Machine Learning
MSE FTP MachLe
Christoph Würsch

V11 Dimensionality Reduction (TSM_MachLE)

Comparison of different methods

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- MSE TSM_MachLe

based on a Jupyter notebook by Aurelien Géron

Setup

First, let's make sure this notebook works well in both python 2 and 3, import a few common modules, ensure MatplotLib plots figures inline and prepare a function to save the figures:

In [1]:
```
# To support both python 2 and python 3
from __future__ import division, print_function, unicode_literals

# 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
import matplotlib.pyplot as plt
plt.rcParams['axes.labelsize'] = 14
plt.rcParams['xtick.labelsize'] = 12
plt.rcParams['ytick.labelsize'] = 12
```

Generate a 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 Scikit-Learn

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

In [3]:
```
from sklearn.decomposition import PCA

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

In [4]:
```
X2D[:5]
```

Out[4]:
```
array([[ 1.26203346,  0.42067648],
       [-0.08001485, -0.35272239],
       [ 1.17545763,  0.36085729],
       [ 0.89305601, -0.30862856],
       [ 0.73016287, -0.25404049]])
```

In [5]:
```
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 [6]:
```
np.allclose(X3D_inv, X)
```

Out[6]:
```
False
```

We can compute the reconstruction error:

In [7]:
```
np.mean(np.sum(np.square(X3D_inv - X), axis=1))
```

Out[7]:
```
0.010170337792848549
```

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

In [8]:
```
pca.components_
```

Out[8]:
```
array([[-0.93636116, -0.29854881, -0.18465208],
       [ 0.34027485, -0.90119108, -0.2684542 ]])
```

Now let's look at the explained variance ratio:

In [9]:
```
pca.explained_variance_ratio_
```

Out[9]:
```
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 [10]:
```
1 - pca.explained_variance_ratio_.sum()
```

Out[10]:
```
0.011195535570688975
```

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

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

In [11]:
```
from matplotlib.patches import FancyArrowPatch
from mpl_toolkits.mplot3d import proj3d

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

    def do_3d_projection(self, renderer=None):
        xs3d, ys3d, zs3d = self._verts3d
        xs, ys, zs = proj3d.proj_transform(xs3d, ys3d, zs3d, self.axes.M)
        self.set_positions((xs[0],ys[0]),(xs[1],ys[1]))

        return np.min(zs)
```

Express the plane as a function of x and y.

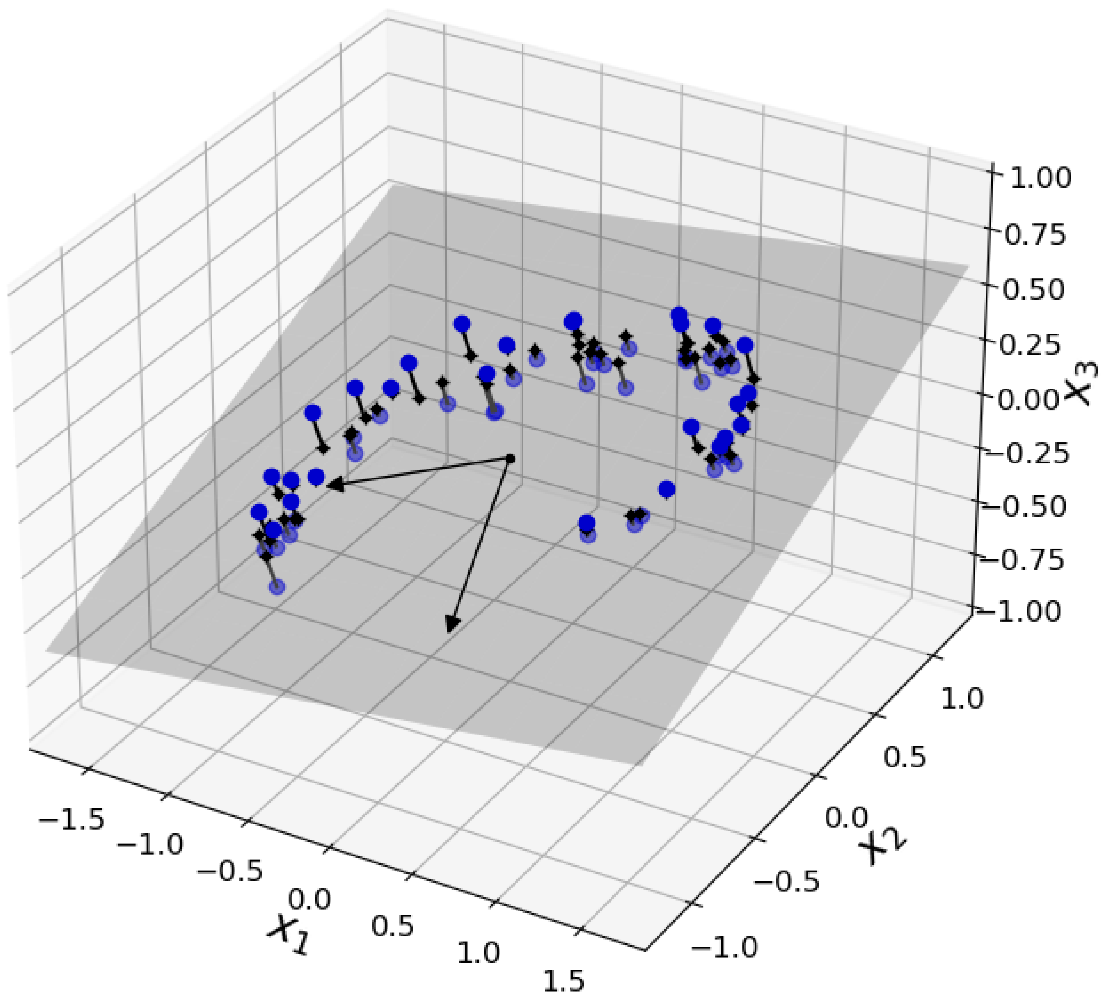
In [12]:
```
axes = [-1.8, 1.8, -1.3, 1.3, -1.0, 1.0]

