EE 046202 - Technion - Unsupervised Learning & Data Analysis

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Tutorial 05 - Dimensionality Reduction - Principle Component Analysis (PCA)

Agenda

- Motivation and Introduction
- Principal Component Analyis (PCA) Recap
  - Algorithm
  - PCA for Compression
  - The Transpose Trick
  - Relation to SVD (Singular Value Decomposition)
- Kernels Motivation

In [6]:
```
# imports for the tutorial
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler
%matplotlib notebook
```

Motivation- Why Dimensionality Reduction?

- Discover Hidden Correlation/Topics - when we reduce dimensions, we sometimes discover correlation between features
  - For example, we can notice two features that occur commonly together
  - *Anomaly Detection*
- Remove Redundant and Noisy Features
  - Not all features are useful and sometimes harm the performance
- Interpretation & Visualiztion
  - For example, when we reduce n-dimensional features to 2 or 3, we can plot them and see the relationship with our eyes
- Easier Storage and Processing of the Data
  - Reduces time and space complexity
  - Yields a more optimized process
- Alleviates **The Curse of Dimensionality**
  - Fewer dimensions $\rightarrow$ less chance of *overfitting* $\rightarrow$ better generalization.

Dimensionality Reduction

- Dimensionality reduction is the process of reducing the dimensionality of the feature space with consideration by obtaining a set of principal features.
  - Dimensionality reduction can be further broken into feature selection and feature extraction.
- Dimensionality Reduction vs. **Feature Selection**
  - Differs from feature selection in 2 ways:
    1. Instead of choosing subset of features, it creates new features (dimensions) defined as functions over all features
    2. Does not consider class labels, just data points
- Main Idea:
  - Given data points in **d**-dimensional space
  - Project the data points into lower dimensional space while **preserving as much information as possible**
    - For example, find the best 2-D approximation to 3/4/104-D data
  - In particular, choose the projection that minimizes the squared error in reconstruction of the original data

Principal Component Analysis (PCA)

PCA is a method for reducing the dimensionality of data.

It uses simple matrix operations from linear algebra and statistics to calculate a projection of the original data into the same number or fewer dimensions.

We can define 2 goals PCA wishes to achieve:

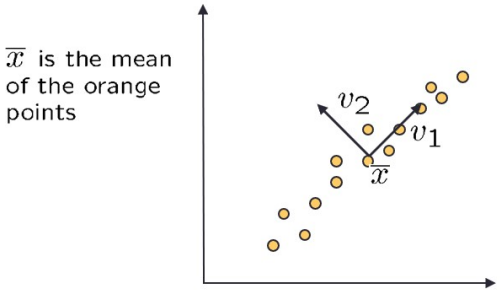
1. Find linearly independent dimensions (or basis of views) which can losslessly represent the data points.
2. Those newly found dimensions should allow us to predict/reconstruct the original dimensions. **The reconstruction/projection error should be minimized.**

More formally, PCA finds a new set of dimensions (or a set of basis of views) such that all the dimensions are **orthogonal** (and hence linearly independent) and ranked according to the variance of data along them. It means that the more important principal axis occurs first (more important = more variance/more spread out data).

Recap of some basics:

- **Variance** - a measure of the variability. Mathematically, it is the average squared deviation from the mean score. We use the following formula to compute variance: $var(x) = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_x)^2$ where μ_x is the mean.
- **Covaraince** - a measure of the extent to which corresponding elements from two sets of ordered data move in the same direction. We use the following formula to compute variance: $cov(x, y) = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu_x)(y_i - \mu_y)$. Replace $\frac{1}{N}$ with $\frac{1}{N-1}$ for the *unbiased* estimation.
- **Covariance matrix** - includes the variance of dimensions on the main diagonal and the rest is the covariance between dimensions. If we have N data points (samples) with d dimensions for each sample and X is an dxN matrix, then: $Cov(X) = \frac{1}{N}(X - \mu_X)(X - \mu_X)^T$ (in PCA, we wish this matrix to be diagonal). We assume the data is centered, thus: $Cov(X) = \frac{1}{N}XX^T$. Replace $\frac{1}{N}$ with $\frac{1}{N-1}$ for the *unbiased* estimation.
- In the PCA case, multiplying by $\frac{1}{N-1}$ will not have much effect on the result, so in the following we will skip this step.

