EE 046202 - Technion - Unsupervised Learning & Data Analysis

Tal Daniel

Tutorial 05 - Dimensionality Reduction - Principle Component Analysis (PCA), Kernels & KPCA

Agenda

In [1]:
```
# 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, KernelPCA
from sklearn.preprocessing import StandardScaler
from sklearn.datasets import make_circles, make_moons
%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 & Visualization
  - 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:

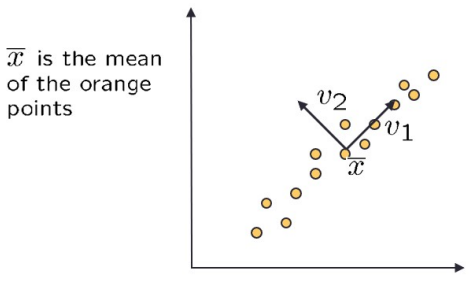
1. Find linearly independent dimensions (or basis of views) which can losslessly represent the data points.
2. Those newly found dimensions should allow us to predict/reconstruct the original dimensions. **The reconstruction/projection error should be minimized.**

- 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:

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

- 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?
  - $\max_v(var(v)) = v_1$

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

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

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

- **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:

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

   Where $\bar{\sigma}_x$ 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 [2]:
```
# 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[2]:

	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean
37	854941	B	13.03	18.42	82.61	523.8	0.08983	0.03766	0.02562
485	913063	B	12.45	16.41	82.85	476.7	0.09514	0.15110	0.15440
116	864726	B	8.95	15.76	58.74	245.2	0.09462	0.12430	0.09263
214	8810955	M	14.19	23.81	92.87	610.7	0.09463	0.13060	0.11150
27	852781	M	18.61	20.25	122.10	1094.0	0.09440	0.10660	0.14900
407	905190	B	12.85	21.37	82.63	514.5	0.07551	0.08316	0.06126
461	911296202	M	27.42	26.27	186.90	2501.0	0.10840	0.19880	0.36350
161	8711803	M	19.19	15.94	126.30	1157.0	0.08694	0.11850	0.11930
462	9113156	B	14.40	26.99	92.25	646.1	0.06995	0.05223	0.03476
264	889719	M	17.19	22.07	111.60	928.3	0.09726	0.08995	0.09061