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 [13]:
```
from mpl_toolkits.mplot3d import Axes3D

fig = plt.figure(figsize=(8, 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, l
ax.add_artist(Arrow3D([0, C[1, 0]],[0, C[1, 1]],[0, C[1, 2]], mutation_scale=15, l
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], X3D_
    else:
        ax.plot([X[i][0], X3D_inv[i][0]], [X[i][1], X3D_inv[i][1]], [X[i][2], X3D_

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)
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])

plt.show()
plt.savefig('PCA-demo.pdf')
```

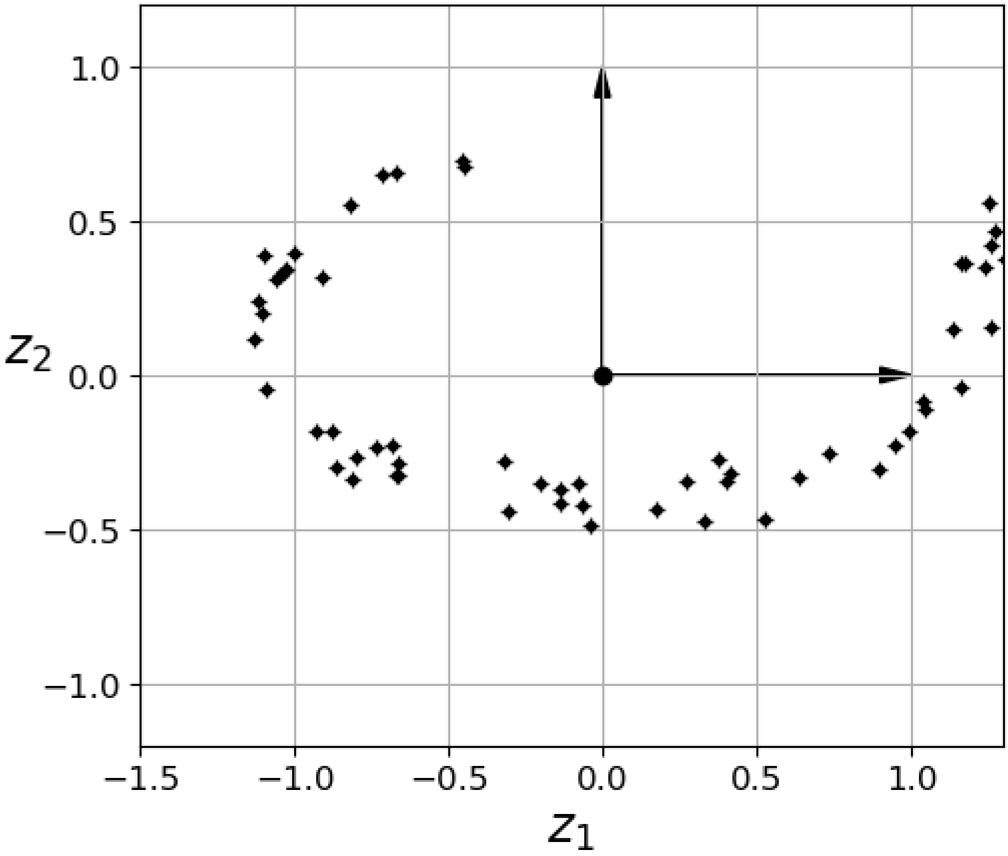
```
C:\Users\christoph.wuersch\AppData\Local\Temp\ipykernel_20592\3871663956.py:21: UserWarning: color is redundantly defined by the 'color' keyword argument and the fmt string "k-" (-> color='k'). The keyword argument will take precedence.
  ax.plot([X[i][0], X3D_inv[i][0]], [X[i][1], X3D_inv[i][1]], [X[i][2], X3D_inv[i][2]], "k-", color="#505050")
```




```
<Figure size 640x480 with 0 Axes>
```

In [14]:

```
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=0.1,
ax.arrow(0, 0, 1, 0, head_width=0.05, length_includes_head=True, head_length=0.1,
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)
plt.savefig('PCA-demo_2D.pdf')
```