PCA Intuition



- Consider the variance along direction v (projection) among all the orange points:

$$var(v) = \sum_{orange\ points\ x} ||(x - \overline{x}) \cdot v||^2$$

- What is the unit vector v that **minimizes** the variance?
  - $\min_v(var(v)) = v_2$
- What is the unit vector v that **maximizes** the variance?
  - $\min_v(var(v)) = v_1$

- $var(v) = var((x - \overline{x})^T \cdot v) = \sum_x ||(x - \overline{x})^T \cdot v||^2 = \sum_x v^T (x - \overline{x})(x - \overline{x})^T v = v^T \left[\sum_x (x - \overline{x})(x - \overline{x})^T\right] v = v^T A v$
- Formally:

$$\max v^T A v$$
$$s.t\ ||v|| = 1$$

, where $A = \sum_x (x - \overline{x})(x - \overline{x})^T = (X - \overline{X})(X - \overline{X})^T$

- **Solution**:
  - v_1 is eigenvector of A with the **largest** eigenvalue
  - v_2 is eigenvector of A with the **smallest** eigenvalue

PCA Algorithm

1. **Normalize/Standartize** (if we use features of different scales, we may get misleading components) and center the data. Given data $X \in \mathcal{R}^{m \times N}$, where m is the number of features and N is the number of samples, normalization:

   $$\tilde{X} = X - \overline{X}$$

   Standartization:

   $$\tilde{X} = \frac{X - \overline{X}}{\overline{\sigma}_x}$$

   Where $\overline{\sigma}_x$ is the empirical standard deviation (the square root of the empirical variance).
2. Calculate the empirical covariance matrix X of data points:

   $$P = \tilde{X}\tilde{X}^T \in \mathcal{R}^{m \times m}$$

   - Note that it is usually better to normalize:

   $$P = \frac{1}{N-1}\tilde{X}\tilde{X}^T$$
3. Calculate eigenvectors and corresponding eigenvalues.
4. Sort the eigenvectors according to their eigenvalues in decreasing order.
5. Choose first k largest eigenvectors and that will be the new k dimensions.
6. Transform the original d dimensional data points into k dimensions.

Example - PCA on Breast Cancer Dataset

The Breast Cancer Wisconsin (Diagnostic) Data Set

This dataset contains features of breast cancer and classify them to benign/malignant. Features are computed from a digitized image of a fine needle aspirate (FNA) of a breast mass. They describe characteristics of the cell nuclei present in the image.

- We will take the first 3 features, and reduce the dimensionality to 2 using PCA.

In [14]:
```
# load the data
dataset = pd.read_csv('./datasets/cancer_dataset.csv')
# print the number of rows in the data set
number_of_rows = len(dataset)
print('Number of rows in the dataset: {}'.format(number_of_rows))
## Show a sample 10 rows
dataset.sample(10)
```

```
Number of rows in the dataset: 569
```

Out[14]:

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	conca
51	857373	B	13.64	16.34	87.21	571.8	0.07685	0.06059	
353	9010018	M	15.08	25.74	98.00	716.6	0.10240	0.09769	
492	914062	M	18.01	20.56	118.40	1007.0	0.10010	0.12890	
368	9011971	M	21.71	17.25	140.90	1546.0	0.09384	0.08562	
542	921644	B	14.74	25.42	94.70	668.6	0.08275	0.07214	
379	9013838	M	11.08	18.83	73.30	361.6	0.12160	0.21540	
335	89742801	M	17.06	21.00	111.80	918.6	0.11190	0.10560	
4	84358402	M	20.29	14.34	135.10	1297.0	0.10030	0.13280	
449	911157302	M	21.10	20.52	138.10	1384.0	0.09684	0.11750	
334	897374	B	12.30	19.02	77.88	464.4	0.08313	0.04202	