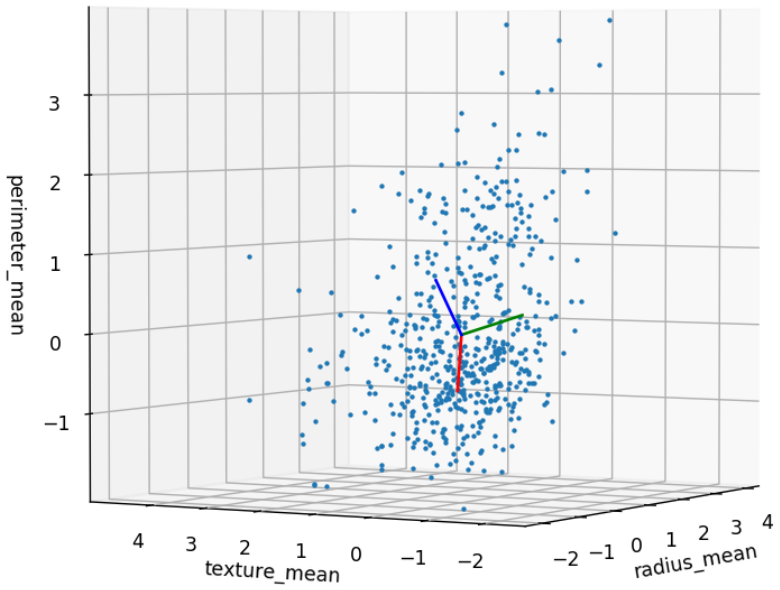
10 rows × 33 columns

In [3]:
```
# 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 [4]:
```
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')
```

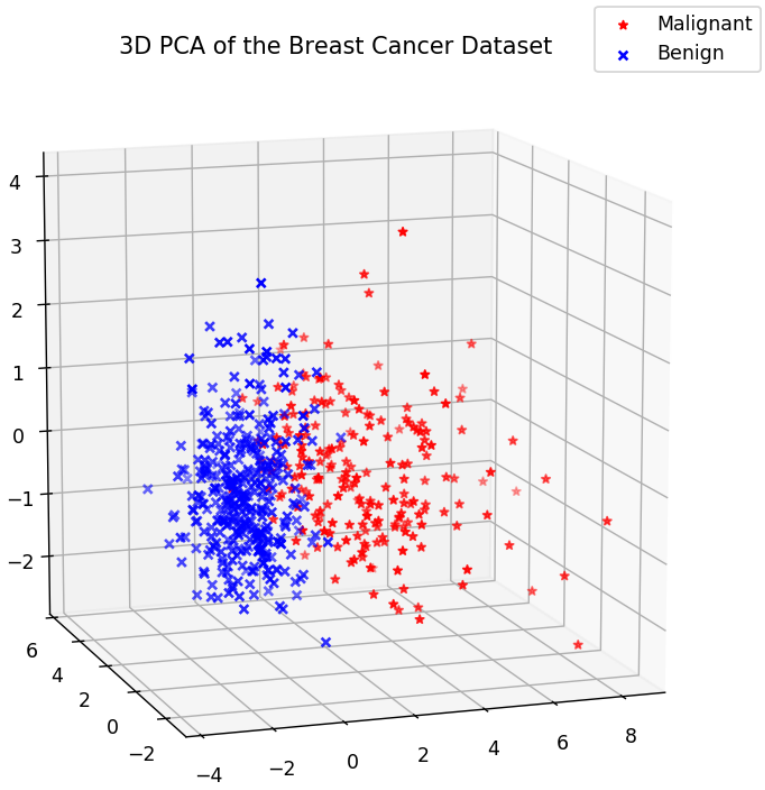
In [5]:
```
%matplotlib notebook
plot_pca()
```



In [6]:
```
# 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 [7]:
```
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 [8]:
```
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:

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

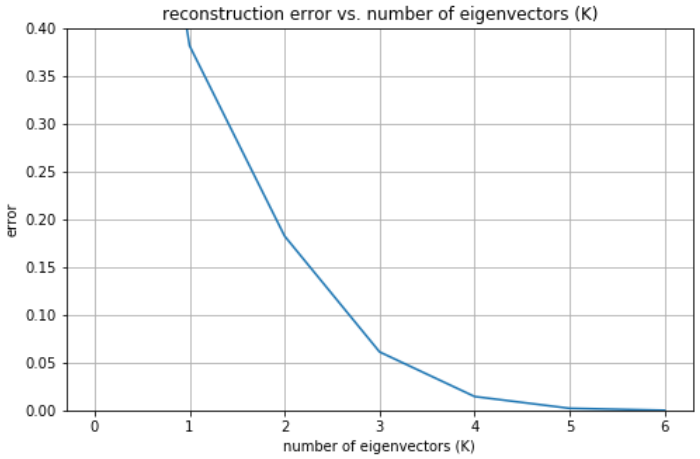
- How to pick k?
  - As a rule of thumb we take the amount of eigenvectors that allows no more than 1% reconstruction error

In [9]:
```
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, err))
```

```
number of eigenvectors (k): 1, reconstruction error: 0.3817772746473096
number of eigenvectors (k): 2, reconstruction error: 0.18251649332420763
number of eigenvectors (k): 3, reconstruction error: 0.061153584222750024
number of eigenvectors (k): 4, reconstruction error: 0.014432620496369605
number of eigenvectors (k): 5, reconstruction error: 0.002089071617164215
number of eigenvectors (k): 6, reconstruction error: 4.1709202569973447e-05
number of eigenvectors (k): 7, reconstruction error: 3.4934265607613812e-31
```

