

plot_lle_digits

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In [ ]: %matplotlib inline
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Manifold learning on handwritten digits: Locally Linear Embedding, Isomap...
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An illustration of various embeddings on the digits dataset.

The RandomTreesEmbedding, from the :mod:sklearn.ensemble module, is not technically a manifold embedding method, as it learn a high-dimensional representation on which we apply a dimensionality reduction method. However, it is often useful to cast a dataset into a representation in which the classes are linearly-separable.

t-SNE will be initialized with the embedding that is generated by PCA in this example, which is not the default setting. It ensures global stability of the embedding, i.e., the embedding does not depend on random initialization.

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print(__doc__)
from time import time

import numpy as np
import matplotlib.pyplot as plt
from matplotlib import offsetbox
from sklearn import (manifold, datasets, decomposition, ensemble,
                     discriminant_analysis, random_projection)

digits = datasets.load_digits(n_class=6)
X = digits.data
y = digits.target
n_samples, n_features = X.shape
n_neighbors = 30

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# Scale and visualize the embedding vectors
def plot_embedding(X, title=None):
    x_min, x_max = np.min(X, 0), np.max(X, 0)
    X = (X - x_min) / (x_max - x_min)

    plt.figure()
    ax = plt.subplot(111)
    for i in range(X.shape[0]):
        plt.text(X[i, 0], X[i, 1], str(digits.target[i]),
                 color=plt.cm.Set1(y[i] / 10.),
                 fontdict={'weight': 'bold', 'size': 9})

    if hasattr(offsetbox, 'AnnotationBbox'):
        # only print thumbnails with matplotlib > 1.0
        shown_images = np.array([[1., 1.]]) # just something big
        for i in range(digits.data.shape[0]):
            dist = np.sum((X[i] - shown_images) ** 2, 1)
            if np.min(dist) < 4e-3:
                # don't show points that are too close
                continue
            shown_images = np.r_[shown_images, [X[i]]]
            imagebox = offsetbox.AnnotationBbox(
                offsetbox.OffsetImage(digits.images[i], cmap=plt.cm.gray_r),
                X[i])
            ax.add_artist(imagebox)
    plt.xticks([], plt.yticks([]))
    if title is not None:
        plt.title(title)

#-----
# Plot images of the digits
n_img_per_row = 20
img = np.zeros((10 * n_img_per_row, 10 * n_img_per_row))
for i in range(n_img_per_row):
    ix = 10 * i + 1
    for j in range(n_img_per_row):
        iy = 10 * j + 1
        img[ix:ix + 8, iy:iy + 8] = X[i * n_img_per_row + j].reshape((8, 8))

plt.imshow(img, cmap=plt.cm.binary)
plt.xticks([])
plt.yticks([])
plt.title('A selection from the 64-dimensional digits dataset')

#-----
# Random 2D projection using a random unitary matrix

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print("Computing random projection")
rp = random_projection.SparseRandomProjection(n_components=2, random_state=42)
X_projected = rp.fit_transform(X)
plot_embedding(X_projected, "Random Projection of the digits")

#-----
# Projection on to the first 2 principal components

print("Computing PCA projection")
t0 = time()
X_pca = decomposition.TruncatedSVD(n_components=2).fit_transform(X)
plot_embedding(X_pca,
               "Principal Components projection of the digits (time %.2fs)" %
               (time() - t0))

#-----
# Projection on to the first 2 linear discriminant components

print("Computing Linear Discriminant Analysis projection")
X2 = X.copy()
X2.flat[:X.shape[1] + 1] += 0.01 # Make X invertible
t0 = time()
X_lda = discriminant_analysis.LinearDiscriminantAnalysis(n_components=2).fit_transform(X)
plot_embedding(X_lda,
               "Linear Discriminant projection of the digits (time %.2fs)" %
               (time() - t0))

#-----
# Isomap projection of the digits dataset
print("Computing Isomap embedding")
t0 = time()
X_iso = manifold.Isomap(n_neighbors, n_components=2).fit_transform(X)
print("Done.")
plot_embedding(X_iso,
               "Isomap projection of the digits (time %.2fs)" %
               (time() - t0))

In [ ]: #-----
# Locally linear embedding of the digits dataset
print("Computing LLE embedding")
clf = manifold.LocallyLinearEmbedding(n_neighbors, n_components=2,
                                     method='standard')

t0 = time()
X_lle = clf.fit_transform(X)
print("Done. Reconstruction error: %g" % clf.reconstruction_error_)
plot_embedding(X_lle,

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        "Locally Linear Embedding of the digits (time %.2fs)" %
        (time() - t0))

#-----
# Modified Locally linear embedding of the digits dataset
print("Computing modified LLE embedding")
clf = manifold.LocallyLinearEmbedding(n_neighbors, n_components=2,
                                     method='modified')

t0 = time()
X_mlle = clf.fit_transform(X)
print("Done. Reconstruction error: %g" % clf.reconstruction_error_)
plot_embedding(X_mlle,
               "Modified Locally Linear Embedding of the digits (time %.2fs)" %
               (time() - t0))

#-----
# HLLC embedding of the digits dataset
print("Computing Hessian LLE embedding")
clf = manifold.LocallyLinearEmbedding(n_neighbors, n_components=2,
                                     method='hessian')

t0 = time()
X_hlle = clf.fit_transform(X)
print("Done. Reconstruction error: %g" % clf.reconstruction_error_)
plot_embedding(X_hlle,
               "Hessian Locally Linear Embedding of the digits (time %.2fs)" %
               (time() - t0))

In [ ]: #-----
# LTSA embedding of the digits dataset
print("Computing LTSA embedding")
clf = manifold.LocallyLinearEmbedding(n_neighbors, n_components=2,
                                     method='ltsa')

t0 = time()
X_lttsa = clf.fit_transform(X)
print("Done. Reconstruction error: %g" % clf.reconstruction_error_)
plot_embedding(X_lttsa,
               "Local Tangent Space Alignment of the digits (time %.2fs)" %
               (time() - t0))

#-----
# MDS embedding of the digits dataset
print("Computing MDS embedding")
clf = manifold.MDS(n_components=2, n_init=1, max_iter=100)

t0 = time()
X_mds = clf.fit_transform(X)
print("Done. Stress: %f" % clf.stress_)

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plot_embedding(X_mds,
               "MDS embedding of the digits (time %.2fs)" %
               (time() - t0))

#-----
# Random Trees embedding of the digits dataset
print("Computing Totally Random Trees embedding")
hasher = ensemble.RandomTreesEmbedding(n_estimators=200, random_state=0,
                                       max_depth=5)

t0 = time()
X_transformed = hasher.fit_transform(X)
pca = decomposition.TruncatedSVD(n_components=2)
X_reduced = pca.fit_transform(X_transformed)

plot_embedding(X_reduced,
               "Random forest embedding of the digits (time %.2fs)" %
               (time() - t0))

In [ ]: #-----
# Spectral embedding of the digits dataset
print("Computing Spectral embedding")
embedder = manifold.SpectralEmbedding(n_components=2, random_state=0,
                                     eigen_solver="arpack")

t0 = time()
X_se = embedder.fit_transform(X)

plot_embedding(X_se,
               "Spectral embedding of the digits (time %.2fs)" %
               (time() - t0))

#-----
# t-SNE embedding of the digits dataset
print("Computing t-SNE embedding")
tsne = manifold.TSNE(n_components=2, init='pca', random_state=0)
t0 = time()
X_tsne = tsne.fit_transform(X)

plot_embedding(X_tsne,
               "t-SNE embedding of the digits (time %.2fs)" %
               (time() - t0))

plt.show()

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