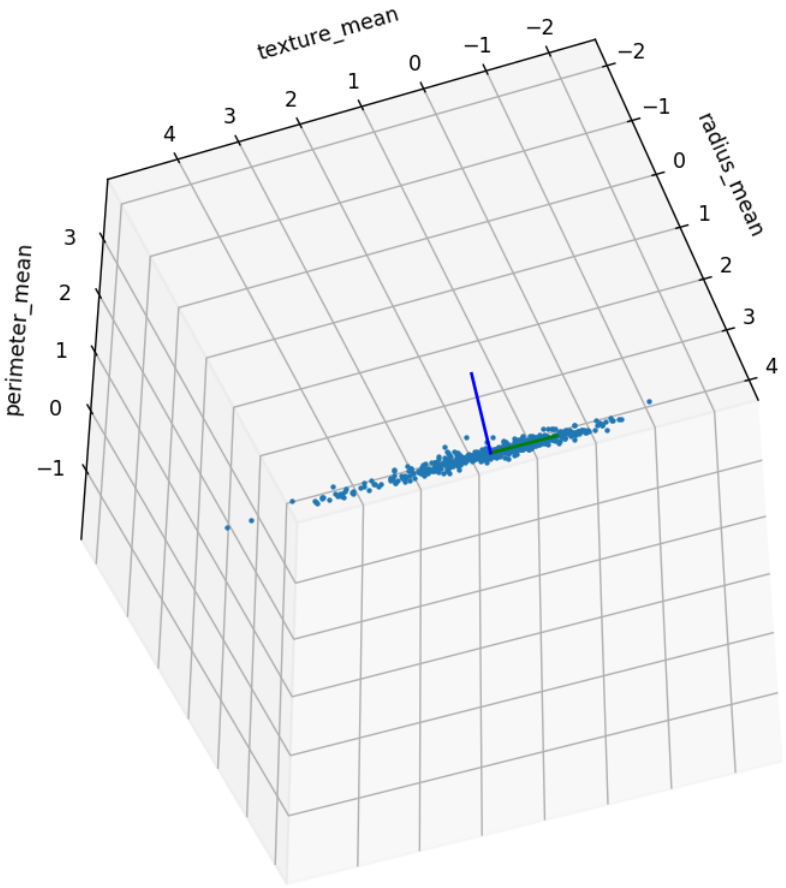
10 rows × 33 columns

In [15]:
```
# take only the first 3 features
x = dataset[['radius_mean', 'texture_mean', 'perimeter_mean']].values
# standartize the data (centering and normalizing), features of different scale!
# note: you can also use scikit-learn's StandardScaler()
x -= x.mean(axis=0, keepdims=True)
x /= x.std(axis=0, keepdims=True)
# calculate the covariance matrix
A = x.T @ x  # x in [N x m]
# calculate eigenvalues and eigenvectors
# NOT ordered in decreasing order
d, v = np.linalg.eig(A)
# sort by decreasing order
v = v[:,np.argsort(-d)]
d = d[np.argsort(-d)]
print("eigenvalues:")
print(d.astype(np.float16))
# the reconstruction of x would be x ~ X @ V @ V.T
# take the 2 most dominant directions
print("projection - dimension reduction (3 to 2):")
x_proj = x @ v[:, :-1]
print(x_proj)
```

```
eigenvalues:
[1.24e+03 4.66e+02 1.21e+00]
projection - dimension reduction (3 to 2):
[[-0.80196001  2.54048135]
 [-2.18555934  1.23675759]
 [-2.23789966  0.38704729]
 ...
 [-1.65154304 -1.54971556]
 [-3.36804781 -1.19009381]
 [ 1.93933426 -2.07217819]]
```

In [16]:
```
def plot_pca():
    # plot
    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(1, 1, 1, projection='3d')
#     ax.axis('equal')
    ax.set_xlabel('radius_mean',)
    ax.set_ylabel('texture_mean')
    ax.set_zlabel('perimeter_mean')
    ax.plot(x[:, 0], x[:, 1], x[:, 2], '.', markersize=3)
    ax.plot([0, v[0, 0]], [0, v[1, 0]], [0, v[2, 0]], 'r') # most dominant eigenvector
    ax.plot([0, v[0, 1]], [0, v[1, 1]], [0, v[2, 1]], 'g')
    ax.plot([0, v[0, 2]], [0, v[1, 2]], [0, v[2, 2]], 'b')
```