In [12]:
```
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, 0.4])
```

In [13]:
```
%matplotlib inline
plot_pca_recon_error(X_normalized, v, d)
```



The Transpose 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

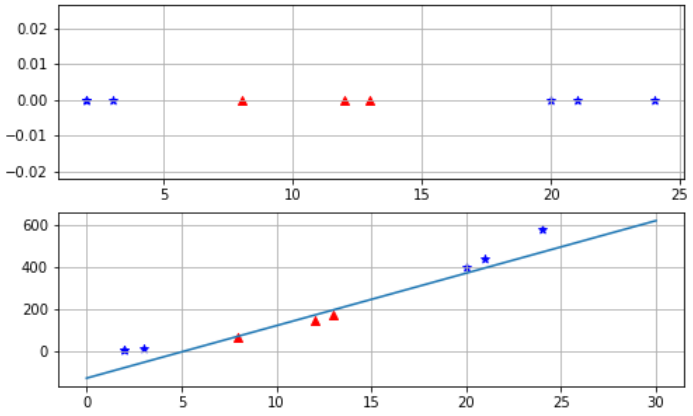
- **Pro**: Optimal reconstruction error in Frobenius norm
- **Con**: Interpretability problem - features lose their previous meaning
  - A singular vector specifies a linear combination of all input columns or rows
  - PCA is **sensitive to outliers** since it is minimizing l_2 norms. The squaring of 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 [14]:
```
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 [15]:
```
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.

The Kernel Trick

- When the **data points**, $\{x^{(i)}\}_{i=1}^{m}$, only appear as **inner (dot) products** - $(x^{(i)})^T x^{(j)}$, we can apply the kernel trick.
- As long as we can calculate the inner product in the **feature space**, we don't need the mapping explicitly.
  - The kernel function, denoted $K(x^{(i)}, x^{(j)}) = \phi(x^{(i)})^T \phi(x^{(j)})$, stands for the inner product in the feature space, and can easily plugged into the optimization.
  - If we could find a function $K(x^{(i)}, x^{(j)})$ that is simple enough, we can actually save us the huge number of calculations required to calculate $\phi(x^{(i)})^T \phi(x^{(j)})$, or even prevent us from the feature extraction itself, $\phi(x)$, this is the **kernel trick**.

- There are no restrictions on the form of $x^{(i)}, x^{(j)}$, but there are restrictions on the kernel function $K(x^{(i)}, x^{(j)})$
  - $K(x^{(i)}, x^{(j)})$ must satisfy the **Mercer Condition** - the $n \times n$ kernel matrix $K(x^{(i)}, x^{(j)})$ is **PSD**
  - This implies that the quadratic optimization is convex
    - It has a uniuqe solution and can be solved efficiently
- **Mercer's Theorem**: *Suppose that $k(x, y)$ is a symmetric real valued function such that $k(x, y) \leq C$ for some $C > 0$. Suppose the linear operator*

$$\mathcal{L}(f)(x) = \int_{\mathcal{R}^D} k(x, y) f(y) dy$$

  is PSD, that is

$$\int \int_{\mathcal{R}^D} k(x, y) f(y) dy dx \geq 0$$

  Let ψ_i be the normalized orthogonal eigenfunctions of $\mathcal{L}$, associated with eigenvalues $\lambda_i > 0$, sorted in non-decreasing order, and let m be the number of non-zero eigenvalues.
- Then, the sequence of eigenvalues is summable, namely $\sum_i \mid \lambda_i \mid < \infty$, and the kernel can be expressed as

$$k(x, y) = \sum_{i=1}^{m} \lambda_i \psi_i(x) \psi_i(y)$$

- *We thus see that by choosing $\phi_i(x) = \sqrt{\lambda_i} \psi_i(x)$, a feature based representation is obtained.*

 The Kernel Trick - Polynomial Kernel Example

- We will now demonstrate the kernel trick for a 2^{nd}-degree polynomial mapping
- Suppose the feature mapping (or extraction) is defined as follows:

$$\phi(u) = \phi(\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}) = \begin{bmatrix} 1 \\ \sqrt{2}u_1 \\ \sqrt{2}u_2 \\ \sqrt{2}u_1 u_2 \\ u_1^2 \\ u_2^2 \end{bmatrix}$$

- The inner product $\phi(u)^T \phi(v)$:

$$\phi(u)^T \phi(v) = 1 + 2u_1 v_1 + 2u_2 v_2 + 2u_1 u_2 v_1 v_2 + u_1^2 v_1^2 + u_2^2 v_2^2 = (1 + u_1 v_1 + u_2 v_2)^2 = (1 + u^T v)^2$$

