Advanced machine learning and data analysis for the physical sciences

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March 20, 2025

Plans for the week March 17-21

1. Discussion of Autoencoders (AEs) and reminder from last week
2. Links between Principal Component Analysis (PCA) and AE
3. Video of Lecture
4. Whiteboard notes

Reading recommendations

1. Goodfellow et al chapter 14.
2. Rashcka et al. Their chapter 17 contains a brief introduction only.
3. Deep Learning Tutorial on AEs from Stanford University at http://ufldl.stanford.edu/tutorial/unsupervised/Autoencoders/
4. Building AEs in Keras at https://blog.keras.io/building-autoencoders-in-keras.html
5. Introduction to AEs in TensorFlow at https://www.tensorflow.org/tutorials/generative/autoencoder
6. Grosse, University of Toronto, Lecture on AEs at http://www.cs.toronto.edu/~rgrosse/courses/csc321_2017/slides/lec20.pdf
7. Bank et al on AEs at https://arxiv.org/abs/2003.05991
8. Baldi and Hornik, Neural networks and principal component analysis: Learning from examples without local minima, Neural

Autoencoders: Overarching view

Autoencoders are artificial neural networks capable of learning efficient representations of the input data (these representations are called codings) without any supervision (i.e., the training set is unlabeled). These codings typically have a much lower dimensionality than the input data, making autoencoders useful for dimensionality reduction.
Autoencoders learn to encode the input data into a lower-dimensional representation, and then decode it back to the original data. The goal of autoencoders is to minimize the reconstruction error, which measures how well the output matches the input. Autoencoders can be seen as a way of learning the latent features or hidden structure of the data, and they can be used for data compression, denoising, anomaly detection, and generative modeling.

Powerful detectors

More importantly, autoencoders act as powerful feature detectors, and they can be used for unsupervised pretraining of deep neural networks.
Lastly, they are capable of randomly generating new data that looks very similar to the training data; this is called a generative model. For example, you could train an autoencoder on pictures of faces, and it would then be able to generate new faces. Surprisingly, autoencoders work by simply learning to copy their inputs to their outputs. This may sound like a trivial task, but we will see that constraining the network in various ways can make it rather difficult. For example, you can limit the size of the internal representation, or you can add noise to the inputs and train the network to recover the original inputs. These constraints prevent the autoencoder from trivially copying the inputs directly to the outputs, which forces it to learn efficient ways of representing the data. In short, the codings are byproducts of the autoencoder's attempt to learn the identity function under some constraints.

First introduction of AEs

Autoencoders were first introduced by Rumelhart, Hinton, and Williams in 1986 with the goal of learning to reconstruct the input observations with the lowest error possible.
Why would one want to learn to reconstruct the input observations? If you have problems imagining what that means, think of having a dataset made of images. An autoencoder would be an algorithm that can give as output an image that is as similar as possible to the input one. You may be confused, as there is no apparent reason of doing so. To better understand why autoencoders are useful we need a more informative (although not yet unambiguous) definition.

An autoencoder is a type of algorithm with the primary purpose of learning an "informative" representation of the data that can be used for different applications (see Bank, D., Koenigstein, N., and Giryes, R., Autoencoders) by learning to reconstruct a set of input observations well enough.

Autoencoder structure

Autoencoders are neural networks where the outputs are its own inputs. They are split into an **encoder part** which maps the input $\boldsymbol{x}$ via a function $f(\boldsymbol{x}, \boldsymbol{W})$ (this is the encoder part) to a **so-called code part** (or intermediate part) with the result $\boldsymbol{h}$

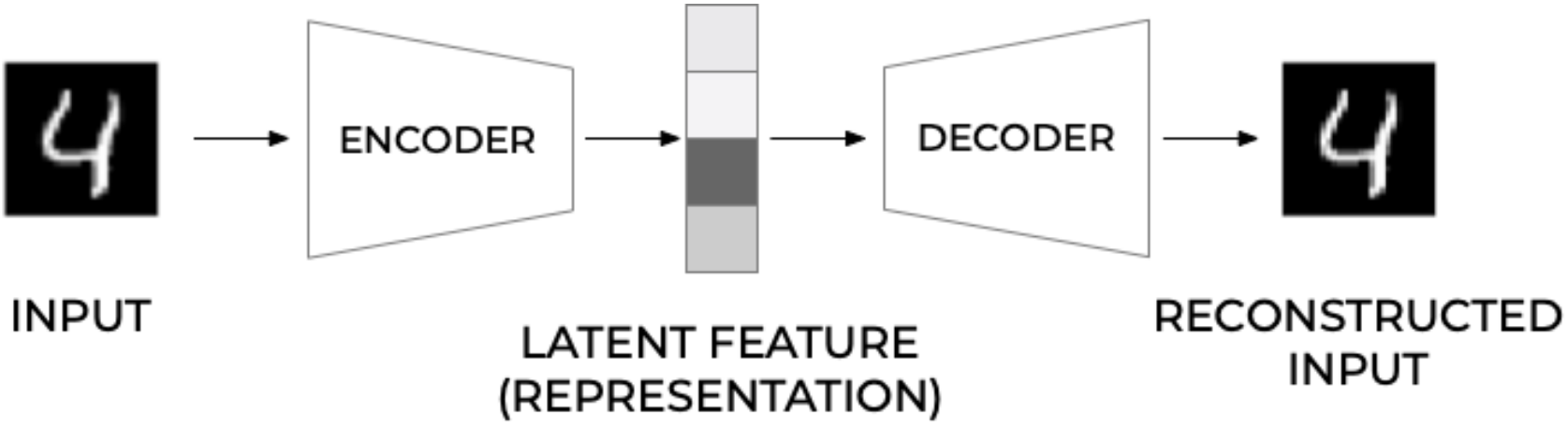
$$\boldsymbol{h} = f(\boldsymbol{x}, \boldsymbol{W})),$$