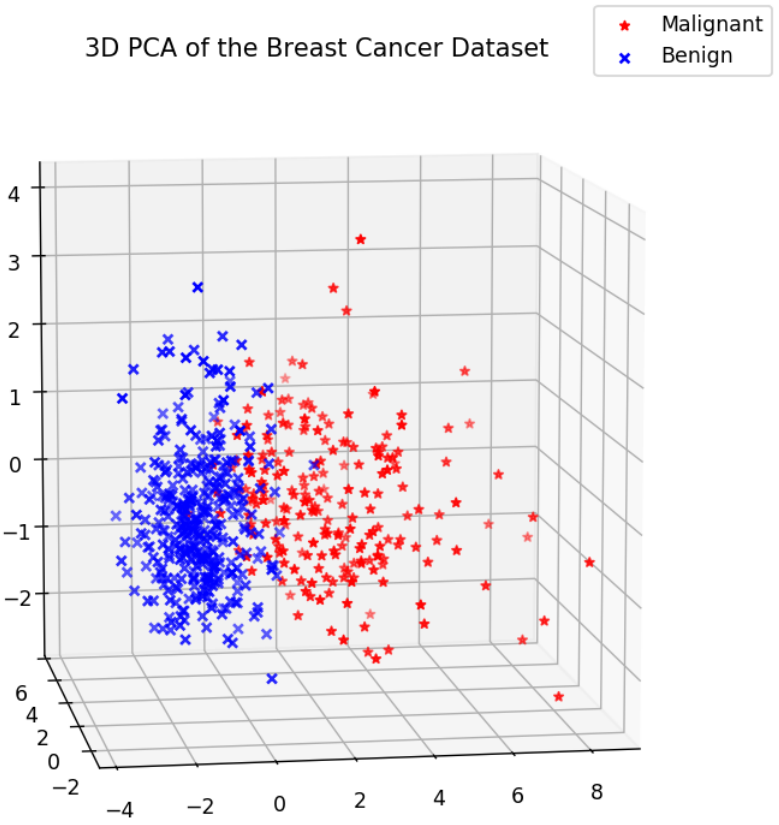
In [17]:
```
%matplotlib notebook
plot_pca()
```



In [18]:
```
# using scikit-learn
scaler = StandardScaler()
X = dataset[['radius_mean', 'texture_mean',
             'perimeter_mean', 'area_mean',
             'smoothness_mean', 'compactness_mean', 'concavity_mean']].values
X = scaler.fit_transform(X)
y = dataset['diagnosis'].values == 'M'
pca = PCA(n_components=3)
X_3d = pca.fit_transform(X)
```

In [19]:
```
def plot_sk_pca():
    # plot
    fig = plt.figure(figsize=(8, 8))
    ax = fig.add_subplot(1, 1, 1, projection='3d')
    ax.scatter(X_3d[y,0], X_3d[y, 1], X_3d[y, 2], color='r', marker='*', label='Malignant')
    ax.scatter(X_3d[~y,0], X_3d[~y, 1], X_3d[~y, 2], color='b', marker='x', label='Benign')
    ax.grid()
    ax.legend()
    ax.set_title("3D PCA of the Breast Cancer Dataset")
```

In [20]:
```
plot_sk_pca()
```



PCA for Compression

- The projection matrix is a matrix composed of the data projected onto the top-K eigenvectors.
- To get a better understanding of the dimensionality reduction quality, we observe the trade-off between the compression and the reconstruction error.
  - The more compression (that is, lower dimension) the larger the reconstruction error and the representation quality is degraded (as our new features don't represent the original data faithfully).

- Measuring the normalized reconstruction error:
  - Denote the top-K eigenvector matrix: $W_k \in \mathcal{R}^{m \times k}$
  - The projection: $Z = XW_K \in \mathcal{R}^{n \times k}$
  - The reconstruction: $\tilde{X} = ZW_k^T = XW_kW_k^T \in \mathcal{R}^{N \times m}$
  - Measure the error by the **Matrix Norm: Frobenius Norm**:

$$||M||_F^2 = \sum_{ij} M_{ij}^2 \rightarrow ||A - B||_F^2 = \sum_{ij} (A_{ij} - B_{ij})^2$$

  - The normalized reconstruction error:

$$err_k = \frac{||XW_kW_k^T - X||_F^2}{||X||_F^2}$$

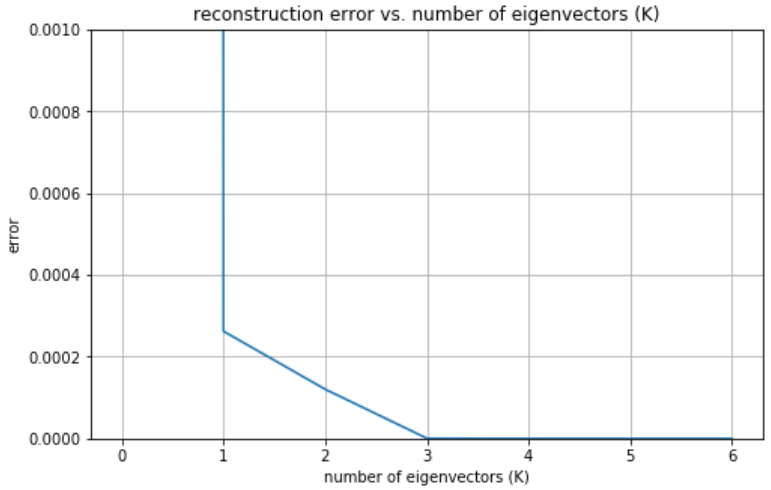
- How to pick k?
  - As a rule of thumb we take the amount of eigenvectors that allows no more than 1% reconstruction error