  - **HOW ABOUT THAT?** - We just found out that we can calculate $\phi(u)^T \phi(v)$ just by calculating the input inner product $u^T v$ and plugging it in $(1 + u^T v)^2$, thus saving us the whole feature mapping calculation process!
- We define **the 2^{nd} polynomial kernel**:

$$K(u, v) = (1 + u^T v)^2$$

  - No need to calculate $\phi(u)^T \phi(v)$ explicitly!
  - The use of kernel function to avoid computing $\phi(\cdot)$ explicitly is known as **the kernel trick**

 Other Kernel Functions

- Linear kernel:

$$K(u, v) = u^T v$$

- Polynomial kernel with degree d:

$$K(u, v) = (\alpha u^T v + \beta)^d$$

  - The feature space is all monomials up to degree d

- **Radial Basis Function** (Gaussian RBF) kernel with width σ:

$$K(u, v) = e^{-\frac{||u-v||^2}{2\sigma^2}} = e^{-\gamma||u-v||^2} = exp(-\gamma||u - v||^2)$$

  - It is also a type of a *similarity function* that measures *how far are two points?*
  - RBF covers the space with "balls" of a fixed radius, where the centers are the support vectors (in SVM).
  - The radius of the "balls" is determined by the parameter $\gamma = \frac{1}{2\sigma^2}$
    - A **smaller** γ means a larger radius, a lower "model complexity"
    - A **larger** γ means a smaller radius, a finer grain coverage which may possibly lead to overfitting.
  - The feature space is **infinite-dimensional** (hint for HW: expand the exponential to an infinite series using Taylor).
- Sigmoid kernel, with parameters κ and θ:

$$K(u, v) = tanh(\kappa u^T v + \theta)$$

  - It does not satisfy the *Mercer* condition on all κ, θ

- Techniques for constructing new kernels (from *Pattern Recognition and Machine Learning*, C.Bishop):

Given valid kernels $k_1(\mathbf{x}, \mathbf{x}')$ and $k_2(\mathbf{x}, \mathbf{x}')$, the following new kernels will also be valid:

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{x}') &= ck_1(\mathbf{x}, \mathbf{x}') && (6.13)\\
k(\mathbf{x}, \mathbf{x}') &= f(\mathbf{x})k_1(\mathbf{x}, \mathbf{x}')f(\mathbf{x}') && (6.14)\\
k(\mathbf{x}, \mathbf{x}') &= q\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.15)\\
k(\mathbf{x}, \mathbf{x}') &= \exp\left(k_1(\mathbf{x}, \mathbf{x}')\right) && (6.16)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}') + k_2(\mathbf{x}, \mathbf{x}') && (6.17)\\
k(\mathbf{x}, \mathbf{x}') &= k_1(\mathbf{x}, \mathbf{x}')k_2(\mathbf{x}, \mathbf{x}') && (6.18)\\
k(\mathbf{x}, \mathbf{x}') &= k_3\left(\phi(\mathbf{x}), \phi(\mathbf{x}')\right) && (6.19)\\
k(\mathbf{x}, \mathbf{x}') &= \mathbf{x}^{\mathrm{T}}\mathbf{A}\mathbf{x}' && (6.20)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a) + k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.21)\\
k(\mathbf{x}, \mathbf{x}') &= k_a(\mathbf{x}_a, \mathbf{x}'_a)k_b(\mathbf{x}_b, \mathbf{x}'_b) && (6.22)
\end{aligned}
$$

where $c > 0$ is a constant, $f(\cdot)$ is any function, $q(\cdot)$ is a polynomial with nonnegative coefficients, $\phi(\mathbf{x})$ is a function from $\mathbf{x}$ to $\mathbb{R}^M$, $k_3(\cdot, \cdot)$ is a valid kernel in $\mathbb{R}^M$, $\mathbf{A}$ is a symmetric positive semidefinite matrix, $\mathbf{x}_a$ and $\mathbf{x}_b$ are variables (not necessarily disjoint) with $\mathbf{x} = (\mathbf{x}_a, \mathbf{x}_b)$, and k_a and k_b are valid kernel functions over their respective spaces.

Exercise - Valid Kernels

Let $k_1(x, y)$ and $k_2(x, y)$ be valid kernels according to Mercer's theorem (that is, they represent an inner product in some transformed space). Prove that the following functions are valid kernels as well:

1. Prove:
$$k(x, y) = k_1(x, y) + k_2(x, y)$$
2. Prove:
$$k(x, y) = f(x)k_1(x, y)f(y) \text{ where } f : \mathcal{R}^D \to \mathcal{R}$$

Solution

The basic trick here is using the initial knowledge that both kernels are valid according to Mercer's theorem.