where $\boldsymbol{W}$ are the weights to be determined. The **decoder** parts maps, via its own parameters (weights given by the matrix $\boldsymbol{V}$ and its own biases) to the final ouput

$$\tilde{\boldsymbol{x}} = g(\boldsymbol{h}, \boldsymbol{V})).$$

The goal is to minimize the construction error.

Schematic image of an Autoencoder



More on the structure

In most typical architectures, the encoder and the decoder are neural networks since they can be easily trained with existing software libraries such as TensorFlow or PyTorch with back propagation.
In general, the encoder can be written as a function g that will depend on some parameters

$$\mathsf{h}_i = g(\mathsf{x}_i),$$

where $\mathsf{h}_i \in \mathbb{R}^q$ (the latent feature representation) is the output of the encoder block where we evaluate it using the input x_i.

Decoder part

Note that we have $g : \mathbb{R}^n \rightarrow \mathbb{R}^q$ The decoder and the output of the network $\tilde{x}_i$ can be written then as a second generic function of the latent features

$$\tilde{x}_i = f\left(h_i\right) = f\left(g\left(x_i\right)\right),$$

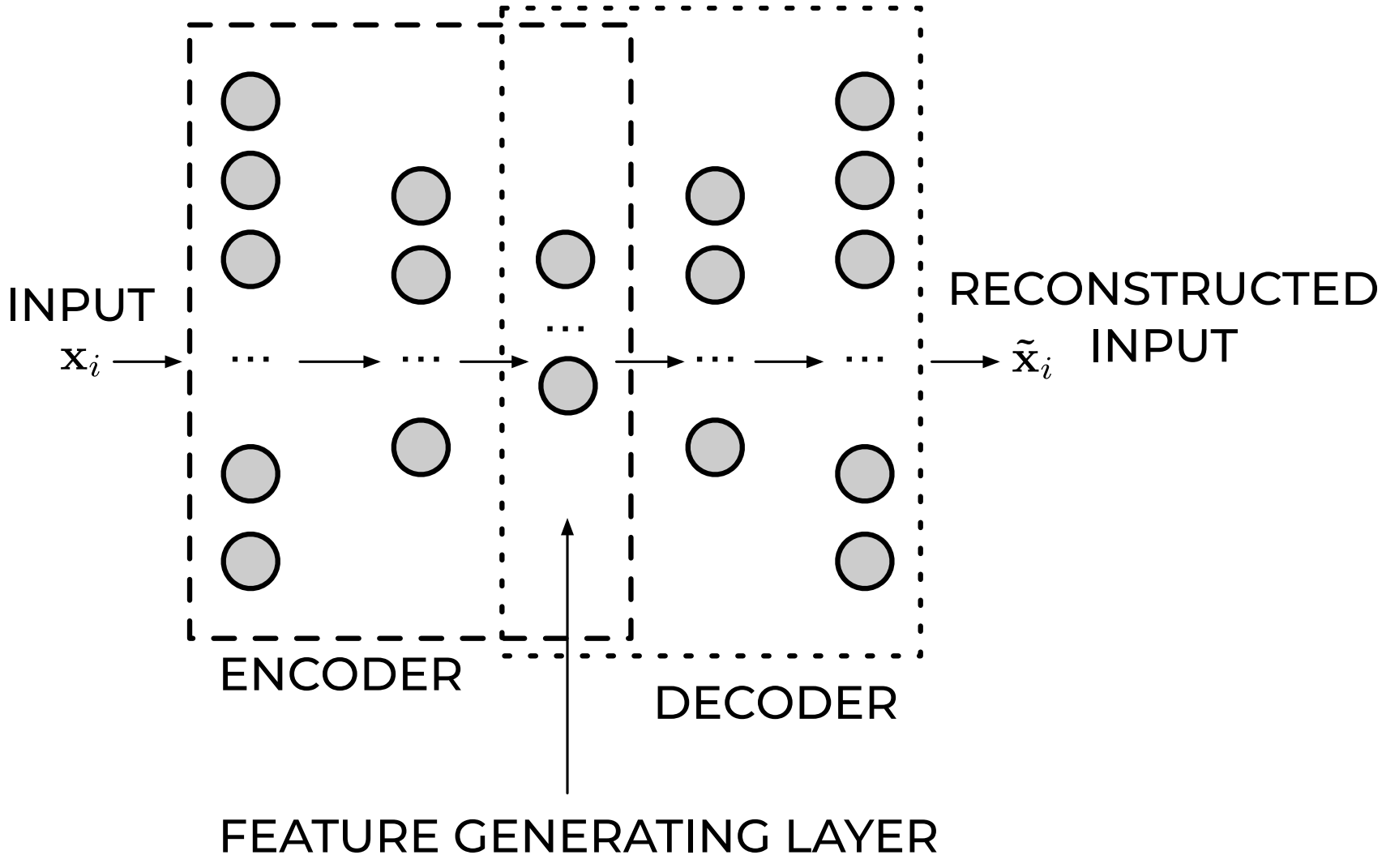
where $\tilde{x}_i \in \mathbb{R}^n$.
Training an autoencoder simply means finding the functions $g(\cdot)$ and $f(\cdot)$ that satisfy

