Chapter 8 – Dimensionality Reduction

This notebook contains all the sample code and solutions to the exercises in chapter 8.

[Run in Google Colab (https://colab.research.google.com/github/ageron/handson-ml2/blob/master/08_dimensionality_reduction.ipynb)](https://colab.research.google.com/github/ageron/handson-ml2/blob/master/08_dimensionality_reduction.ipynb)

Setup

First, let's import a few common modules, ensure MatplotLib plots figures inline and prepare a function to save the figures. We also check that Python 3.5 or later is installed (although Python 2.x may work, it is deprecated so we strongly recommend you use Python 3 instead), as well as Scikit-Learn ≥0.20.

In [1]:
```
# Python ≥3.5 is required
import sys
assert sys.version_info >= (3, 5)

# Scikit-Learn ≥0.20 is required
import sklearn
assert sklearn.__version__ >= "0.20"

# Common imports
import numpy as np
import os

# to make this notebook's output stable across runs
np.random.seed(42)

# To plot pretty figures
%matplotlib inline
import matplotlib as mpl
import matplotlib.pyplot as plt
mpl.rc('axes', labelsize=14)
mpl.rc('xtick', labelsize=12)
mpl.rc('ytick', labelsize=12)

# Where to save the figures
PROJECT_ROOT_DIR = "."
CHAPTER_ID = "dim_reduction"
IMAGES_PATH = os.path.join(PROJECT_ROOT_DIR, "images", CHAPTER_ID)
os.makedirs(IMAGES_PATH, exist_ok=True)

def save_fig(fig_id, tight_layout=True, fig_extension="png", resolution=300):
    path = os.path.join(IMAGES_PATH, fig_id + "." + fig_extension)
    print("Saving figure", fig_id)
    if tight_layout:
        plt.tight_layout()
    plt.savefig(path, format=fig_extension, dpi=resolution)

# Ignore useless warnings (see SciPy issue #5998)
import warnings
warnings.filterwarnings(action="ignore", message="^internal gelsd")
```

Projection methods

Build 3D dataset:

In [2]:
```
np.random.seed(4)
m = 60
w1, w2 = 0.1, 0.3
noise = 0.1

angles = np.random.rand(m) * 3 * np.pi / 2 - 0.5
X = np.empty((m, 3))
X[:, 0] = np.cos(angles) + np.sin(angles)/2 + noise * np.random.randn(m) / 2
X[:, 1] = np.sin(angles) * 0.7 + noise * np.random.randn(m) / 2
X[:, 2] = X[:, 0] * w1 + X[:, 1] * w2 + noise * np.random.randn(m)
```

PCA using SVD decomposition

In [3]:
```
X_centered = X - X.mean(axis=0)
U, s, Vt = np.linalg.svd(X_centered)
c1 = Vt.T[:, 0]
c2 = Vt.T[:, 1]
```

In [4]:
```
m, n = X.shape

S = np.zeros(X_centered.shape)
S[:n, :n] = np.diag(s)
```

In [5]:
```
np.allclose(X_centered, U.dot(S).dot(Vt))
```

Out[5]:
```
True
```

In [6]:
```
W2 = Vt.T[:, :2]
X2D = X_centered.dot(W2)
```

In [7]:
```
X2D_using_svd = X2D
```

PCA using Scikit-Learn

With Scikit-Learn, PCA is really trivial. It even takes care of mean centering for you:

In [8]:
```
from sklearn.decomposition import PCA

pca = PCA(n_components = 2)
X2D = pca.fit_transform(X)
```

In [9]:
```
X2D[:5]
```

Out[9]:
```
array([[ 1.26203346,  0.42067648],
       [-0.08001485, -0.35272239],
       [ 1.17545763,  0.36085729],
       [ 0.89305601, -0.30862856],
       [ 0.73016287, -0.25404049]])
```

In [10]:
```
X2D_using_svd[:5]
```

Out[10]:
```
array([[-1.26203346, -0.42067648],
       [ 0.08001485,  0.35272239],
       [-1.17545763, -0.36085729],
       [-0.89305601,  0.30862856],
       [-0.73016287,  0.25404049]])
```

Notice that running PCA multiple times on slightly different datasets may result in different results. In general the only difference is that some axes may be flipped. In this example, PCA using Scikit-Learn gives the same projection as the one given by the SVD approach, except both axes are flipped:

In [11]:
```
np.allclose(X2D, -X2D_using_svd)
```
Out[11]:
```
True
```

Recover the 3D points projected on the plane (PCA 2D subspace).