Section 1

- Prove for:
$$k(x, y) = k_1(x, y) + k_2(x, y)$$

Using Mercer's theorem we know that there exists mappings $\phi_1(x)$ and $\phi_2(x)$ such that:

$$
\begin{aligned}
k_1(x, y) &= \phi_1(x)^T\phi_1(y)\\
k_2(x, y) &= \phi_2(x)^T\phi_2(y)
\end{aligned}
$$

Thus,

$$
\begin{aligned}
k(x, y) &= k_1(x, y) + k_2(x, y)\\
&= \phi_1(x)^T\phi_1(y) + \phi_2(x)^T\phi_2(y)\\
&= [\phi_1(x), \phi_2(x)]^T[\phi_1(y), \phi_2(y)] = \Phi(x)^T\Phi(y)
\end{aligned}
$$

- $[\phi_1(x), \phi_2(x)]$ is a concatentanion of the vectors $\phi_1(x), \phi_2(x)$:
$$[\ \phi_{11}(x) \quad \dots \quad \phi_{1n}(x) \quad \phi_{21}(x) \quad \dots \quad \phi_{2m}(x)\ ]^T$$
- Thus, $k(x, y)$ represents an inner product in some transformed space.

Section 2

- Prove for:
$$k(x, y) = f(x)k_1(x, y)f(y) \text{ where } f : \mathcal{R}^D \to \mathcal{R}$$

Again, using Mercer's theorem:

$$
\begin{aligned}
k(x, y) &= f(x)k_1(x, y)f(y)\\
&= f(x)\phi_1(x)^T\phi_1(y)f(y)\\
&= \Phi(x)^T\Phi(y)
\end{aligned}
$$

where $\Phi(x) = f(x)\phi_1(x)$.

- Recall that $\phi_1(x)$ is a vector and $f(x)$ is a **scalar**.
- Thus, $k(x, y)$ represents an inner product in some transformed space.

Nonlinear PCA - NLPCA (& Kernel PCA)

- The main shortcoming of PCA is that it is **unable to capture nonlinear structures in the data**.
- The basic idea behind Kernel PCA is that by embedding the data into a high-dimensional space for which linear sub-spaces capture the relavant structures.
- Mathematically:

$$x \in \mathcal{R}^D \xrightarrow{\text{nonlinear}} \phi(x) \in \mathcal{R}^m \xrightarrow{\text{linear}} y \in \mathcal{R}^d, m \geq D > d$$

(and usually $m >> D$)

- The basic steps of Nonlinear PCA:
  - Using the mapping $\phi(x)$, we map each data point $x_i \rightarrow \phi(x_i),\ i = 1, \ldots, n$.
  - As in regular PCA, we center (or normalize/standartize) the data. We define:

$$\Phi = \left(\phi(x_1) - \overline{\phi}, \ldots, \phi(x_n) - \overline{\phi}\right) \in \mathcal{R}^{m \times n}$$
$$\overline{\phi} = \frac{1}{n}\sum_{j=1}^{n}\phi(x_j)$$

  - Define the sample covariance matrix:

$$\hat{P}_{\phi(x)} = \frac{1}{n}\sum_{j=1}^{n}\left(\phi(x_j) - \overline{\phi}\right)\left(\phi(x_j) - \overline{\phi}\right)^T = \frac{1}{n}\Phi\Phi^T \in \mathcal{R}^{m \times m}$$

  - Perform the *eigen-decomposition* of the sample covariance matrix:

$$\hat{P}_{\phi(x)}u_i = \lambda_i u_i,\ i = 1, \ldots, m$$

    - The d *nonlinear* Principal Components (PCs):

$$y_i = u_i^T\left(\phi(x) - \overline{\phi}\right) \in \mathcal{R},\ u_i \in \mathcal{R}^m,\ i = 1, \ldots, d$$