$$\arg\min_{f,g} < [\Delta(x_i, f(g\left(x_i\right))] > .$$

Typical AEs

The standard setup is done via a standard feed forward neural network (FFNN), or what is called a Feed Forward Autoencoder.
A typical FFNN architecture has an odd number of layers and is symmetrical with respect to the middle layer.
Typically, the first layer has a number of neurons $n_1 = n$ which equals the size of the input observation x_i.
As we move toward the center of the network, the number of neurons in each layer drops in some measure. The middle layer usually has the smallest number of neurons. The fact that the number of neurons in this layer is smaller than the size of the input, is often called the **bottleneck**.

Feed Forward Autoencoder



Mirroring

In almost all practical applications, the layers after the middle one are a mirrored version of the layers before the middle one. For example, an autoencoder with three layers could have the following numbers of neurons:
$n_1 = 10$, $n_2 = 5$ and then $n_3 = n_1 = 10$ where the input dimension is equal to ten.
All the layers up to and including the middle one, make what is called the encoder, and all the layers from and including the middle one (up to the output) make what is called the decoder.
If the FFNN training is successful, the result will be a good approximation of the input $\tilde{x}_i \approx x_i$.
What is essential to notice is that the decoder can reconstruct the input by using only a much smaller number of features than the input observations initially have.

Output of middle layer

The output of the middle layer h_i are also called a **learned representation** of the input observation x_i.
The encoder can reduce the number of dimensions of the input observation and create a learned representation h_i) of the input that has a smaller dimension $q < n$.
This learned representation is enough for the decoder to reconstruct the input accurately (if the autoencoder training was successful as intended).

Activation Function of the Output Layer

In autoencoders based on neural networks, the output layer's activation function plays a particularly important role. The most used functions are ReLU and Sigmoid.

ReLU

The ReLU activation function can assume all values in the range $[0, \infty]$. As a remainder, its formula is

$$\mathrm{ReLU}\,(x) = \max\,(0, x)\,.$$

This choice is good when the input observations x_i assume a wide range of positive values. If the input x_i can assume negative values, the ReLU is, of course, a terrible choice, and the identity function is a much better choice. It is then common to replace to the ReLU with the so-called **Leaky ReLu** or just modified ReLU.
The ReLU activation function for the output layer is well suited for cases when the input observations x_i assume a wide range of positive real values.

Sigmoid

The sigmoid function σ can assume all values in the range $[0, 1]$,

$$\sigma(x) = \frac{1}{1 + e^{-x}}.$$

This activation function can only be used if the input observations x_i are all in the range $[0, 1]$ or if you have normalized them to be in that range. Consider as an example the MNIST dataset. Each value of the input observation x_i (one image) is the gray values of the pixels that can assume any value from 0 to 255. Normalizing the data by dividing the pixel values by 255 would make each observation (each image) have only pixel values between 0 and 1. In this case, the sigmoid would be a good choice for the output layer's activation function.