In [10]:
```
X_normalized = X - X.mean(axis=0, keepdims=True)
X_norm = np.linalg.norm(X_normalized, ord='fro')
# calculate the covariance matrix
A = X_normalized.T @ X_normalized  # x in [N x m]
d, v = np.linalg.eig(A)
# sort by decreasing order
v = v[:,np.argsort(-d)]
d = d[np.argsort(-d)]
for k in range(1, X_normalized.shape[1] + 1):
    Z = X_normalized @ v[:,:k]
    err = np.square(np.linalg.norm(Z @ v[:,:k].T - X_normalized, ord='fro') / X_norm)
    print("number of eigenvectors (k): {}, reconstruction error: {}".format(k + 1, err))
```

```
number of eigenvectors (k): 2, reconstruction error: 0.00026239486787054983
number of eigenvectors (k): 3, reconstruction error: 0.0001204728931473307
number of eigenvectors (k): 4, reconstruction error: 4.2466242287813953e-07
number of eigenvectors (k): 5, reconstruction error: 1.0554210768301531e-08
number of eigenvectors (k): 6, reconstruction error: 2.7565644447137836e-09
number of eigenvectors (k): 7, reconstruction error: 6.737174895338786e-10
number of eigenvectors (k): 8, reconstruction error: 4.83758706698729e-29
```

In [11]:
```
def plot_pca_recon_error(X, v, d):
    k_s = list(range(X.shape[1]))
    X_norm = np.linalg.norm(X, ord='fro')
    errs = []
    for k in k_s:
        Z = X @ v[:,:k]
        err = np.square(np.linalg.norm(Z @ v[:,:k].T - X, ord='fro') / X_norm)
        errs.append(err)
    fig = plt.figure(figsize=(8, 5))
    ax = fig.add_subplot(111)
    ax.plot(k_s, errs)
    ax.grid()
    ax.set_xlabel("number of eigenvectors (K)")
    ax.set_ylabel("error")
    ax.set_title("reconstruction error vs. number of eigenvectors (K)")
    ax.set_ylim([0, 0.001])
```

In [12]:
```
%matplotlib inline
plot_pca_recon_error(X_normalized, v, d)
```



The Tranpose Trick

- What happens when the number of features is very large and much larger than the number of samples, that is, $m >> N$?
  - Calculating the $m \times m$ covariance matrix is computationally expensive ($O(m^2N)$).
- **The Transpose Trick**: ($X \in \mathcal{R}^{m \times N}$)
  - Instead of calculating the eigenvalues and eigenvectors of $\frac{1}{N}XX^T$ we compute the eigenvalues and eigenvectors of
    $$\frac{1}{m}X^TX$$
  - *Why???*
    - If v is an eigenvector of XX^T, then:
      $$XX^Tv = \lambda v$$
    - Left-multiplying by X^T, we get
      $$X^TX(X^Tv) = \lambda(X^Tv)$$
      - $\rightarrow X^Tv$ is an **eigenvector** of X^TX with **eigenvalue** λ.
    - In order to compute v, which is really what we want:
      - Denote the eigenvector of X^TX by w.
      - We get:
        $$Xw = XX^Tv = \lambda v \rightarrow v = \lambda^{-1}Xw$$

The Relationship Between PCA & SVD

- The PCA viewpoint requires that one compute the eigenvalues and eigenvectors of the covariance matrix, which is the product XX^T, where X is the data matrix. Since the covariance matrix is symmetric, the matrix is diagonalizable, and the eigenvectors can be normalized such that they are orthonormal: $XX^T = WAW^T$
- On the other hand, applying SVD to the data matrix X as follows: $X = U\Sigma V^T$, and attempting to construct the covariance matrix from this decomposition gives:
  $$XX^T = (U\Sigma V^T)(U\Sigma V^T)^T = U\Sigma^2U^T$$
  the last transition is due to V being orthonormal ($VV^T = I$). Thus, the square roots of the eigenvalues of XX^T are the singular values of X.
- Using the SVD to perform PCA makes much better sense numerically than forming the covariance matrix to begin with, since the formation of $XX^\top$ can cause loss of precision. But performing SVD is slower.