- Compuational cost:
  - Computing the eigenvectors of a $m \times m$ matrix requires (in general) $O(m^3)$ steps - very expensive for large m!
- **Note** - the features $\phi(x_i)$ need to be centered even if the x_i are centered, since the mapping ϕ is **nonlinear**.
- Reducing the computational cost using the **Transpose Trick**:
  - The dimension m of the feature space may be very large which may be very expensive computationally.
  - Using the *transpose trick* which is based on the relation between the eigen-decomposition of $\Phi\Phi^T$ and $\Phi^T\Phi$, we can reduce the cost.
    - Recall the the **eigenvalues** of $\Phi\Phi^T$ and $\Phi^T\Phi$ are equal.
  - Doing the same derivation as before (look up...) we get that if w is an eigen-vector of $\Phi^T\Phi$ and v is an eigen-vector of $\Phi\Phi^T$ then:

$$u = \lambda^{-1}\Phi w$$

    - It is much cheaper to compute as the number of samples $n << m$.
  - The d *nonlinear* Principal Components (PCs):

$$y_i = u_i^T\left(\phi(x) - \overline{\phi}\right) = \lambda_i^{-1}w_i^T\Phi^T\left(\phi(x) - \overline{\phi}\right) \in \mathcal{R}, u_i \in \mathcal{R}^m,\ i = 1, \ldots, d$$

Kernel PCA

- Notice that the nonlinear PCs only require the computation of *inner products* between the features ϕ. This indicates that we can use **the kernel trick** to calculate these inner products.
- We define the kernel and *centered kernel functions*:

$$k(x, y) = \phi(x)^T\phi(y)$$
$$\tilde{k}(x, y) = \left(\phi(x) - \overline{\phi}\right)^T\left(\phi(y) - \overline{\phi}\right)$$

  - Note that:

$$\tilde{k}(x, y) = k(x, y) - \frac{1}{n}\sum_{j=1}^{n}k(x, x_j) - \frac{1}{n}\sum_{i=1}^{n}k(x_i, y) + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}k(x_i, y_j)$$

  - Define the kernel and centered *kernel matrices*, which are defined w.r.t. the data points:

$$K = \left[k_{ij}\right],\ \ k_{ij} = k(x_i, x_j)$$
$$\tilde{K} = \Phi^T\Phi = \left[\tilde{k}_{ij}\right],\ \ \tilde{k}_{ij} = \tilde{k}(x_i, x_j)$$

Claim

The nonlinear PCs can be computed directly in terms of the matrix $\tilde{K}$.

- It can be shown that:
$$\tilde{K} = \big(I - \frac{1}{n}11^T\big)K\big(I - \frac{1}{n}11^T\big) = JKJ$$
  - $1 = (1, 1, \dots, 1)^T \in \mathcal{R}^n$

- We also define the vectors:
$$k_x = [k(x_1, x), \dots, k(x_n, x)]^T$$
$$\tilde{k_x} = \Phi^T(\phi(x) - \overline{\phi}) = [\tilde{k}(x_1, x), \dots, \tilde{k}(x_n, x)]^T$$
- The nonlinear PCs can then be computed as:
$$y_i = w_i^T\Phi^T\big(\phi(x) - \overline{\phi}\big) = w_i^T\tilde{k}_x, \;\; i = 1, 2, \dots, d$$
  - w_i are the **eignevectors** of $\tilde{K}$:
$$\tilde{K}w_i = \lambda_i w_i$$
$$||w_i||^2 = \lambda_i^{-1}, \;\; [w_1, \dots, w_d] = V_d\Lambda_d^{-\frac{1}{2}}$$
  - V_d and Λ_d are obtained from the top-d eigenvectors of $\tilde{K}$'s eigen-decomposition:
$$\tilde{K} = V_{\tilde{K}}\Lambda_{\tilde{K}}V_{\tilde{K}}^T$$
  - Concatenating the components y_i we get (the projection):
$$Y = (y_1, y_2, \dots, y_d)^T = \Lambda_d^{-\frac{1}{2}}V_d^T\tilde{K}$$
    - Notice that $\Lambda_d^{-\frac{1}{2}}$ is the normaliztion factor (recall that Λ_d is a diagonal matrix with the eigenvalues on the diagonal).