Cost/Loss Function

If an autoencoder is trying to solve a regression problem, the most common choice as a loss function is the Mean Square Error

$$L_{\mathrm{MSE}} = \mathrm{MSE} = \frac{1}{n} \sum_{i=1}^{n} ||\mathrm{x}_i - \tilde{\mathrm{x}}_i| \,|_2^2.$$

Binary Cross-Entropy

If the activation function of the output layer of the AE is a sigmoid function, thus limiting neuron outputs to be between 0 and 1, and the input features are normalized to be between 0 and 1 we can use as loss function the binary cross-entropy. This cots/loss function is typically used in classification problems, but it works well for autoencoders. The formula for it is

$$L_{\mathrm{CE}} = -\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{p}[x_{j,i}\log\tilde{x}_{j,i} + (1-x_{j,i})\log(1-\tilde{x}_{j,i})].$$

Reconstruction Error

The reconstruction error (RE) is a metric that gives you an indication of how good (or bad) the autoencoder was able to reconstruct the input observation x_i. The most typical RE used is the MSE

$$\mathrm{RE} \equiv \mathrm{MSE} = \frac{1}{n} \sum_{i=1}^{n} ||x_i - \tilde{x}_i| \, |_2^2.$$

Towards the PCA theorem

We have from last week that the covariance matrix (the correlation matrix involves a simple rescaling) is given as

$$\boldsymbol{C}[\boldsymbol{x}] = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X} = \mathbb{E}[\boldsymbol{X}^T\boldsymbol{X}].$$

Let us now assume that we can perform a series of orthogonal transformations where we employ some orthogonal matrices $\boldsymbol{S}$. These matrices are defined as $\boldsymbol{S} \in \mathbb{R}^{p\times p}$ and obey the orthogonality requirements $\boldsymbol{S}\boldsymbol{S}^T = \boldsymbol{S}^T\boldsymbol{S} = \boldsymbol{I}$. The matrix can be written out in terms of the column vectors $\boldsymbol{s}_i$ as $\boldsymbol{S} = [\boldsymbol{s}_0, \boldsymbol{s}_1, \dots, \boldsymbol{s}_{p-1}]$ and $\boldsymbol{s}_i \in \mathbb{R}^p$.

More details

Assume also that there is a transformation $\boldsymbol{S}^T\boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S} = \boldsymbol{C}[\boldsymbol{y}]$ such that the new matrix $\boldsymbol{C}[\boldsymbol{y}]$ is diagonal with elements $[\lambda_0, \lambda_1, \lambda_2, \dots, \lambda_{p-1}]$.
That is we have

$$\boldsymbol{C}[\boldsymbol{y}] = \mathbb{E}[\boldsymbol{S}^T\boldsymbol{X}^T\boldsymbol{X}\boldsymbol{T}\boldsymbol{S}] = \boldsymbol{S}^T\boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S},$$

since the matrix $\boldsymbol{S}$ is not a data dependent matrix. Multiplying with $\boldsymbol{S}$ from the left we have

$$\boldsymbol{S}\boldsymbol{C}[\boldsymbol{y}] = \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S},$$

and since $\boldsymbol{C}[\boldsymbol{y}]$ is diagonal we have for a given eigenvalue i of the covariance matrix that

$$\boldsymbol{S}_i\lambda_i = \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S}_i.$$

More on the PCA Theorem

In the derivation of the PCA theorem we will assume that the eigenvalues are ordered in descending order, that is $\lambda_0 > \lambda_1 > \cdots > \lambda_{p-1}$.
The eigenvalues tell us then how much we need to stretch the corresponding eigenvectors. Dimensions with large eigenvalues have thus large variations (large variance) and define therefore useful dimensions. The data points are more spread out in the direction of these eigenvectors. Smaller eigenvalues mean on the other hand that the corresponding eigenvectors are shrunk accordingly and the data points are tightly bunched together and there is not much variation in these specific directions. Hopefully then we could leave it out dimensions where the eigenvalues are very small. If p is very large, we could then aim at reducing p to $l << p$ and handle only l features/predictors.

The Algorithm before the Theorem

Here's how we would proceed in setting up the algorithm for the PCA, see also discussion below here.

- Set up the datapoints for the design/feature matrix $\boldsymbol{X}$ with $\boldsymbol{X} \in \mathbb{R}^{n\times p}$, with the predictors/features p referring to the column numbers and the entries n being the row elements.

$$\boldsymbol{X} = \begin{bmatrix} x_{0,0} & x_{0,1} & x_{0,2} & \dots & \dots x_{0,p-1} \\ x_{1,0} & x_{1,1} & x_{1,2} & \dots & \dots x_{1,p-1} \\ x_{2,0} & x_{2,1} & x_{2,2} & \dots & \dots x_{2,p-1} \\ \dots & \dots & \dots & \dots\dots & \dots \\ x_{n-2,0} & x_{n-2,1} & x_{n-2,2} & \dots & \dots x_{n-2,p-1} \\ x_{n-1,0} & x_{n-1,1} & x_{n-1,2} & \dots & \dots x_{n-1,p-1} \end{bmatrix},$$