In [12]:
```
X3D_inv = pca.inverse_transform(X2D)
```

Of course, there was some loss of information during the projection step, so the recovered 3D points are not exactly equal to the original 3D points:

In [13]:
```
np.allclose(X3D_inv, X)
```
Out[13]:
```
False
```

We can compute the reconstruction error:

In [14]:
```
np.mean(np.sum(np.square(X3D_inv - X), axis=1))
```
Out[14]:
```
0.010170337792848549
```

The inverse transform in the SVD approach looks like this:

In [15]:
```
X3D_inv_using_svd = X2D_using_svd.dot(Vt[:2, :])
```

The reconstructions from both methods are not identical because Scikit-Learn's `PCA` class automatically takes care of reversing the mean centering, but if we subtract the mean, we get the same reconstruction:

In [16]:
```
np.allclose(X3D_inv_using_svd, X3D_inv - pca.mean_)
```
Out[16]:
```
True
```

The `PCA` object gives access to the principal components that it computed:

In [17]:
```
pca.components_
```
Out[17]:
```
array([[-0.93636116, -0.29854881, -0.18465208],
       [ 0.34027485, -0.90119108, -0.2684542 ]])
```

Compare to the first two principal components computed using the SVD method:

In [18]:
```
Vt[:2]
```
Out[18]:
```
array([[ 0.93636116,  0.29854881,  0.18465208],
       [-0.34027485,  0.90119108,  0.2684542 ]])
```

Notice how the axes are flipped.

Now let's look at the explained variance ratio:

In [19]:
```
pca.explained_variance_ratio_
```
Out[19]:
```
array([0.84248607, 0.14631839])
```

The first dimension explains 84.2% of the variance, while the second explains 14.6%.

By projecting down to 2D, we lost about 1.1% of the variance:

In [20]:
```
1 - pca.explained_variance_ratio_.sum()
```

Out[20]: 0.011195535570688975

Here is how to compute the explained variance ratio using the SVD approach (recall that `s` is the diagonal of the matrix `S`):

In [21]:
```
np.square(s) / np.square(s).sum()
```

Out[21]: array([0.84248607, 0.14631839, 0.01119554])

Next, let's generate some nice figures! :)

Utility class to draw 3D arrows (copied from [http://stackoverflow.com/questions/11140163 (http://stackoverflow.com/questions/11140163)](http://stackoverflow.com/questions/11140163))

In [22]:
```
from matplotlib.patches import FancyArrowPatch
from mpl_toolkits.mplot3d import proj3d

class Arrow3D(FancyArrowPatch):
    def __init__(self, xs, ys, zs, *args, **kwargs):
        FancyArrowPatch.__init__(self, (0,0), (0,0), *args, **kwargs)
        self._verts3d = xs, ys, zs

    def draw(self, renderer):
        xs3d, ys3d, zs3d = self._verts3d
        xs, ys, zs = proj3d.proj_transform(xs3d, ys3d, zs3d, renderer.M)
        self.set_positions((xs[0],ys[0]),(xs[1],ys[1]))
        FancyArrowPatch.draw(self, renderer)
```

Express the plane as a function of x and y.

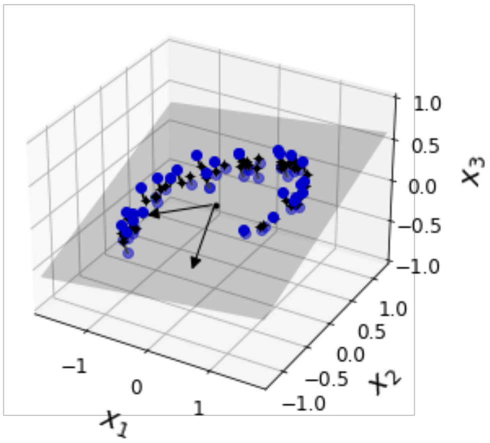
In [23]:
```
axes = [-1.8, 1.8, -1.3, 1.3, -1.0, 1.0]

x1s = np.linspace(axes[0], axes[1], 10)
x2s = np.linspace(axes[2], axes[3], 10)
x1, x2 = np.meshgrid(x1s, x2s)

C = pca.components_
R = C.T.dot(C)
z = (R[0, 2] * x1 + R[1, 2] * x2) / (1 - R[2, 2])
```

Plot the 3D dataset, the plane and the projections on that plane.