- The low-dimensional nonlinear representation is obtained from the top-d eigenvectors of the matrix $\tilde{K}$.
  - The problem has been solved in the high-dimensional feature space ϕ while not explicitly computing ϕ or even working in $\mathcal{R}^m$

NLPCA Algorithm (Kernel PCA - KPCA)

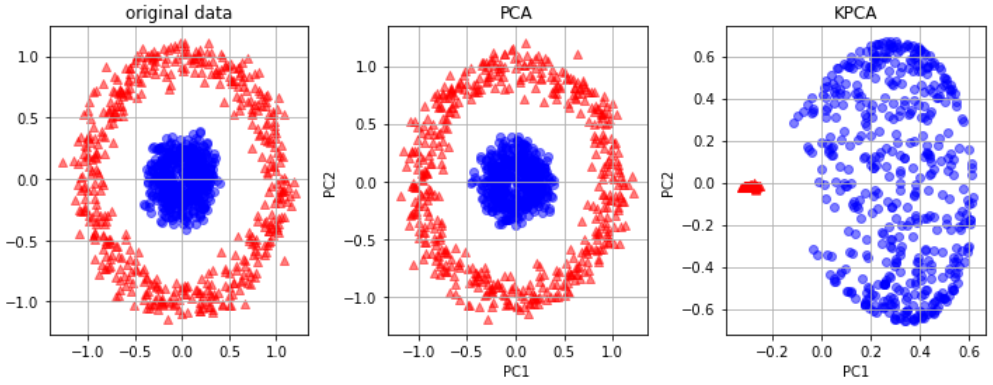
- **Input**: A set of points $\mathcal{X} = \{x_1, x_2, \dots, x_N\} \subset \mathcal{R}^D$, and a mapping $\phi : \mathcal{R}^D \to \mathcal{R}^M$ **or** a symmetric positive definite kernel function $k : \mathcal{R}^D \times \mathcal{R}^D \to \mathcal{R}$

1. Compute $\overline{\phi} = \frac{1}{N}\sum_j \phi(x_j)$ and the centered embedded data matrix Φ **or** the kernel matrix K.
2. Compute the centered kernel *matrix*:
$$\tilde{\mathcal{K}} = \Phi^T\Phi \text{ or } \tilde{\mathcal{K}} = \big(I - \frac{1}{n}11^T\big)K\big(I - \frac{1}{n}11^T\big) = JKJ \text{ or } \big(\tilde{k}(x_i, x_j)\big) \in \mathcal{R}^{N\times N}$$
3. Compute the eigenvectors $w_i \in \mathcal{R}^N$ of $\tilde{\mathcal{K}}$:
$$\tilde{\mathcal{K}}w_i = \lambda_i w_i$$
and normalize so that $||w_i||^2 = \lambda_i^{-1}$ (can be done as in step 4).
   - For every data point x, its i^{th} nonlinear principal component is given by:
$$y_i = w_i^T\Phi^T(\phi(x) - \overline{\phi}) \text{ or } w_i^T[\tilde{k}(x_1, x), \dots, \tilde{k}(x_N, x)]^T$$
   for $i = 1, 2, \dots, d$
4. The projection is given by:
$$Y = (y_1, y_2, \dots, y_d)^T = \Lambda_d^{-\frac{1}{2}}V_d^T\tilde{K}$$

- **Output**: A set of points $\{y_j\}_{j=1}^N$ lying in $\mathcal{R}^d$, where y_{ij} in the i^{th} nonlinear principal component of x_j for $i = 1, \dots, d$ and $j = 1, \dots, N$

