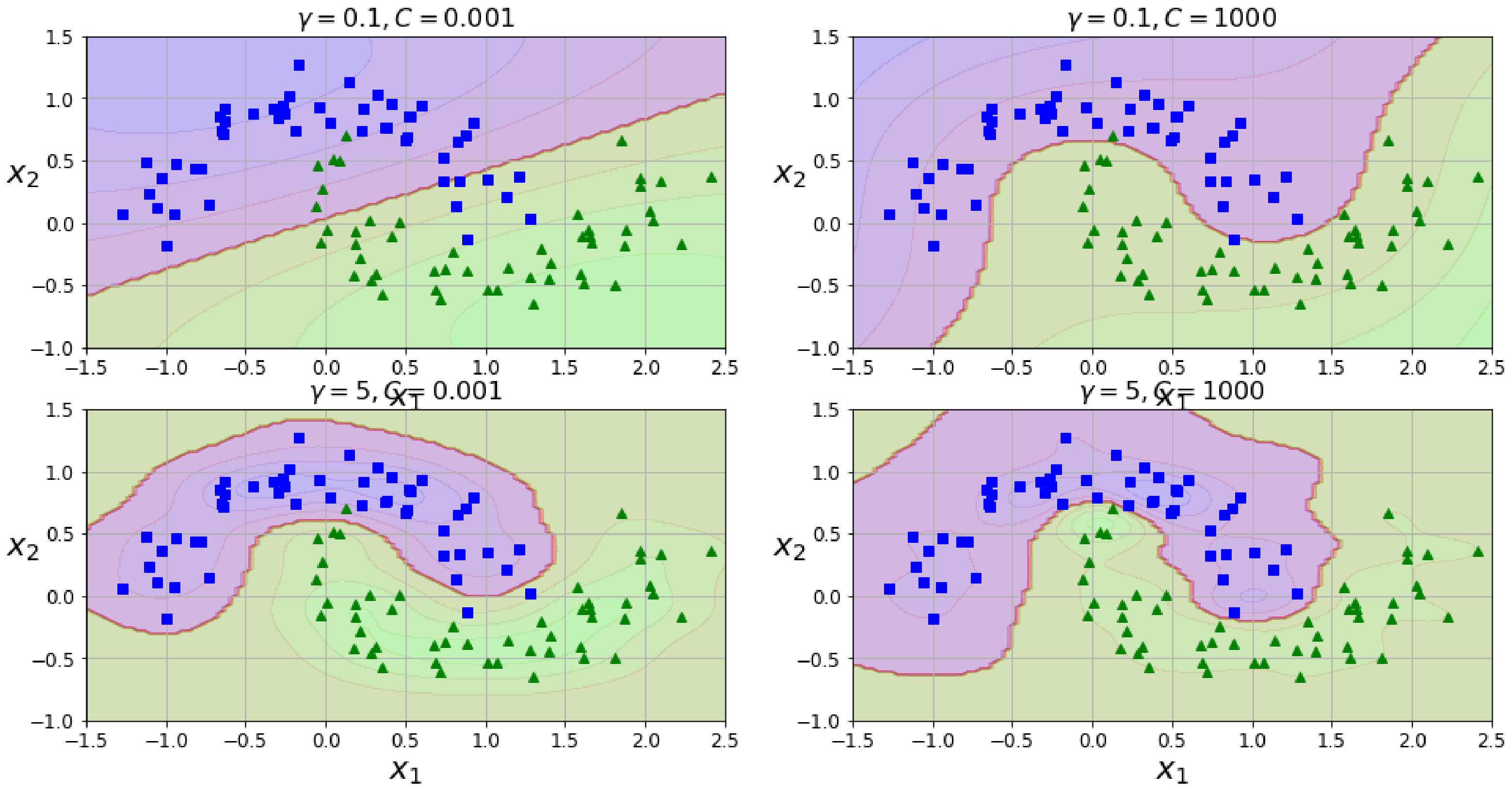
2D example (from above)