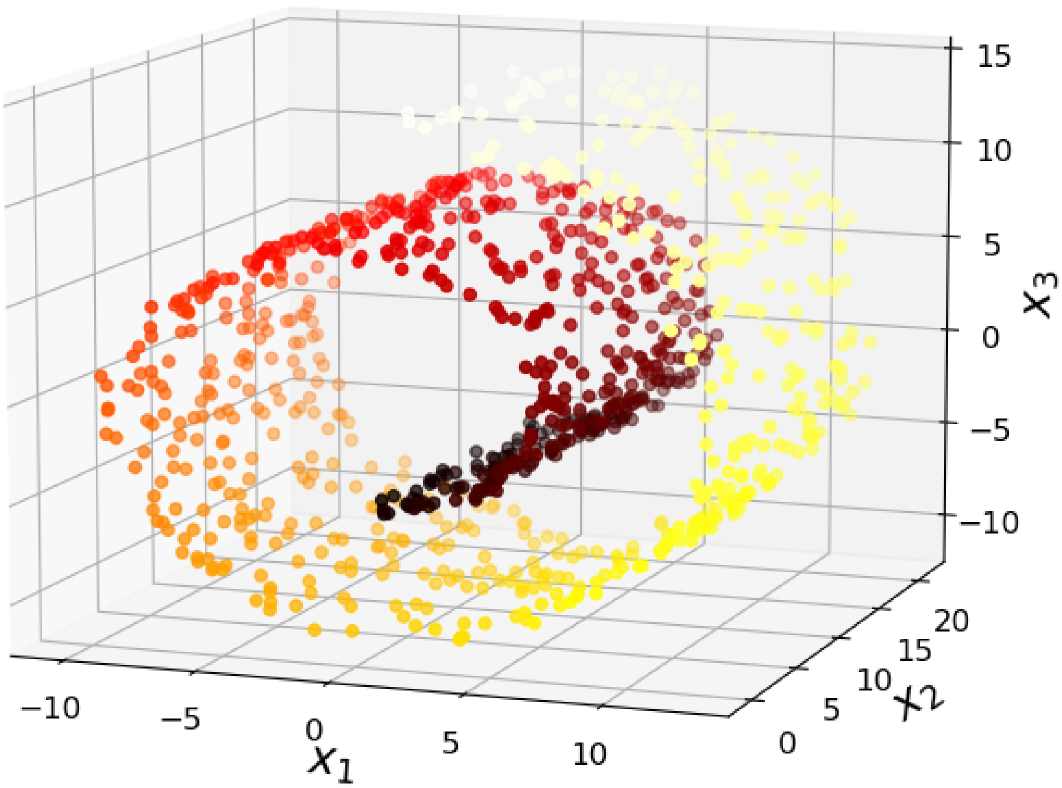


Manifold learning

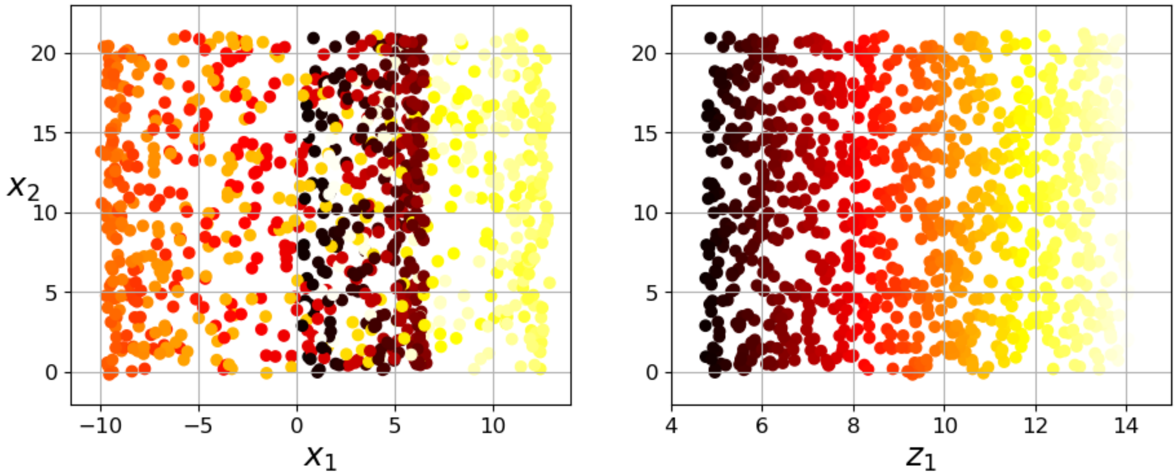
Swiss roll:

In [15]:
```
from sklearn.datasets import make_swiss_roll
X, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=42)
```

In [16]:
```
axes = [-11.5, 14, -2, 23, -12, 15]

fig = plt.figure(figsize=(8, 8))
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])

plt.savefig('SwissRoll.pdf')
plt.show()
```