Further steps

- Center the data by subtracting the mean value for each column. This leads to a new matrix $\boldsymbol{X} \rightarrow \overline{\boldsymbol{X}}$.
- Compute then the covariance/correlation matrix $\mathbb{E}[\overline{\boldsymbol{X}}^T\overline{\boldsymbol{X}}]$.
- Find the eigenpairs of $\boldsymbol{C}$ with eigenvalues $[\lambda_0, \lambda_1, \ldots, \lambda_{p-1}]$ and eigenvectors $[\boldsymbol{s}_0, \boldsymbol{s}_1, \ldots, \boldsymbol{s}_{p-1}]$.
- Order the eigenvalue (and the eigenvectors accordingly) in order of decreasing eigenvalues.
- Keep only those l eigenvalues larger than a selected threshold value, discarding thus $p - l$ features since we expect small variations in the data here.

Writing our own PCA code

We will use a simple example first with two-dimensional data drawn from a multivariate normal distribution with the following mean and covariance matrix (we have fixed these quantities but will play around with them below):

$$\mu = (-1, 2) \qquad \Sigma = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}$$

Note that the mean refers to each column of data. We will generate $n = 10000$ points $X = \{x_1, \ldots, x_N\}$ from this distribution, and store them in the 1000×2 matrix $\boldsymbol{X}$. This is our design matrix where we have forced the covariance and mean values to take specific values.

Implementing it

The following Python code aids in setting up the data and writing out the design matrix. Note that the function **multivariate** returns also the covariance discussed above and that it is defined by dividing by $n-1$ instead of n.

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from IPython.display import display
n = 10000
mean = (-1, 2)
cov = [[4, 2], [2, 2]]
X = np.random.multivariate_normal(mean, cov, n)
```

Now we are going to implement the PCA algorithm. We will break it down into various substeps.

First Step

The first step of PCA is to compute the sample mean of the data and use it to center the data. Recall that the sample mean is

$$\mu_n = \frac{1}{n}\sum_{i=1}^{n} x_i$$

and the mean-centered data $\bar{X} = \{\bar{x}_1, \ldots, \bar{x}_n\}$ takes the form

$$\bar{x}_i = x_i - \mu_n.$$

When you are done with these steps, print out μ_n to verify it is close to μ and plot your mean centered data to verify it is centered at the origin! The following code elements perform these operations using **pandas** or using our own functionality for doing so. The latter, using **numpy** is rather simple through the **mean()** function.

```
df = pd.DataFrame(X)
# Pandas does the centering for us
df = df -df.mean()
# we center it ourselves
X_centered = X - X.mean(axis=0)
```

Scaling

Alternatively, we could use the functions we discussed earlier for scaling the data set. That is, we could have used the **StandardScaler** function in **Scikit-Learn**, a function which ensures that for each feature/predictor we study the mean value is zero and the variance is one (every column in the design/feature matrix). You would then not get the same results, since we divide by the variance. The diagonal covariance matrix elements will then be one, while the non-diagonal ones need to be divided by $2\sqrt{2}$ for our specific case.

Centered Data

Now we are going to use the mean centered data to compute the sample covariance of the data by using the following equation

$$\Sigma_n = \frac{1}{n-1}\sum_{i=1}^{n} \bar{x}_i^T \bar{x}_i = \frac{1}{n-1}\sum_{i=1}^{n} (x_i - \mu_n)^T (x_i - \mu_n)$$

where the data points $x_i \in \mathbb{R}^p$ (here in this example $p = 2$) are column vectors and x^T is the transpose of x. We can write our own code or simply use either the functionaly of **numpy** or that of **pandas**, as follows

```
print(df.cov())
print(np.cov(X_centered.T))
```

Note that the way we define the covariance matrix here has a factor $n-1$ instead of n. This is included in the **cov()** function by **numpy** and **pandas**. Our own code here is not very elegant and asks for obvious improvements. It is tailored to this specific 2×2 covariance matrix.

```
# extract the relevant columns from the centered design matrix of dim
x = X_centered[:,0]
y = X_centered[:,1]
Cov = np.zeros((2,2))
```

Exploring

Depending on the number of points n, we will get results that are close to the covariance values defined above. The plot shows how the data are clustered around a line with slope close to one. Is this expected? Try to change the covariance and the mean values. For example, try to make the variance of the first element much larger than that of the second diagonal element. Try also to shrink the covariance (the non-diagonal elements) and see how the data points are distributed.

Diagonalize the sample covariance matrix to obtain the principal components

Now we are ready to solve for the principal components! To do so we diagonalize the sample covariance matrix Σ. We can use the function **np.linalg.eig** to do so. It will return the eigenvalues and eigenvectors of Σ. Once we have these we can perform the following tasks:

- We compute the percentage of the total variance captured by the first principal component
- We plot the mean centered data and lines along the first and second principal components
- Then we project the mean centered data onto the first and second principal components, and plot the projected data.
- Finally, we approximate the data as

$$x_i \approx \tilde{x}_i = \mu_n + \langle x_i, v_0 \rangle v_0$$

where v_0 is the first principal component.

Collecting all Steps

Collecting all these steps we can write our own PCA function and compare this with the functionality included in **Scikit-Learn**.

The code here outlines some of the elements we could include in the analysis. Feel free to extend upon this in order to address the above questions.

```
# diagonalize and obtain eigenvalues, not necessarily sorted
EigValues, EigVectors = np.linalg.eig(Cov)
# sort eigenvectors and eigenvalues
#permute = EigValues.argsort()
#EigValues = EigValues[permute]
#EigVectors = EigVectors[:,permute]
print("Eigenvalues of Covariance matrix")
for i in range(2):
    print(EigValues[i])
FirstEigvector = EigVectors[:,0]
SecondEigvector = EigVectors[:,1]
print("First eigenvector")
print(FirstEigvector)
print("Second eigenvector")
print(SecondEigvector)
#thereafter we do a PCA with Scikit-learn
from sklearn.decomposition import PCA
pca = PCA(n_components = 2)
X2Dsl = pca.fit_transform(X)
print("Eigenvector of largest eigenvalue")
print(pca.components_.T[:, 0])
```

Classical PCA Theorem

We assume now that we have a design matrix $\boldsymbol{X}$ which has been centered as discussed above. For the sake of simplicity we skip the overline symbol. The matrix is defined in terms of the various column vectors $[\boldsymbol{x}_0, \boldsymbol{x}_1, \dots, \boldsymbol{x}_{p-1}]$ each with dimension $\boldsymbol{x} \in \mathbb{R}^n$. The PCA theorem states that minimizing the above reconstruction error corresponds to setting $\boldsymbol{W} = \boldsymbol{S}$, the orthogonal matrix which diagonalizes the empirical covariance(correlation) matrix. The optimal low-dimensional encoding of the data is then given by a set of vectors $\boldsymbol{z}_i$ with at most l vectors, with $l << p$, defined by the orthogonal projection of the data onto the columns spanned by the eigenvectors of the covariance(correlations matrix).

The PCA Theorem

To show the PCA theorem let us start with the assumption that there is one vector $\boldsymbol{s}_0$ which corresponds to a solution which minimized the reconstruction error J. This is an orthogonal vector. It means that we now approximate the reconstruction error in terms of $\boldsymbol{w}_0$ and $\boldsymbol{z}_0$ as

We are almost there, we have obtained a relation between minimizing the reconstruction error and the variance and the covariance matrix. Minimizing the error is equivalent to maximizing the variance of the projected data.

We could trivially maximize the variance of the projection (and thereby minimize the error in the reconstruction function) by letting the norm-2 of $\boldsymbol{w}_0$ go to infinity. However, this norm since we want the matrix $\boldsymbol{W}$ to be an orthogonal matrix, is constrained by $||\boldsymbol{w}_0||_2^2 = 1$. Imposing this condition via a Lagrange multiplier we can then in turn maximize

$$J(\boldsymbol{w}_0) = \boldsymbol{w}_0^T \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{w}_0 + \lambda_0(1 - \boldsymbol{w}_0^T \boldsymbol{w}_0).$$

Taking the derivative with respect to $\boldsymbol{w}_0$ we obtain

Geometric Interpretation and link with Singular Value Decomposition

For a detailed demonstration of the geometric interpretation, see Vidal, Ma and Sastry, section 2.1.2.

Principal Component Analysis (PCA) is by far the most popular dimensionality reduction algorithm. First it identifies the hyperplane that lies closest to the data, and then it projects the data onto it.

The following Python code uses NumPy's **svd()** function to obtain all the principal components of the training set, then extracts the first two principal components. First we center the data using either **pandas** or our own code

```
import numpy as np
import pandas as pd
from IPython.display import display
np.random.seed(100)
# setting up a 10 x 5 vanilla matrix
rows = 10
cols = 5
X = np.random.randn(rows,cols)
df = pd.DataFrame(X)
# Pandas does the centering for us
df = df -df.mean()
display(df)
```

PCA and scikit-learn

Scikit-Learn's PCA class implements PCA using SVD decomposition just like we did before. The following code applies PCA to reduce the dimensionality of the dataset down to two dimensions (note that it automatically takes care of centering the data):

```
#thereafter we do a PCA with Scikit-learn
from sklearn.decomposition import PCA
pca = PCA(n_components = 2)
X2D = pca.fit_transform(X)
print(X2D)
```

After fitting the PCA transformer to the dataset, you can access the principal components using the components variable (note that it contains the PCs as horizontal vectors, so, for example, the first principal component is equal to

```
pca.components_.T[:, 0]
```

Another very useful piece of information is the explained variance ratio of each principal component, available via the *explained_variance_ratio* variable. It indicates the proportion of the dataset's variance that lies along the axis of each principal component.

Example of Cancer Data

We can now repeat the above but applied to real data, in this case the Wisconsin breast cancer data. Here we compute performance scores on the training data using logistic regression.

```
import matplotlib.pyplot as plt
import numpy as np
from sklearn.model_selection import  train_test_split
from sklearn.datasets import load_breast_cancer
from sklearn.linear_model import LogisticRegression
cancer = load_breast_cancer()

X_train, X_test, y_train, y_test = train_test_split(cancer.data,cancer

logreg = LogisticRegression()
logreg.fit(X_train, y_train)
print("Train set accuracy from Logistic Regression: {:.2f}".format(log
# We scale the data
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
# Then perform again a log reg fit
logreg.fit(X_train_scaled, y_train)
print("Train set accuracy scaled data: {:.2f}".format(logreg.score(X_t
#thereafter we do a PCA with Scikit-learn
from sklearn.decomposition import PCA
pca = PCA(n_components = 2)
```

Incremental PCA

One problem with the preceding implementation of PCA is that it requires the whole training set to fit in memory in order for the SVD algorithm to run. Fortunately, Incremental PCA (IPCA) algorithms have been developed: you can split the training set into mini-batches and feed an IPCA algorithm one minibatch at a time. This is useful for large training sets, and also to apply PCA online (i.e., on the fly, as new instances arrive).

Randomized PCA. Scikit-Learn offers yet another option to perform PCA, called Randomized PCA. This is a stochastic algorithm that quickly finds an approximation of the first d principal components. Its computational complexity is $O(m \times d^2) + O(d^3)$, instead of $O(m \times n^2) + O(n^3)$, so it is dramatically faster than the previous algorithms when d is much smaller than n.

Kernel PCA. The kernel trick is a mathematical technique that implicitly maps instances into a very high-dimensional space (called the feature space), enabling nonlinear classification and regression with Support Vector Machines. Recall that a linear decision boundary in the high-dimensional feature space corresponds to a complex nonlinear decision boundary in the original space. It turns

Other techniques

There are many other dimensionality reduction techniques, several of which are available in Scikit-Learn.

Here are some of the most popular:

- **Multidimensional Scaling (MDS)** reduces dimensionality while trying to preserve the distances between the instances.
- **Isomap** creates a graph by connecting each instance to its nearest neighbors, then reduces dimensionality while trying to preserve the geodesic distances between the instances.
- **t-Distributed Stochastic Neighbor Embedding** (t-SNE) reduces dimensionality while trying to keep similar instances close and dissimilar instances apart. It is mostly used for visualization, in particular to visualize clusters of instances in high-dimensional space (e.g., to visualize the MNIST images in 2D).
- Linear Discriminant Analysis (LDA) is actually a classification algorithm, but during training it learns the most discriminative axes between the classes, and these axes can then be used to define a hyperplane onto which to project the data. The

Back to Autoencoders: Linear Autoencoders

These examples here are based the codes from A. Geron's textbook. They can be easily modified and adapted to different data sets. The first example is a straightforward AE.

```
import sys
assert sys.version_info >= (3, 5)

# Is this notebook running on Colab or Kaggle?
IS_COLAB = "google.colab" in sys.modules
IS_KAGGLE = "kaggle_secrets" in sys.modules

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

# TensorFlow >= 2.0 is required
import tensorflow as tf
from tensorflow import keras
assert tf.__version__ >= "2.0"

if not tf.config.list_physical_devices('GPU'):
    print("No GPU was detected. LSTMs and CNNs can be very slow withou
    if IS_COLAB:
        print("Go to Runtime > Change runtime and select a GPU hardwar
    if IS_KAGGLE:
        print("Go to Settings > Accelerator and select GPU.")

# Common imports
```

More advanced features, stacked AEs

```
# You can select the so-called fashion data as well, here we just use
#(X_train_full, y_train_full), (X_test, y_test) = keras.datasets.fashi
(X_train_full, y_train_full), (X_test, y_test) = keras.datasets.mnist.
X_train_full = X_train_full.astype(np.float32) / 255
X_test = X_test.astype(np.float32) / 255
X_train, X_valid = X_train_full[:-5000], X_train_full[-5000:]
y_train, y_valid = y_train_full[:-5000], y_train_full[-5000:]
```

We can now train all layers at once by building a stacked AE with 3 hidden layers and 1 output layer (i.e., 2 stacked Autoencoders).

```
def rounded_accuracy(y_true, y_pred):
    return keras.metrics.binary_accuracy(tf.round(y_true), tf.round(y_
tf.random.set_seed(42)
np.random.seed(42)

stacked_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(30, activation="selu"),
])
stacked_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
stacked_ae = keras.models.Sequential([stacked_encoder, stacked_decoder
stacked_ae.compile(loss="binary_crossentropy",
```

Using Convolutional Layers Instead of Dense Layers

```
tf.random.set_seed(42)
np.random.seed(42)

conv_encoder = keras.models.Sequential([
    keras.layers.Reshape([28, 28, 1], input_shape=[28, 28]),
    keras.layers.Conv2D(16, kernel_size=3, padding="SAME", activation=
    keras.layers.MaxPool2D(pool_size=2),
    keras.layers.Conv2D(32, kernel_size=3, padding="SAME", activation=
    keras.layers.MaxPool2D(pool_size=2),
    keras.layers.Conv2D(64, kernel_size=3, padding="SAME", activation=
    keras.layers.MaxPool2D(pool_size=2)
])
conv_decoder = keras.models.Sequential([
    keras.layers.Conv2DTranspose(32, kernel_size=3, strides=2, padding
                                 input_shape=[3, 3, 64]),
    keras.layers.Conv2DTranspose(16, kernel_size=3, strides=2, padding
    keras.layers.Conv2DTranspose(1, kernel_size=3, strides=2, padding=
    keras.layers.Reshape([28, 28])
])
conv_ae = keras.models.Sequential([conv_encoder, conv_decoder])

conv_ae.compile(loss="binary_crossentropy", optimizer=keras.optimizers
                metrics=[rounded_accuracy])
history = conv_ae.fit(X_train, X_train, epochs=5,
                      validation_data=(X_valid, X_valid))

conv_encoder.summary()
conv_decoder.summary()
```

Recurrent Autoencoders

```
recurrent_encoder = keras.models.Sequential([
    keras.layers.LSTM(100, return_sequences=True, input_shape=[28, 28]
    keras.layers.LSTM(30)
])
recurrent_decoder = keras.models.Sequential([
    keras.layers.RepeatVector(28, input_shape=[30]),
    keras.layers.LSTM(100, return_sequences=True),
    keras.layers.TimeDistributed(keras.layers.Dense(28, activation="si
])
recurrent_ae = keras.models.Sequential([recurrent_encoder, recurrent_d
recurrent_ae.compile(loss="binary_crossentropy", optimizer=keras.optim
                     metrics=[rounded_accuracy])
history = recurrent_ae.fit(X_train, X_train, epochs=10, validation_dat

show_reconstructions(recurrent_ae)
plt.show()
```

Stacked denoising Autoencoder with Gaussian noise

```
tf.random.set_seed(42)
np.random.seed(42)

denoising_encoder = keras.models.Sequential([
    keras.layers.Flatten(input_shape=[28, 28]),
    keras.layers.GaussianNoise(0.2),
    keras.layers.Dense(100, activation="selu"),
    keras.layers.Dense(30, activation="selu")
])
denoising_decoder = keras.models.Sequential([
    keras.layers.Dense(100, activation="selu", input_shape=[30]),
    keras.layers.Dense(28 * 28, activation="sigmoid"),
    keras.layers.Reshape([28, 28])
])
denoising_ae = keras.models.Sequential([denoising_encoder, denoising_d
denoising_ae.compile(loss="binary_crossentropy", optimizer=keras.optim
                     metrics=[rounded_accuracy])
history = denoising_ae.fit(X_train, X_train, epochs=10,
                           validation_data=(X_valid, X_valid))

tf.random.set_seed(42)
np.random.seed(42)

noise = keras.layers.GaussianNoise(0.2)
show_reconstructions(denoising_ae, noise(X_valid, training=True))
plt.show()
```

PyTorch example

We will continue with the MNIST database, which has 60000 training examples and a test set of 10000 handwritten numbers. The images have only one color channel and have a size of 28×28 pixels. We start by uploading the data set.

```
# import the Torch packages
# transforms are used to preprocess the images, e.g. crop, rotate, nor
import torch
from torchvision import datasets,transforms

# specify the data path in which you would like to store the downloade
# ToTensor() here is used to convert data type to tensor

train_dataset = datasets.MNIST(root='./mnist_data/', train=True, trans
test_dataset = datasets.MNIST(root='./mnist_data/', train=False, trans
print(train_dataset)
batchSize=128

#only after packed in DataLoader, can we feed the data into the neural
train_loader = torch.utils.data.DataLoader(dataset=train_dataset, batc
test_loader = torch.utils.data.DataLoader(dataset=test_dataset, batch_
```

We visualize the images here using the *imshow* function function and the *make_grid* function from PyTorch to arrange and display them.

```
# package we used to manipulate matpip
```