In [31]:

```
from sklearn.svm import SVC

gamma1, gamma2 = 0.1, 5
C1, C2 = 0.001, 1000
hyperparams = (gamma1, C1), (gamma1, C2), (gamma2, C1), (gamma2, C2)

svm_clfs = []
for gamma, C in hyperparams:
    rbf_kernel_svm_clf = Pipeline((
            ("scaler", StandardScaler()),
            ("svm_clf", SVC(kernel="rbf", gamma=gamma, C=C))
        ))
    rbf_kernel_svm_clf.fit(X, y)
    svm_clfs.append(rbf_kernel_svm_clf)
```

In [32]:

```
plt.figure(figsize=(16, 8))

for i, svm_clf in enumerate(svm_clfs):
    plt.subplot(221 + i)
    plot_predictions(svm_clf, [-1.5, 2.5, -1, 1.5])
    plot_dataset(X, y, [-1.5, 2.5, -1, 1.5])
    gamma, C = hyperparams[i]
    plt.title(r"$\gamma = {}, C = {}$".format(gamma, C), fontsize=16)
```



Regression

Regression

Can also use SVMs to perform regression, in addition to classification.

General idea is to reverse the objective: rather than fitting the largest possible margin between two classes, SVM regression fits as many instances as possible within the margin.

The width of the margin is controlled by the hyperparameter \epsilon.

Linear regression

In [33]:

```
np.random.seed(42)
m = 50
X = 2 * np.random.rand(m, 1)
y = (4 + 3 * X + np.random.randn(m, 1)).ravel()
```

In [34]:

```
from sklearn.svm import LinearSVR

svm_reg1 = LinearSVR(epsilon=1.5, random_state=42)
svm_reg2 = LinearSVR(epsilon=0.5, random_state=42)
svm_reg1.fit(X, y)
svm_reg2.fit(X, y)

def find_support_vectors(svm_reg, X, y):
    y_pred = svm_reg.predict(X)
    off_margin = (np.abs(y - y_pred) >= svm_reg.epsilon)
    return np.argwhere(off_margin)

svm_reg1.support_ = find_support_vectors(svm_reg1, X, y)
svm_reg2.support_ = find_support_vectors(svm_reg2, X, y)

eps_x1 = 1
eps_y_pred = svm_reg1.predict([[eps_x1]])
```

In [35]:

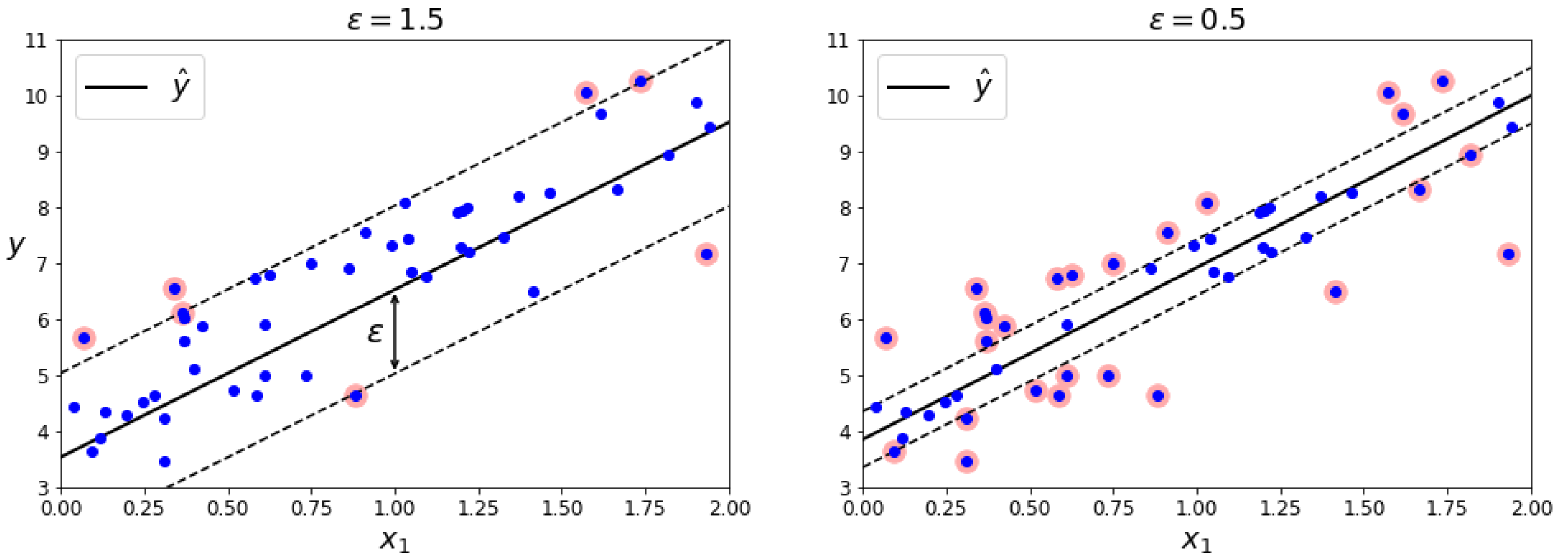
```
eps_y_pred
```

Out[35]:

```
array([6.52640746])
```

In [36]:

```
def plot_svm_regression(svm_reg, X, y, axes):
    x1s = np.linspace(axes[0], axes[1], 100).reshape(100, 1)
    y_pred = svm_reg.predict(x1s)
    plt.plot(x1s, y_pred, "k-", linewidth=2, label=r"$\hat{y}$")
    plt.plot(x1s, y_pred + svm_reg.epsilon, "k--")
    plt.plot(x1s, y_pred - svm_reg.epsilon, "k--")
    plt.scatter(X[svm_reg.support_], y[svm_reg.support_], s=180, facecolors='#FFAA
AA')
    plt.plot(X, y, "bo")
    plt.xlabel(r"$x_1$", fontsize=18)
    plt.legend(loc="upper left", fontsize=18)
    plt.axis(axes)

plt.figure(figsize=(16, 5))
plt.subplot(121)
plot_svm_regression(svm_reg1, X, y, [0, 2, 3, 11])
plt.title(r"$\epsilon = {}$".format(svm_reg1.epsilon), fontsize=18)
plt.ylabel(r"$y$", fontsize=18, rotation=0)
#plt.plot([eps_x1, eps_x1], [eps_y_pred, eps_y_pred - svm_reg1.epsilon], "k-", lin
ewidth=2)
plt.annotate(
        '', xy=(eps_x1, eps_y_pred), xycoords='data',
        xytext=(eps_x1, eps_y_pred - svm_reg1.epsilon),
        textcoords='data', arrowprops={'arrowstyle': '<->', 'linewidth': 1.5}
    )
plt.text(0.91, 5.6, r"$\epsilon$", fontsize=20)
plt.subplot(122)
plot_svm_regression(svm_reg2, X, y, [0, 2, 3, 11])
plt.title(r"$\epsilon = {}$".format(svm_reg2.epsilon), fontsize=18);
```



$\varepsilon = 1.5$
$\varepsilon = 0.5$
$\hat{y}$
ε
y
x_1

Non-linear regression

In [37]:
```
np.random.seed(42)
m = 100
X = 2 * np.random.rand(m, 1) - 1
y = (0.2 + 0.1 * X + 0.5 * X**2 + np.random.randn(m, 1)/10).ravel()
```

In [38]:

```python
from sklearn.svm import SVR

svm_poly_reg1 = SVR(kernel="poly", degree=2, C=100, epsilon=0.1)
svm_poly_reg2 = SVR(kernel="poly", degree=2, C=0.01, epsilon=0.1)
svm_poly_reg1.fit(X, y);
svm_poly_reg2.fit(X, y);
```

In [39]:

```
plt.figure(figsize=(16, 5))
plt.subplot(121)
plot_svm_regression(svm_poly_reg1, X, y, [-1, 1, 0, 1])
plt.title(r"$degree={}, C={}, \epsilon = {}$".format(svm_poly_reg1.degree, svm_pol
y_reg1.C, svm_poly_reg1.epsilon), fontsize=18)
plt.ylabel(r"$y$", fontsize=18, rotation=0)
plt.subplot(122)
plot_svm_regression(svm_poly_reg2 , X, y, [-1, 1, 0, 1])
plt.title(r"$degree={}, C={}, \epsilon = {}$".format(svm_poly_reg2.degree, svm_pol
y_reg2.C, svm_poly_reg2.epsilon), fontsize=18);
```