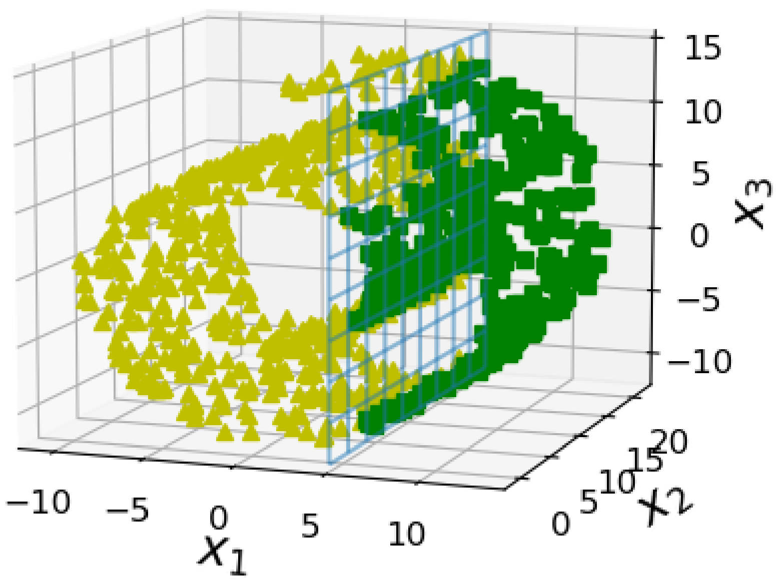


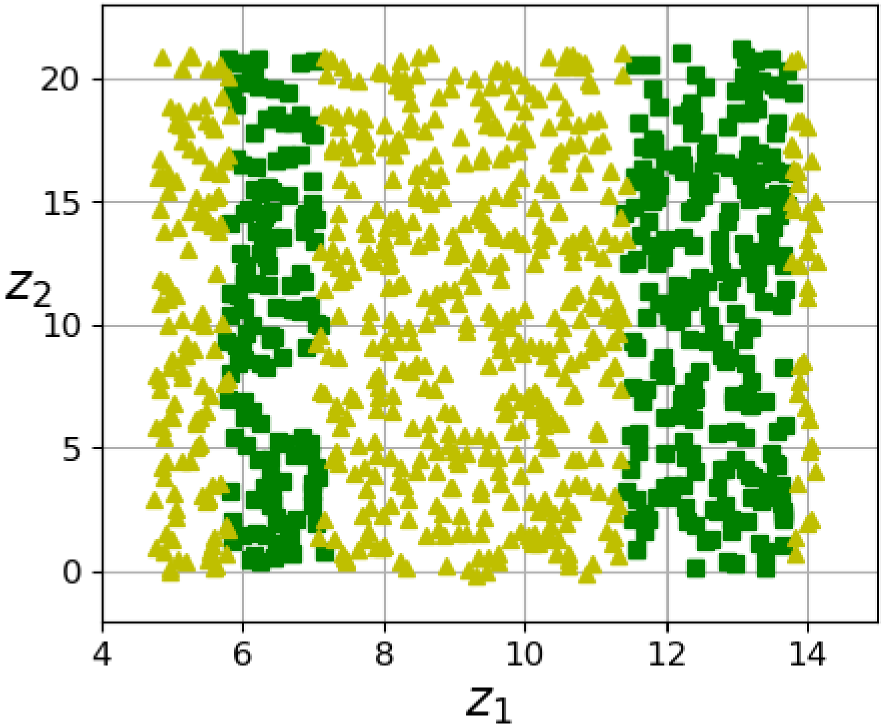
In [17]:
```
plt.figure(figsize=(11, 4))

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)

plt.savefig('squished_swiss_roll_plot.pdf')
plt.show()
```

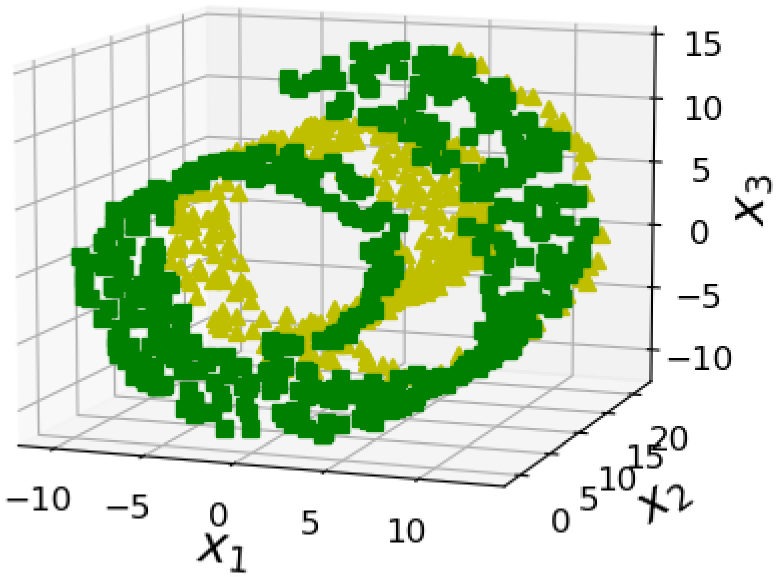


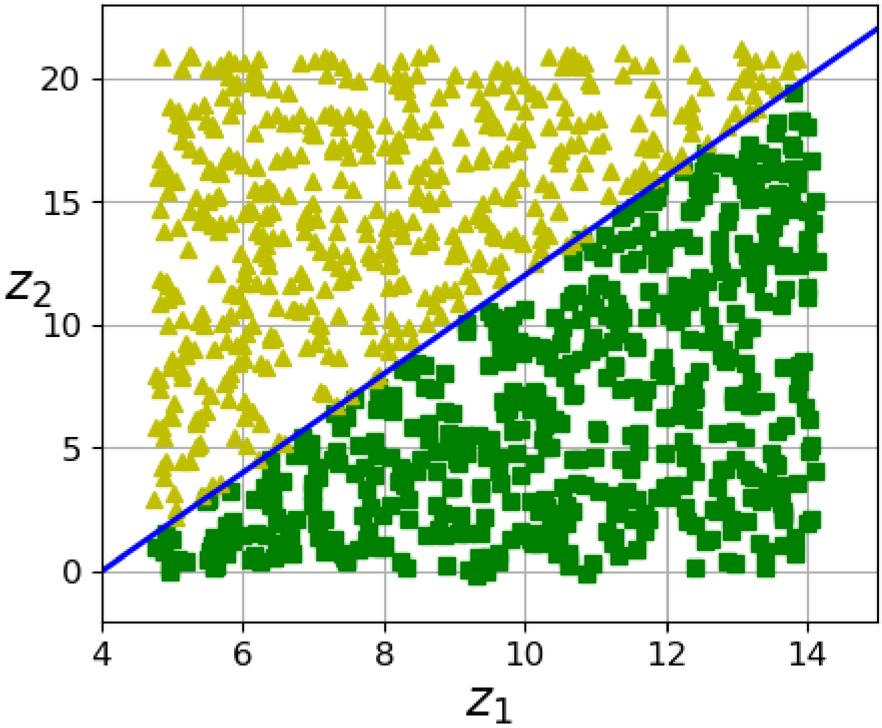
In [18]:
```
from matplotlib import gridspec

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])

plt.savefig('manifold_decision_boundary_1.pdf')
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)

plt.savefig('manifold_decision_boundary_2.pdf')
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])

plt.savefig('manifold_decision_boundary_3.pdf')
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)

plt.savefig('manifold_decision_boundary_4.pdf')
plt.show()
```