In [24]:
```
from mpl_toolkits.mplot3d import Axes3D

fig = plt.figure(figsize=(6, 3.8))
ax = fig.add_subplot(111, projection='3d')

X3D_above = X[X[:, 2] > X3D_inv[:, 2]]
X3D_below = X[X[:, 2] <= X3D_inv[:, 2]]

ax.plot(X3D_below[:, 0], X3D_below[:, 1], X3D_below[:, 2], "bo", alpha=0.5)

ax.plot_surface(x1, x2, z, alpha=0.2, color="k")
np.linalg.norm(C, axis=0)
ax.add_artist(Arrow3D([0, C[0, 0]],[0, C[0, 1]],[0, C[0, 2]], mutation_scale=15
ax.add_artist(Arrow3D([0, C[1, 0]],[0, C[1, 1]],[0, C[1, 2]], mutation_scale=15
ax.plot([0], [0], [0], "k.")
```

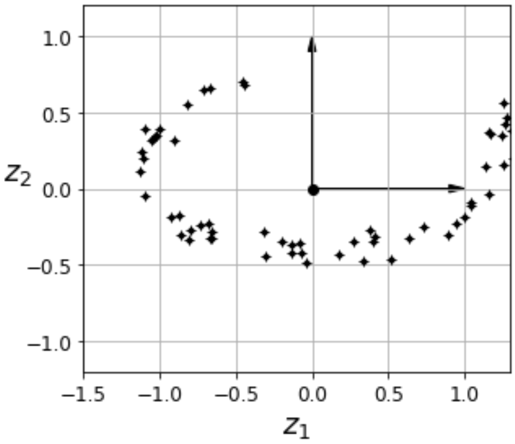
```
for i in range(m):
    if X[i, 2] > X3D_inv[i, 2]:
        ax.plot([X[i][0], X3D_inv[i][0]], [X[i][1], X3D_inv[i][1]], [X[i][2], X
    else:
        ax.plot([X[i][0], X3D_inv[i][0]], [X[i][1], X3D_inv[i][1]], [X[i][2], X

ax.plot(X3D_inv[:, 0], X3D_inv[:, 1], X3D_inv[:, 2], "k+")
ax.plot(X3D_inv[:, 0], X3D_inv[:, 1], X3D_inv[:, 2], "k.")
ax.plot(X3D_above[:, 0], X3D_above[:, 1], X3D_above[:, 2], "bo")
ax.set_xlabel("$x_1$", fontsize=18, labelpad=10)
ax.set_ylabel("$x_2$", fontsize=18, labelpad=10)
ax.set_zlabel("$x_3$", fontsize=18, labelpad=10)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])

# Note: If you are using Matplotlib 3.0.0, it has a bug and does not
# display 3D graphs properly.
# See https://github.com/matplotlib/matplotlib/issues/12239
# You should upgrade to a later version. If you cannot, then you can
# use the following workaround before displaying each 3D graph:
# for spine in ax.spines.values():
#     spine.set_visible(False)

save_fig("dataset_3d_plot")
plt.show()
```

```
Saving figure dataset_3d_plot
```



In [25]:
```
fig = plt.figure()
ax = fig.add_subplot(111, aspect='equal')

ax.plot(X2D[:, 0], X2D[:, 1], "k+")
ax.plot(X2D[:, 0], X2D[:, 1], "k.")
ax.plot([0], [0], "ko")
ax.arrow(0, 0, 0, 1, head_width=0.05, length_includes_head=True, head_length=0.
ax.arrow(0, 0, 1, 0, head_width=0.05, length_includes_head=True, head_length=0.
ax.set_xlabel("$z_1$", fontsize=18)
ax.set_ylabel("$z_2$", fontsize=18, rotation=0)
ax.axis([-1.5, 1.3, -1.2, 1.2])
ax.grid(True)
save_fig("dataset_2d_plot")
```

```
Saving figure dataset_2d_plot
```