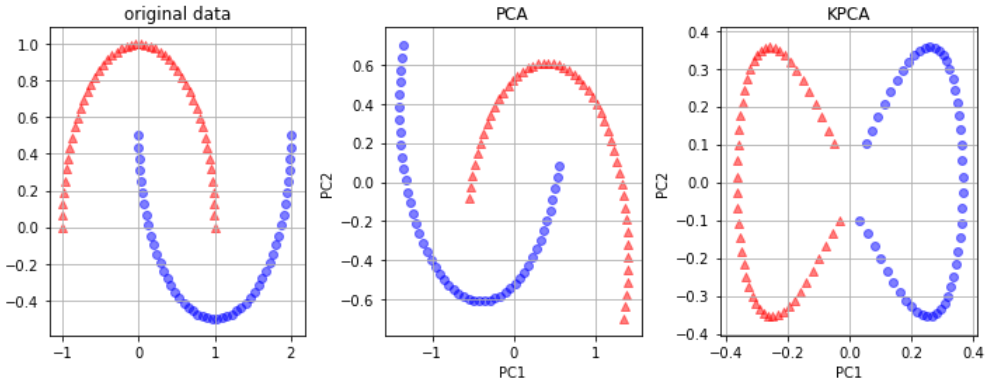
In [4]:
```
def plot_circles_example():
    # example - circles
    X, y = make_circles(n_samples=1000, random_state=123, noise=0.1, factor=0.2)
    pca = PCA(n_components=2)
    kpca = KernelPCA(n_components=2, kernel='rbf', gamma=15)  # Radial Basis Function kernel
    X_pca = pca.fit_transform(X)
    X_kpca = kpca.fit_transform(X)

    # plot
    fig = plt.figure(figsize=(10,4))

    # original data
    ax1 = fig.add_subplot(1,3,1)
    ax1.scatter(X[y==0, 0], X[y==0, 1], color='red', marker='^', alpha=0.5)
    ax1.scatter(X[y==1, 0], X[y==1, 1], color='blue', marker='o', alpha=0.5)
    ax1.grid()
    ax1.set_title("original data")

    # pca
    ax2 = fig.add_subplot(1,3,2)
    ax2.scatter(X_pca[y==0, 0], X_pca[y==0, 1], color='red', marker='^', alpha=0.5)
    ax2.scatter(X_pca[y==1, 0], X_pca[y==1, 1], color='blue', marker='o', alpha=0.5)
    ax2.grid()
    ax2.set_title("PCA")
    ax2.set_xlabel("PC1")
    ax2.set_ylabel("PC2")

    # kpca
    ax3 = fig.add_subplot(1,3,3)
    ax3.scatter(X_kpca[y==0, 0], X_kpca[y==0, 1], color='red', marker='^', alpha=0.5)
    ax3.scatter(X_kpca[y==1, 0], X_kpca[y==1, 1], color='blue', marker='o', alpha=0.5)
    ax3.grid()
    ax3.set_title("KPCA")
    ax3.set_xlabel("PC1")
    ax3.set_ylabel("PC2")

    plt.tight_layout()
```

In [5]:
```
plot_circles_example()
```



In [6]:
```
def plot_moons_example():
    # example - moons
    X, y = make_moons(n_samples=100, random_state=123)
    pca = PCA(n_components=2)
    kpca = KernelPCA(n_components=2, kernel='rbf', gamma=15)  # Radial Basis Function kernel
    X_pca = pca.fit_transform(X)
    X_kpca = kpca.fit_transform(X)

    # plot
    fig = plt.figure(figsize=(10,4))

    # original data
    ax1 = fig.add_subplot(1,3,1)
    ax1.scatter(X[y==0, 0], X[y==0, 1], color='red', marker='^', alpha=0.5)
    ax1.scatter(X[y==1, 0], X[y==1, 1], color='blue', marker='o', alpha=0.5)
    ax1.grid()
    ax1.set_title("original data")

    # pca
    ax2 = fig.add_subplot(1,3,2)
    ax2.scatter(X_pca[y==0, 0], X_pca[y==0, 1], color='red', marker='^', alpha=0.5)
    ax2.scatter(X_pca[y==1, 0], X_pca[y==1, 1], color='blue', marker='o', alpha=0.5)
    ax2.grid()
    ax2.set_title("PCA")
    ax2.set_xlabel("PC1")
    ax2.set_ylabel("PC2")

    # kpca
    ax3 = fig.add_subplot(1,3,3)
    ax3.scatter(X_kpca[y==0, 0], X_kpca[y==0, 1], color='red', marker='^', alpha=0.5)
    ax3.scatter(X_kpca[y==1, 0], X_kpca[y==1, 1], color='blue', marker='o', alpha=0.5)
    ax3.grid()
    ax3.set_title("KPCA")
    ax3.set_xlabel("PC1")
    ax3.set_ylabel("PC2")

    plt.tight_layout()
```

In [7]:
```
plot_moons_example()
```



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)
- The Kernel Trick - Machine Learning Fundamentals - The Kernel Trick (https://www.youtube.com/watch?v=JiM_LXpAtLc)
- Kernel PCA - David Thompson: Nonlinear Dimensionality Reduction: KPCA (https://www.youtube.com/watch?v=HbDHohXPLnU)

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/)