20
15
10
5
0
z_2
4
6
8
10
12
14
z_1

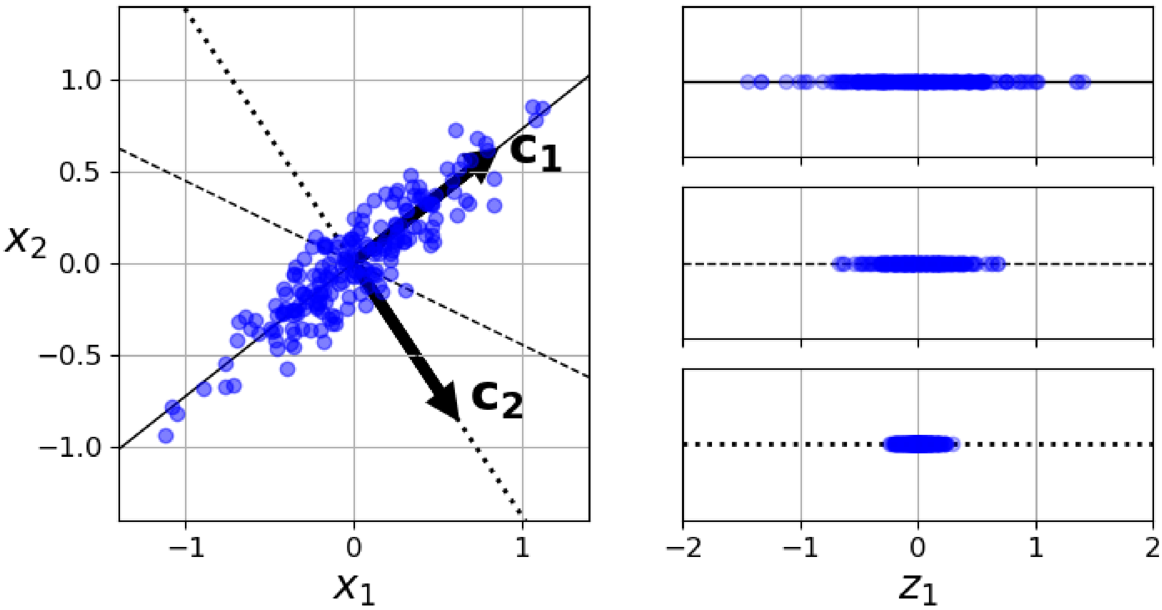

15
10
5
0
−5
−10
x_3
−10
−5
0
5
10
x_1
0
5
10
15
20
x_2



PCA

In [19]:
```
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)]]) # rot

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=Tr
plt.arrow(0, 0, u3[0], u3[1], head_width=0.1, linewidth=5, length_includes_head=Tr
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)

plt.savefig('pca_best_projection.pdf')
plt.show()
```