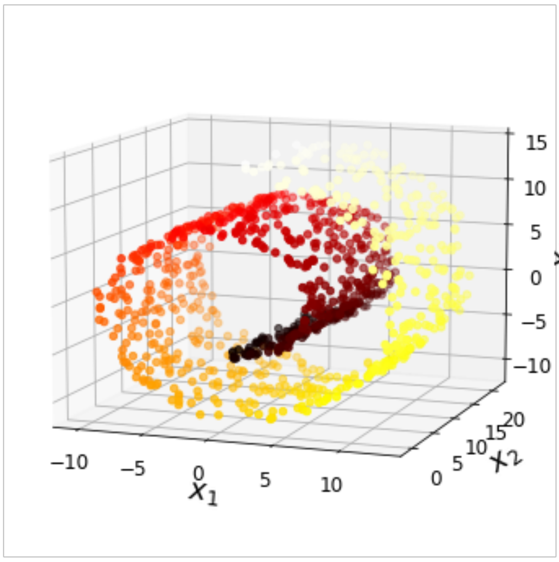
Manifold learning

Swiss roll:

In [26]:
```
from sklearn.datasets import make_swiss_roll
X, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=42)
```

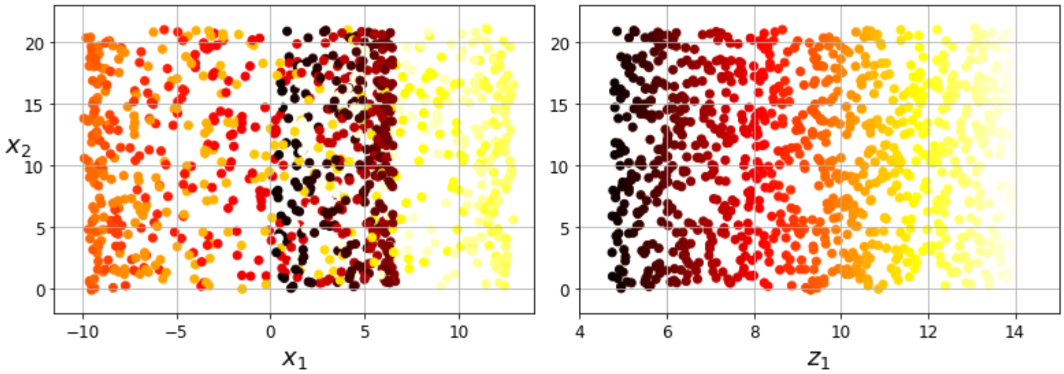
In [27]:
```
axes = [-11.5, 14, -2, 23, -12, 15]

fig = plt.figure(figsize=(6, 5))
ax = fig.add_subplot(111, projection='3d')

ax.scatter(X[:, 0], X[:, 1], X[:, 2], c=t, cmap=plt.cm.hot)
ax.view_init(10, -70)
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])

save_fig("swiss_roll_plot")
plt.show()
```

```
Saving figure swiss_roll_plot
```



In [28]:
```
plt.figure(figsize=(11, 4))

plt.subplot(121)
plt.scatter(X[:, 0], X[:, 1], c=t, cmap=plt.cm.hot)
plt.axis(axes[:4])
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$x_2$", fontsize=18, rotation=0)
plt.grid(True)

plt.subplot(122)
plt.scatter(t, X[:, 1], c=t, cmap=plt.cm.hot)
plt.axis([4, 15, axes[2], axes[3]])
plt.xlabel("$z_1$", fontsize=18)
plt.grid(True)

save_fig("squished_swiss_roll_plot")
plt.show()
```

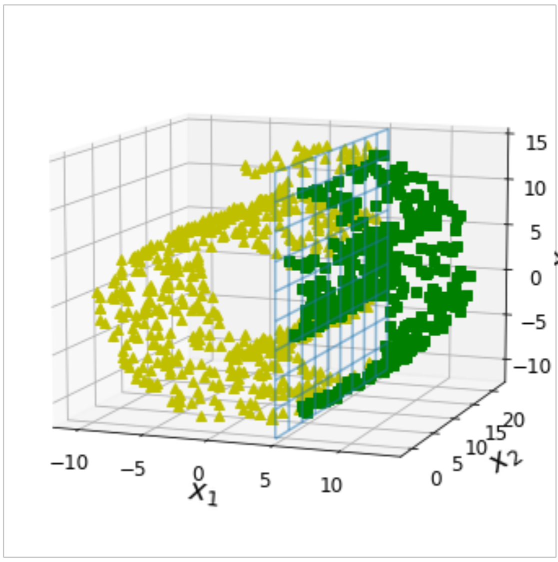
```
Saving figure squished_swiss_roll_plot
```