PCA as Dimensionality Reduction Technique

- **Pro**: Optimal reconstruction error in Frobenius norm
- **Con**: Interpretability problem - features lose their previous meaning
  - A singular vector specifies a linear combination of all input columns or rows
  - PCA is **sensitive to outliers** since it is minimizing l_2 norms. The squaring of deviations from the outliers, they will dominate the total norm and therefore will drive the PCA components.
- **When will PCA work?**
  - PCA assumes **linear** realtionships among variables
  - Clouds of points in *p*-dimensional space has linear dimensions that can be effectively summarized by the principal axes
  - If the structure in the data is **non-linear** (the cloud of points twists and curves its way through *p*-dimensional space), the principal axes will not be an efficient and informative summary of the data.

Kernels Motivation

- The main shortcoming of PCA is that it is unable to capture nonlinear structures in the data.
- Consider the following example of linearly inseparatable 1-D set of exmaples and then extracting polynimial (second order) features:

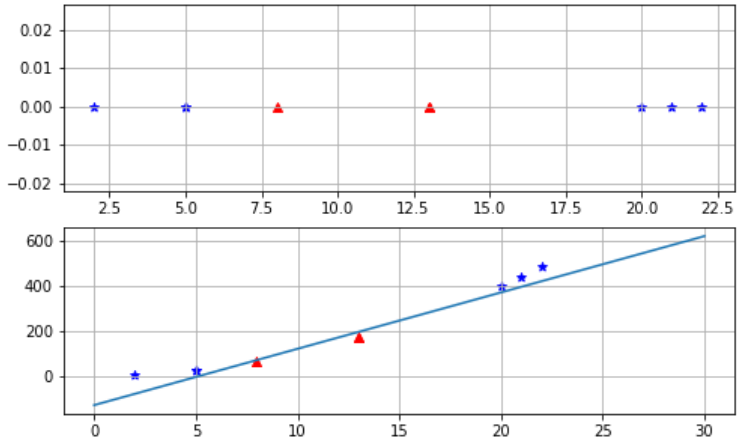
In [13]:
```
def plot_kernel_example():
    x_1 = np.random.randint(0,6, size=(3,))
    x_2 = np.random.randint(8,14, size=(3,))
    x_3 = np.random.randint(20,25, size=(3,))

    x_1_p = x_1 ** 2
    x_2_p = x_2 ** 2
    x_3_p = x_3 ** 2

    x_class = np.linspace(0, 30, 400)
    y_class = 25 * x_class - 130

    fig = plt.figure(figsize=(8,5))
    ax_1 = fig.add_subplot(211)
    ax_1.scatter(x_1, np.zeros_like(x_1), marker='*', color='b')
    ax_1.scatter(x_2, np.zeros_like(x_2), marker='^', color='r')
    ax_1.scatter(x_3, np.zeros_like(x_3), marker='*', color='b')
    ax_1.grid()
    ax_2 = fig.add_subplot(212)
    ax_2.scatter(x_1, x_1_p, marker='*', color='b')
    ax_2.scatter(x_2, x_2_p, marker='^', color='r')
    ax_2.scatter(x_3, x_3_p, marker='*', color='b')
    ax_2.plot(x_class, y_class)
    ax_2.grid()
```

In [14]:
```
plot_kernel_example()
```



- Adding polynomial features is simple to implement and can work great with all sorts of ML algorithms.
- At a **low polynomial** degree it cannot deal with more complex datasets.
- At a **high polynomial** degree there are a lot of features, which makes the computation very slow.
  - Computation in the feature space can be costly because it is high dimensional (even go to infinity).
- **The Kernel Trick** comes to the rescue!
  - It makes it possible to get the same result as if you added many features (even in high dimension), **without actually adding them**!
    - So there is no computational disaster resulting from the large number of features.

Recommended Videos

Warning!

- These videos do not replace the lectures and tutorials.
- Please use these to get a better understanding of the material, and not as an alternative to the written material.

Video By Subject

- PCA (1) - StatQuest: Principal Component Analysis (PCA), Step-by-Step (https://www.youtube.com/watch?v=FgakZw6K1QQ)
- PCA (2) - Principal Component Analysis (PCA) - Computerphile (https://www.youtube.com/watch?v=TJdH6rPA-TI)

Credits

- Icons from Icon8.com (https://icons8.com/) - https://icons8.com (https://icons8.com)
- Datasets from Kaggle (https://www.kaggle.com/) - https://www.kaggle.com/ (https://www.kaggle.com/)