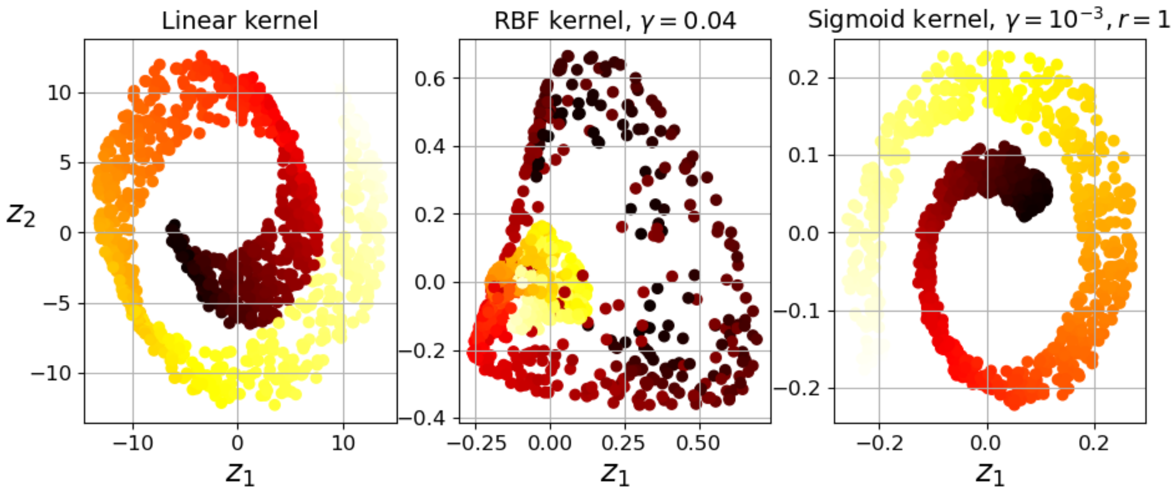
Kernel PCA

In [20]:
```
X, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=42)
```

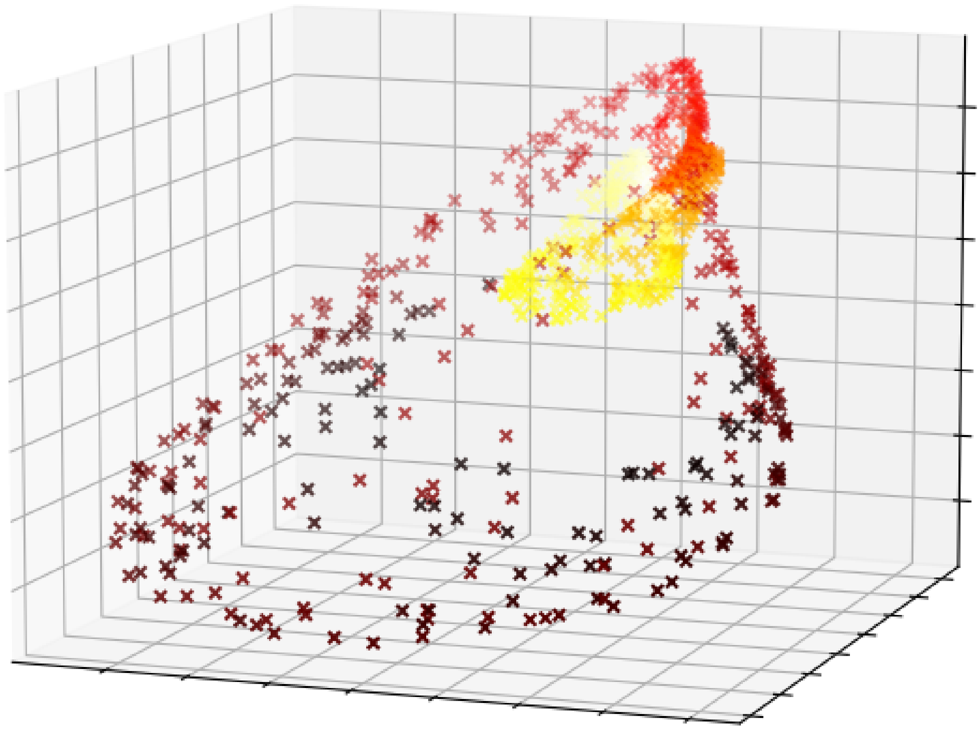
In [21]:
```
from sklearn.decomposition import KernelPCA

rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.04)
X_reduced = rbf_pca.fit_transform(X)
```

In [22]:
```
from sklearn.decomposition import KernelPCA

lin_pca = KernelPCA(n_components = 2, kernel="linear", fit_inverse_transform=True)
rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.0433, fit_inverse_tran
sig_pca = KernelPCA(n_components = 2, kernel="sigmoid", gamma=0.001, coef0=1, fit_

y = t > 6.9
```

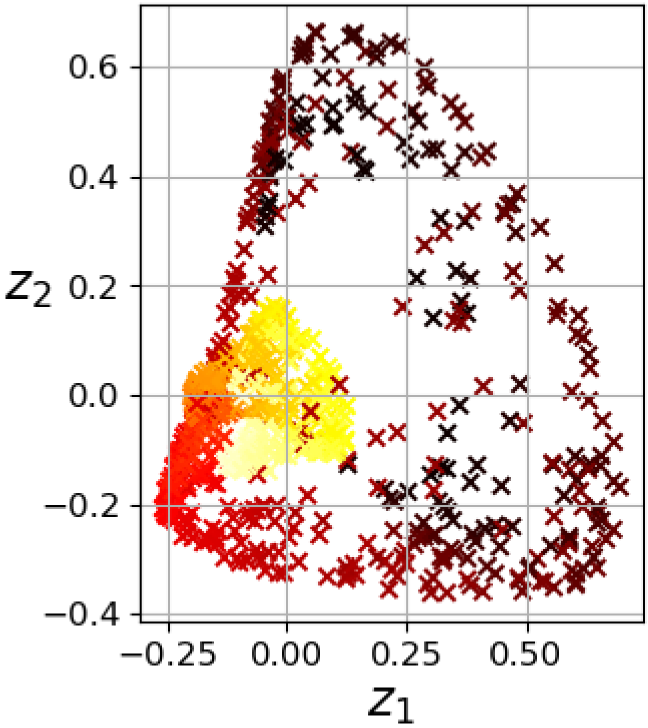
```
plt.figure(figsize=(11, 4))
for subplot, pca, title in ((131, lin_pca, "Linear kernel"), (132, rbf_pca, "RBF k
    X_reduced = pca.fit_transform(X)
    if subplot == 132:
        X_reduced_rbf = X_reduced

    plt.subplot(subplot)
    #plt.plot(X_reduced[y, 0], X_reduced[y, 1], "gs")
    #plt.plot(X_reduced[~y, 0], X_reduced[~y, 1], "y^")
    plt.title(title, fontsize=14)
    plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=t, cmap=plt.cm.hot)
    plt.xlabel("$z_1$", fontsize=18)
    if subplot == 131:
        plt.ylabel("$z_2$", fontsize=18, rotation=0)
    plt.grid(True)

plt.savefig('kernel_pca_plot.pdf')
plt.show()
```