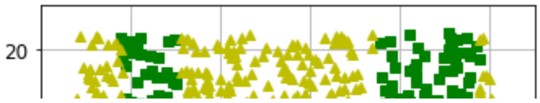
In [29]:
```
from matplotlib import gridspec

axes = [-11.5, 14, -2, 23, -12, 15]

x2s = np.linspace(axes[2], axes[3], 10)
x3s = np.linspace(axes[4], axes[5], 10)
x2, x3 = np.meshgrid(x2s, x3s)

fig = plt.figure(figsize=(6, 5))
ax = plt.subplot(111, projection='3d')

positive_class = X[:, 0] > 5
X_pos = X[positive_class]
X_neg = X[~positive_class]
ax.view_init(10, -70)
ax.plot(X_neg[:, 0], X_neg[:, 1], X_neg[:, 2], "y^")
ax.plot_wireframe(5, x2, x3, alpha=0.5)
ax.plot(X_pos[:, 0], X_pos[:, 1], X_pos[:, 2], "gs")
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])

save_fig("manifold_decision_boundary_plot1")
plt.show()

fig = plt.figure(figsize=(5, 4))
ax = plt.subplot(111)

plt.plot(t[positive_class], X[positive_class, 1], "gs")
plt.plot(t[~positive_class], X[~positive_class, 1], "y^")
```

```
plt.axis([4, 15, axes[2], axes[3]])
plt.xlabel("$z_1$", fontsize=18)
plt.ylabel("$z_2$", fontsize=18, rotation=0)
plt.grid(True)

save_fig("manifold_decision_boundary_plot2")
plt.show()

fig = plt.figure(figsize=(6, 5))
ax = plt.subplot(111, projection='3d')

positive_class = 2 * (t[:] - 4) > X[:, 1]
X_pos = X[positive_class]
X_neg = X[~positive_class]
ax.view_init(10, -70)
ax.plot(X_neg[:, 0], X_neg[:, 1], X_neg[:, 2], "y^")
ax.plot(X_pos[:, 0], X_pos[:, 1], X_pos[:, 2], "gs")
ax.set_xlabel("$x_1$", fontsize=18)
ax.set_ylabel("$x_2$", fontsize=18)
ax.set_zlabel("$x_3$", fontsize=18)
ax.set_xlim(axes[0:2])
ax.set_ylim(axes[2:4])
ax.set_zlim(axes[4:6])

save_fig("manifold_decision_boundary_plot3")
plt.show()

fig = plt.figure(figsize=(5, 4))
ax = plt.subplot(111)

plt.plot(t[positive_class], X[positive_class, 1], "gs")
plt.plot(t[~positive_class], X[~positive_class, 1], "y^")
plt.plot([4, 15], [0, 22], "b-", linewidth=2)
plt.axis([4, 15, axes[2], axes[3]])
plt.xlabel("$z_1$", fontsize=18)
plt.ylabel("$z_2$", fontsize=18, rotation=0)
plt.grid(True)

save_fig("manifold_decision_boundary_plot4")
plt.show()
```

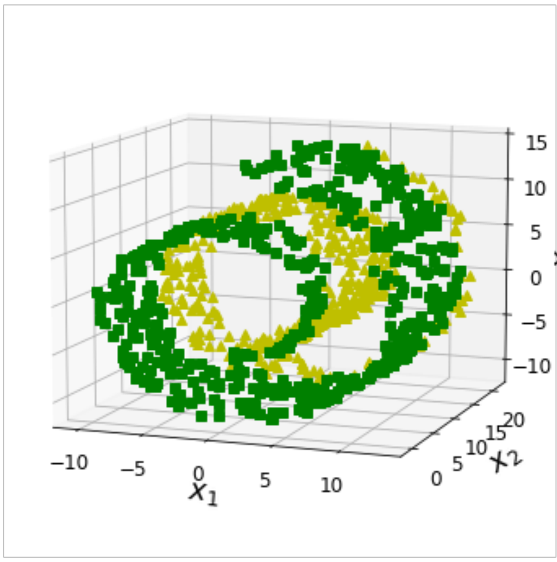
```
Saving figure manifold_decision_boundary_plot1
```



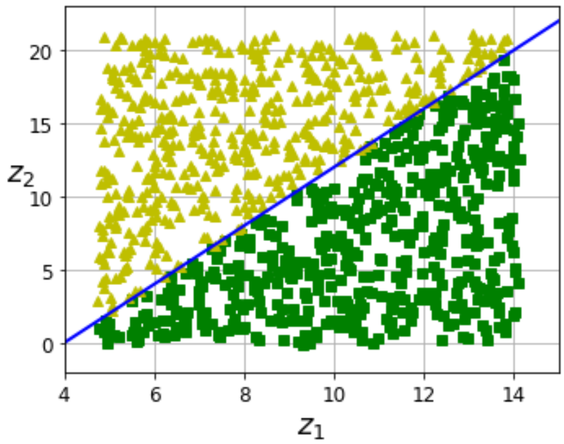

```
Saving figure manifold_decision_boundary_plot2
```



```
Saving figure manifold_decision_boundary_plot3
```




```
Saving figure manifold_decision_boundary_plot4
```



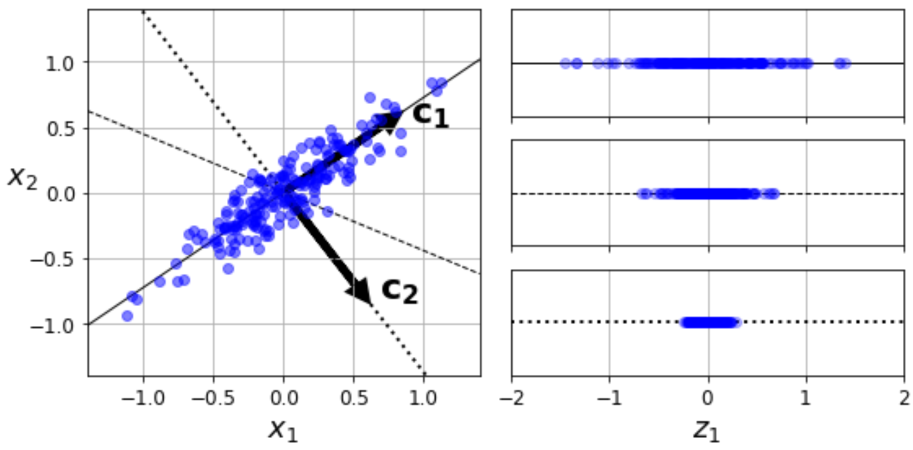
PCA

In [30]:

```python
angle = np.pi / 5
stretch = 5
m = 200

np.random.seed(3)
X = np.random.randn(m, 2) / 10
X = X.dot(np.array([[stretch, 0],[0, 1]])) # stretch
X = X.dot([[np.cos(angle), np.sin(angle)], [-np.sin(angle), np.cos(angle)]]) #

u1 = np.array([np.cos(angle), np.sin(angle)])
u2 = np.array([np.cos(angle - 2 * np.pi/6), np.sin(angle - 2 * np.pi/6)])
u3 = np.array([np.cos(angle - np.pi/2), np.sin(angle - np.pi/2)])

X_proj1 = X.dot(u1.reshape(-1, 1))
X_proj2 = X.dot(u2.reshape(-1, 1))
X_proj3 = X.dot(u3.reshape(-1, 1))

plt.figure(figsize=(8,4))
plt.subplot2grid((3,2), (0, 0), rowspan=3)
plt.plot([-1.4, 1.4], [-1.4*u1[1]/u1[0], 1.4*u1[1]/u1[0]], "k-", linewidth=1)
plt.plot([-1.4, 1.4], [-1.4*u2[1]/u2[0], 1.4*u2[1]/u2[0]], "k--", linewidth=1)
```

```
plt.plot([-1.4, 1.4], [-1.4*u3[1]/u3[0], 1.4*u3[1]/u3[0]], "k:", linewidth=2)
plt.plot(X[:, 0], X[:, 1], "bo", alpha=0.5)
plt.axis([-1.4, 1.4, -1.4, 1.4])
plt.arrow(0, 0, u1[0], u1[1], head_width=0.1, linewidth=5, length_includes_head
plt.arrow(0, 0, u3[0], u3[1], head_width=0.1, linewidth=5, length_includes_head
plt.text(u1[0] + 0.1, u1[1] - 0.05, r"$\mathbf{c_1}$", fontsize=22)
plt.text(u3[0] + 0.1, u3[1], r"$\mathbf{c_2}$", fontsize=22)
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$x_2$", fontsize=18, rotation=0)
plt.grid(True)

plt.subplot2grid((3,2), (0, 1))
plt.plot([-2, 2], [0, 0], "k-", linewidth=1)
plt.plot(X_proj1[:, 0], np.zeros(m), "bo", alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-2, 2, -1, 1])
plt.grid(True)

plt.subplot2grid((3,2), (1, 1))
plt.plot([-2, 2], [0, 0], "k--", linewidth=1)
plt.plot(X_proj2[:, 0], np.zeros(m), "bo", alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.gca().get_xaxis().set_ticklabels([])
plt.axis([-2, 2, -1, 1])
plt.grid(True)

plt.subplot2grid((3,2), (2, 1))
plt.plot([-2, 2], [0, 0], "k:", linewidth=2)
plt.plot(X_proj3[:, 0], np.zeros(m), "bo", alpha=0.3)
plt.gca().get_yaxis().set_ticks([])
plt.axis([-2, 2, -1, 1])
plt.xlabel("$z_1$", fontsize=18)
plt.grid(True)

save_fig("pca_best_projection_plot")
plt.show()
```

Saving figure pca_best_projection_plot



MNIST compression

In [31]:
```
from sklearn.datasets import fetch_openml

mnist = fetch_openml('mnist_784', version=1)
mnist.target = mnist.target.astype(np.uint8)
```

In [32]:
```
from sklearn.model_selection import train_test_split
```

```
X = mnist["data"]
y = mnist["target"]

X_train, X_test, y_train, y_test = train_test_split(X, y)
```

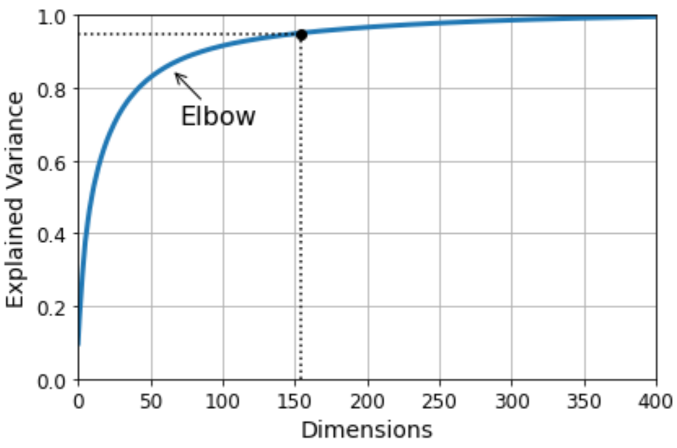
In [33]:
```
pca = PCA()
pca.fit(X_train)
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.95) + 1
```

In [34]:
```
d
```

Out[34]: 154

In [35]:
```
plt.figure(figsize=(6,4))
plt.plot(cumsum, linewidth=3)
plt.axis([0, 400, 0, 1])
plt.xlabel("Dimensions")
plt.ylabel("Explained Variance")
plt.plot([d, d], [0, 0.95], "k:")
plt.plot([0, d], [0.95, 0.95], "k:")
plt.plot(d, 0.95, "ko")
plt.annotate("Elbow", xy=(65, 0.85), xytext=(70, 0.7),
             arrowprops=dict(arrowstyle="->"), fontsize=16)
plt.grid(True)
save_fig("explained_variance_plot")
plt.show()
```

Saving figure explained_variance_plot



In [36]:
```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X_train)
```

In [37]:
```
pca.n_components_
```

Out[37]: 154

In [38]:
```
np.sum(pca.explained_variance_ratio_)
```

Out[38]: 0.9504334914295706

LLE

In [39]:
```
X, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=41)
```

In [40]:
```
from sklearn.manifold import LocallyLinearEmbedding

lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10, random_state=42)
```

```
X_reduced = lle.fit_transform(X)
```

In [41]:
```
plt.title("Unrolled swiss roll using LLE", fontsize=14)
plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=t, cmap=plt.cm.hot)
plt.xlabel("$z_1$", fontsize=18)
plt.ylabel("$z_2$", fontsize=18)
plt.axis([-0.065, 0.055, -0.1, 0.12])
plt.grid(True)

save_fig("lle_unrolling_plot")
plt.show()
```

```
Saving figure lle_unrolling_plot
```