In [23]:
```
plt.figure(figsize=(8,8))

X_inverse = pca.inverse_transform(X_reduced_rbf)

ax = plt.subplot(111, projection='3d')
ax.view_init(10, -70)
ax.scatter(X_inverse[:, 0], X_inverse[:, 1], X_inverse[:, 2], c=t, cmap=plt.cm.hot
ax.set_xlabel("")
ax.set_ylabel("")
ax.set_zlabel("")
ax.set_xticklabels([])
ax.set_yticklabels([])
ax.set_zticklabels([])

plt.savefig('preimage_plot.pdf')
plt.show()
```



In [24]:
```
X_reduced = rbf_pca.fit_transform(X)

plt.figure(figsize=(11, 4))
plt.subplot(132)
plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=t, cmap=plt.cm.hot, marker="x")
plt.xlabel("$z_1$", fontsize=18)
plt.ylabel("$z_2$", fontsize=18, rotation=0)
plt.grid(True)
```



In [25]:
```
from sklearn.model_selection import GridSearchCV
from sklearn.linear_model import LogisticRegression
from sklearn.pipeline import Pipeline

clf = Pipeline([
        ("kpca", KernelPCA(n_components=2)),
        ("log_reg", LogisticRegression(solver='lbfgs'))
    ])

param_grid = [{
        "kpca__gamma": np.linspace(0.03, 0.05, 10),
        "kpca__kernel": ["rbf", "sigmoid"]
    }]

grid_search = GridSearchCV(clf, param_grid, cv=3)
grid_search.fit(X, y)
```

Out[25]:
```
GridSearchCV(cv=3,
             estimator=Pipeline(steps=[('kpca', KernelPCA(n_components=2)),
                                       ('log_reg', LogisticRegression())]),
             param_grid=[{'kpca__gamma': array([0.03      , 0.03222222, 0.0344444
4, 0.03666667, 0.03888889,
       0.04111111, 0.04333333, 0.04555556, 0.04777778, 0.05      ]),
                          'kpca__kernel': ['rbf', 'sigmoid']}])
```

In [26]:
```
print(grid_search.best_params_)
```

```
{'kpca__gamma': 0.043333333333333335, 'kpca__kernel': 'rbf'}
```

In [27]:
```
rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.0433,
                    fit_inverse_transform=True)
X_reduced = rbf_pca.fit_transform(X)
X_preimage = rbf_pca.inverse_transform(X_reduced)
```

In [28]:
```
from sklearn.metrics import mean_squared_error

mean_squared_error(X, X_preimage)
```

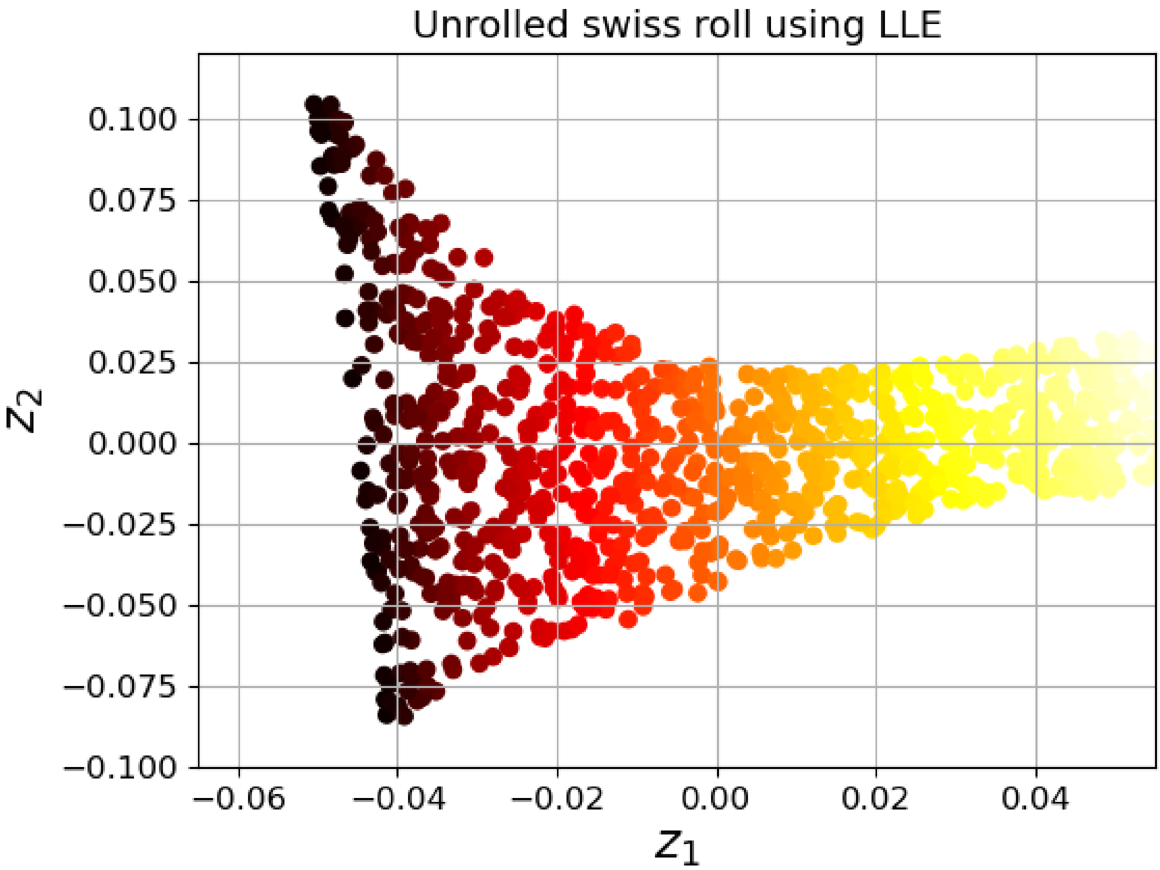
Out[28]:
```
32.78630879576608
```

LLE

In [29]:
```
X, t = make_swiss_roll(n_samples=1000, noise=0.2, random_state=41)
```

In [30]:
```
from sklearn.manifold import LocallyLinearEmbedding

lle = LocallyLinearEmbedding(n_components=2, n_neighbors=10, random_state=42)
X_reduced = lle.fit_transform(X)
```

In [31]:
```
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)

plt.savefig('lle_unrolling_plot.pdf')
plt.show()
```



MDS, Isomap and t-SNE

In [32]:
```
from sklearn.manifold import MDS

mds = MDS(n_components=2, random_state=42)
X_reduced_mds = mds.fit_transform(X)
```

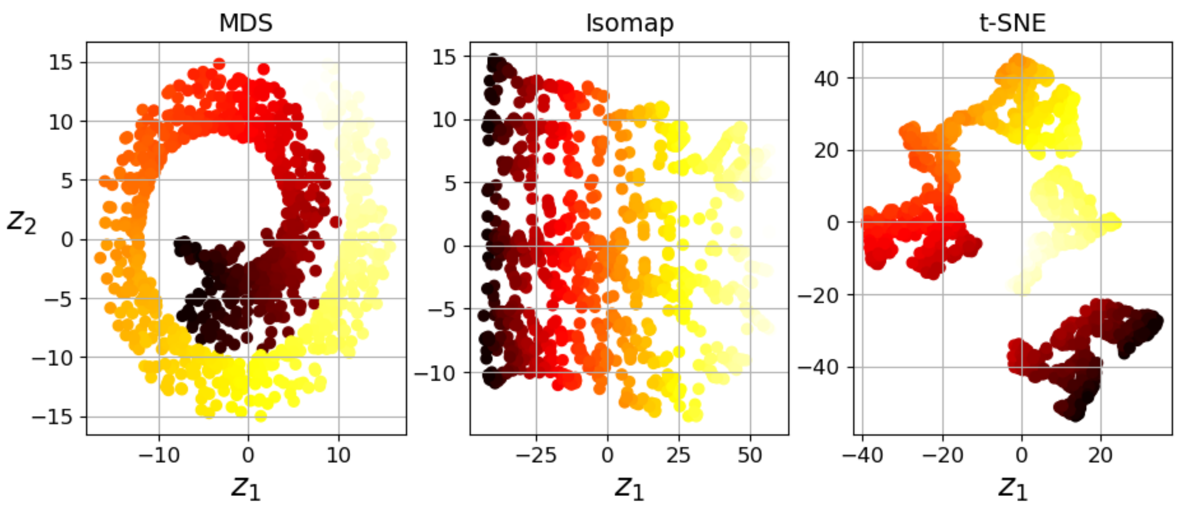
In [33]:
```
from sklearn.manifold import Isomap
```

```
isomap = Isomap(n_components=2)
X_reduced_isomap = isomap.fit_transform(X)
```

In [34]:
```
from sklearn.manifold import TSNE

tsne = TSNE(n_components=2, random_state=42)
X_reduced_tsne = tsne.fit_transform(X)
```

```
C:\Users\christoph.wuersch\.conda\envs\ML\lib\site-packages\sklearn\manifold\_t_sn
e.py:780: FutureWarning: The default initialization in TSNE will change from 'rand
om' to 'pca' in 1.2.
  warnings.warn(
C:\Users\christoph.wuersch\.conda\envs\ML\lib\site-packages\sklearn\manifold\_t_sn
e.py:790: FutureWarning: The default learning rate in TSNE will change from 200.0
to 'auto' in 1.2.
  warnings.warn(
```

In [35]:
```
titles = ["MDS", "Isomap", "t-SNE"]

plt.figure(figsize=(11,4))

for subplot, title, X_reduced in zip((131, 132, 133), titles,
                                     (X_reduced_mds, X_reduced_isomap, X_reduced_t
    plt.subplot(subplot)
    plt.title(title, fontsize=14)
    plt.scatter(X_reduced[:, 0], X_reduced[:, 1], c=t, cmap=plt.cm.hot)
    plt.xlabel("$z_1$", fontsize=18)
    if subplot == 131:
        plt.ylabel("$z_2$", fontsize=18, rotation=0)
    plt.grid(True)

plt.savefig('other_dim_reduction_plot.pdf')
plt.show()
```



In [ ]: