code-file

November 4, 2023

Exercise1: 'Kernel properties' (10 points) 1. Provide some python code to illustrate the relation of a kernel on centered data and the eigen-decomposition of uncentered data. How do some results of the eigendecomposition change / or not change?

[2]:
```
import numpy as np
import pandas as pd

# Function to compute inner-product kernel matrix
def compute_kernel_matrix(data):
    n = data.shape[0]
    kernel_matrix = np.zeros((n, n))
    for i in range(n):
        for j in range(n):
            kernel_matrix[i, j] = np.dot(data[i], data[j])  # Using inner␣
 ↪product
    return kernel_matrix

# Function to center a kernel matrix
def center_kernel_matrix(K):
    n = K.shape[0]
    one_n = np.ones((n, n)) / n
    centered_K = K - one_n.dot(K) - K.dot(one_n) + one_n.dot(K).dot(one_n)
    return centered_K

# Load data from file
file_path = '/content/sample_data/krein.cvs'
data = pd.read_csv(file_path)


data_values = data.values

# Compute the uncentered kernel matrix
uncentered_kernel = compute_kernel_matrix(data_values)

# Center the kernel matrix
centered_kernel = center_kernel_matrix(uncentered_kernel)

# Perform eigen-decomposition of the uncentered kernel matrix
```

```python
eigvals_uncentered, eigvecs_uncentered = np.linalg.eig(uncentered_kernel)

# Perform eigen-decomposition of the centered kernel matrix
eigvals_centered, eigvecs_centered = np.linalg.eig(centered_kernel)

# Compare some results of the eigen-decomposition
print("Eigenvalues of the uncentered kernel matrix:")
print(eigvals_uncentered)
print("\nEigenvalues of the centered kernel matrix:")
print(eigvals_centered)
```

```
Eigenvalues of the uncentered kernel matrix:
[3.67262729e+10 2.74598861e+10 2.01021408e+10 1.18488675e+03
 8.14186337e+02 6.32976296e+02 4.10141472e+02 2.52573529e+02
 2.27433769e+02 1.49193573e+02 1.15354334e+02 7.92387545e+01
 6.90990723e+01 5.88200733e+01 4.49577312e+01 4.10905256e+01
 3.26242603e+01 2.77085615e+01 2.42662757e+01 2.08563446e+01
 1.80444543e+01 1.49106569e+01 1.34298617e+01 1.17655648e+01
 1.05598983e+01 1.04101302e+01 9.23433708e+00 8.38173558e+00
 7.72728431e+00 6.96918558e+00 6.58402296e+00 6.03917536e+00
 5.42969190e+00 5.07177794e+00 4.86631829e+00 4.46764119e+00
 4.29417769e+00 3.78319712e+00 3.49413290e+00 3.35081162e+00
 3.23322372e+00 3.02296964e+00 2.88759710e+00 2.70377510e+00
 2.67961291e+00 2.51390197e+00 2.32836385e+00 2.34795561e+00
 2.27165374e+00 2.14170253e+00 2.02541581e+00 1.95334870e+00
 1.87940430e+00 1.84960153e+00 1.74581053e+00 1.69889162e+00
 1.64857782e+00 1.59668366e+00 1.53886961e+00 1.44258556e+00
 1.40044734e+00 1.34574929e+00 1.31899277e+00 1.28213556e+00
 1.22354625e+00 1.20323356e+00 1.14518743e+00 1.11732897e+00
 1.07691032e+00 1.05956806e+00 1.02539440e+00 1.01277929e+00
 9.85954258e-01 9.35352279e-01 9.01794170e-01 8.97532990e-01
 8.38736343e-01 8.21207922e-01 7.78504449e-01 7.84165044e-01
 8.07310820e-01 8.02207767e-01 7.56850652e-01 7.29989814e-01
 7.10773170e-01 6.83167992e-01 6.77896777e-01 6.43546039e-01
 6.25513049e-01 6.13798635e-01 5.85220472e-01 5.91184896e-01
 5.60374853e-01 5.50573275e-01 5.42707517e-01 5.28522768e-01
 4.97734564e-01 4.94178625e-01 4.84382424e-01 4.43985413e-01
 4.37346968e-01 4.27611900e-01 4.17167034e-01 4.13489509e-01
 3.91617999e-01 3.85703319e-01 3.81313664e-01 3.70171091e-01
 3.40540290e-01 3.36650215e-01 3.50396618e-01 3.55953567e-01
 3.60130756e-01 3.13253197e-01 3.21323258e-01 3.00628897e-01
 2.91317203e-01 2.83434213e-01 2.12288242e-01 2.13259815e-01
 2.26989845e-01 2.29970855e-01 2.70077859e-01 2.63482686e-01
 2.60500468e-01 2.42999890e-01 2.45787073e-01 2.52768028e-01
 2.00058546e-01 1.82581755e-01 1.86030852e-01 1.73814928e-01
 1.68618148e-01 1.65712229e-01 1.56763031e-01 1.52184106e-01
 1.46859128e-01 1.38795953e-01 1.37355314e-01 1.33168173e-01
```

```
 1.22011185e-01 1.19694467e-01 1.15120429e-01 1.16011906e-01
 1.09370252e-01 1.05139215e-01 9.94165809e-02 9.70300404e-02
 9.01852043e-02 9.21089492e-02 9.56025023e-02 8.03989161e-02
 7.75400045e-02 7.23680692e-02 7.07483592e-02 6.42410247e-02
 6.94664495e-02 5.99597575e-02 5.39518165e-02 6.27858190e-02
 5.02164955e-02 5.11084995e-02 4.60461142e-02 5.67197841e-02
 3.91434389e-02 4.08835266e-02 4.13271545e-02 3.37118741e-02
 1.99958749e-05 1.18901011e-04 2.66161502e-04 4.22534014e-04
 5.36200355e-04 1.09096117e-03 1.66398178e-03 3.12546169e-02
 2.60010102e-03 2.42982295e-02 1.82552632e-02 1.55450013e-02
 1.97014150e-02 1.27275265e-02 2.30982900e-03 3.56418281e-03
 1.16309512e-02 5.65741807e-03 8.16733934e-03 6.99742325e-03
 4.19176381e-03 3.97286760e-03 1.05689097e-02 9.60193757e-03
 2.95935849e-02 3.02879573e-02 2.33425396e-02 2.74788911e-02
 2.08287244e-02 2.24585082e-02 6.49593816e-03]

Eigenvalues of the centered kernel matrix:
[ 3.67258766e+10  2.74598057e+10  2.01002180e+10  1.18487600e+03
  8.14185617e+02  6.32958816e+02  4.10128453e+02  2.52570081e+02
  2.27427719e+02  1.49193540e+02  1.15354312e+02  7.92387528e+01
  6.90974749e+01  5.88188834e+01  4.49574624e+01  4.10903845e+01
  3.26237013e+01  2.77061043e+01  2.42657767e+01  2.08562920e+01
  1.80437675e+01  1.49106569e+01  1.34298511e+01  1.17652964e+01
  1.05568259e+01  1.04101085e+01  9.23173509e+00  8.38013821e+00
  7.72728389e+00  6.96899447e+00  6.58319750e+00  6.03839312e+00
  5.42968861e+00  5.07175911e+00  4.86575675e+00  4.46722451e+00
  4.29391825e+00  3.78286793e+00  3.49409898e+00  3.34978206e+00
  3.23263825e+00  3.02270399e+00  2.88517247e+00  2.70376153e+00
  2.67860712e+00  2.51323724e+00  2.32793894e+00  2.34773766e+00
  2.27156871e+00  2.14049295e+00  2.02484086e+00  1.95329189e+00
  1.87776776e+00  1.84958897e+00  1.74510834e+00  1.69888253e+00
  1.64788470e+00  1.59668232e+00  1.53869982e+00  1.44171925e+00
  1.39952791e+00  1.34574133e+00  1.31886216e+00  1.28163984e+00
  1.22349127e+00  1.20321053e+00  1.14504683e+00  1.11699880e+00
  1.07610859e+00  1.05865769e+00  1.02465899e+00  1.01248102e+00
  9.85651773e-01  9.35224332e-01  9.01761975e-01  8.96358933e-01
  8.21115572e-01  8.37836625e-01  8.07063084e-01  8.01883419e-01
  7.82180700e-01  7.76606819e-01  7.55333494e-01  7.29926222e-01
  7.10767704e-01  6.83078601e-01  6.76979304e-01  6.43528839e-01
  6.25341441e-01  6.13742785e-01  5.91125229e-01  5.83165804e-01
  5.60074490e-01  5.49581601e-01  5.42575159e-01  5.28207885e-01
  4.97734475e-01  4.93686545e-01  4.84291585e-01  4.43826555e-01
  4.37310149e-01  4.26198175e-01  4.17144327e-01  4.13463701e-01
  3.91600464e-01  3.83875341e-01  3.80231974e-01  3.70066399e-01
  3.60125757e-01  3.55580346e-01  3.50218315e-01  3.40516759e-01
  3.36598383e-01  3.13228680e-01  3.21322395e-01  3.00190075e-01
  2.90880351e-01  2.82931980e-01  2.69912446e-01  2.62180875e-01
  2.60397124e-01  2.52255307e-01  2.45638452e-01  2.42282127e-01
```

```
 1.68594875e-01  1.72427068e-01  2.29759308e-01  2.26754761e-01
 1.82556022e-01  1.85113906e-01  1.99504760e-01  2.12833686e-01
 2.11521465e-01  1.65509454e-01  1.56595182e-01  1.52138964e-01
 1.46027976e-01  1.38615614e-01  1.35857872e-01  1.32403734e-01
 1.21790027e-01  1.19671300e-01  1.15158927e-01  1.13380507e-01
 1.09344275e-01  1.04816022e-01  9.94107683e-02  9.70260979e-02
 9.55750194e-02  9.18703577e-02  9.01493287e-02  8.03985322e-02
 7.75323473e-02  7.07873156e-02  6.99334151e-02  6.94149780e-02
 6.41149327e-02  5.96852177e-02  6.26998865e-02  5.66429955e-02
 5.39511894e-02  5.03149677e-02  4.56439655e-02  4.79286901e-02
 3.91434824e-02  4.07308792e-02  4.10914000e-02  3.36641353e-02
 2.90966213e-02  2.74476100e-02  1.91798644e-02  2.01700953e-02
 2.33404672e-02  1.56435997e-02  3.03306509e-02  3.01709766e-02
 2.42797974e-02  2.23213649e-02  1.27746202e-02  1.23693007e-02
 8.14320251e-03  1.09800848e-02  1.05646197e-02  9.45920697e-03
 6.82937134e-03  5.24531923e-03  1.08231286e-03  5.03870362e-04
-9.06669851e-07  6.46404616e-03  3.82884429e-05  3.53913536e-03
 2.33309627e-03  1.79560480e-03  1.25918847e-04  2.75845054e-04
 1.66042001e-03  3.87775105e-03  3.99082471e-03]
```

Exercise2: ‘Frobenius norm of a matrix’ (10 points) 1. Provide some python code to calculate the Frobenius norm of a matrix A and evaluate its relation to the sum of the (squared) singular values of A

[3]:
```python
import numpy as np
import pandas as pd

# Function to calculate Frobenius norm
def frobenius_norm(matrix):
    return np.sqrt(np.sum(matrix ** 2))

# Load data from file
file_path = '/content/sample_data/krein.cvs'
data = pd.read_csv(file_path)

matrix_data = data.values

# Calculate Frobenius norm directly
frobenius_norm_direct = frobenius_norm(matrix_data)

# Calculate Frobenius norm using singular value decomposition (SVD)
u, s, vh = np.linalg.svd(matrix_data)
frobenius_norm_svd = np.sqrt(np.sum(s**2))

# Compare the norms
print("Frobenius Norm of matrix A:", frobenius_norm_direct)
print("Sum of squared singular values of matrix A (from SVD):",␣
 ↪frobenius_norm_svd)
```

```
Frobenius Norm of matrix A: 290324.48089291924
Sum of squared singular values of matrix A (from SVD): 290324.4808929191
```

Exercise3: 'Correction of non-psd similarities' (10 points) 1. Provide some python code to illustrate that adding an offset indeed shifts the eigenvalues

[4]:
```python
import numpy as np
import pandas as pd

# Function to calculate the eigenvalues of a symmetric matrix
def calculate_eigenvalues(matrix):
    eigenvalues, _ = np.linalg.eig(matrix)
    return eigenvalues

# Load data from file
file_path = '/content/sample_data/krein.cvs'
data = pd.read_csv(file_path)


matrix_data = data.values

# Make a symmetric matrix from the data
symmetric_matrix = np.dot(matrix_data, matrix_data.T)

# Calculate eigenvalues of the original matrix
original_eigenvalues = calculate_eigenvalues(symmetric_matrix)

# Add an offset to the diagonal
offset = 5  # Change this to alter the offset value
offset_matrix = symmetric_matrix + np.eye(symmetric_matrix.shape[0]) * offset

# Calculate eigenvalues of the matrix with the offset
offset_eigenvalues = calculate_eigenvalues(offset_matrix)

# Show the eigenvalues
print("Original Eigenvalues:")
print(original_eigenvalues)
print("\nEigenvalues with Offset:")
print(offset_eigenvalues)
```

```
Original Eigenvalues:
[3.67262729e+10 2.74598861e+10 2.01021408e+10 1.18488675e+03
 8.14186337e+02 6.32976296e+02 4.10141472e+02 2.52573529e+02
 2.27433769e+02 1.49193573e+02 1.15354334e+02 7.92387543e+01
 6.90990719e+01 5.88200736e+01 4.49577311e+01 4.10905254e+01
 3.26242605e+01 2.77085614e+01 2.42662756e+01 2.08563443e+01
 1.80444544e+01 1.49106574e+01 1.34298615e+01 1.17655651e+01
 1.05598978e+01 1.04101303e+01 9.23433730e+00 8.38173563e+00
```

```
 7.72728417e+00 6.96918575e+00 6.58402326e+00 6.03917512e+00
 5.42969193e+00 5.07177781e+00 4.86631856e+00 4.46764115e+00
 4.29417797e+00 3.78319714e+00 3.49413292e+00 3.35081194e+00
 3.23322360e+00 3.02297017e+00 2.88759707e+00 2.70377525e+00
 2.67961307e+00 2.51390203e+00 2.32836403e+00 2.34795574e+00
 2.27165364e+00 2.14170257e+00 2.02541591e+00 1.95334863e+00
 1.87940407e+00 1.84960148e+00 1.74581100e+00 1.69889168e+00
 1.64857768e+00 1.59668375e+00 1.53886950e+00 1.44258576e+00
 1.40044690e+00 1.34574914e+00 1.31899271e+00 1.28213579e+00
 1.22354626e+00 1.20323362e+00 1.14518727e+00 1.11732893e+00
 1.07691069e+00 1.05956796e+00 1.02539438e+00 1.01277929e+00
 9.85954140e-01 9.35352130e-01 9.01794210e-01 8.97532969e-01
 8.38735969e-01 8.21208057e-01 7.78504607e-01 7.84165001e-01
 8.07310903e-01 8.02207575e-01 7.56850528e-01 7.29990058e-01
 7.10772966e-01 6.83168003e-01 6.77897167e-01 6.43546199e-01
 6.25512650e-01 6.13798659e-01 5.85220292e-01 5.91184942e-01
 5.60374864e-01 5.50573035e-01 5.42707895e-01 5.28522581e-01
 4.97734739e-01 4.94178660e-01 4.84382532e-01 4.43985355e-01
 4.37346853e-01 4.27611546e-01 4.17167168e-01 4.13489474e-01
 3.91618206e-01 3.85703225e-01 3.81313491e-01 3.70170720e-01
 3.40540463e-01 3.36650220e-01 3.50396800e-01 3.55953635e-01
 3.60130887e-01 3.13252748e-01 3.21323191e-01 3.00628984e-01
 2.91317306e-01 2.83433793e-01 2.12288535e-01 2.13259898e-01
 2.26989773e-01 2.29970676e-01 2.70077777e-01 2.63482851e-01
 2.60500808e-01 2.43000034e-01 2.45787030e-01 2.52767936e-01
 2.00058520e-01 1.82581888e-01 1.86030803e-01 1.73815102e-01
 1.68618007e-01 1.65712212e-01 1.56762787e-01 1.52184014e-01
 1.46859121e-01 1.38795481e-01 1.37355046e-01 1.33168133e-01
 1.22011130e-01 1.19694752e-01 1.15120763e-01 1.16012035e-01
 1.09370218e-01 1.05139142e-01 9.94164302e-02 9.70300898e-02
 9.01854559e-02 9.21090322e-02 9.56022442e-02 8.03988987e-02
 7.75401876e-02 7.23679645e-02 7.07488311e-02 6.42409950e-02
 6.94663903e-02 5.99598730e-02 5.39516191e-02 6.27857297e-02
 5.02165506e-02 5.11081670e-02 4.60458111e-02 5.67200850e-02
 4.08837946e-02 3.91433592e-02 4.13270574e-02 1.99093609e-05
 1.18753944e-04 2.66185893e-04 4.22674006e-04 5.36041795e-04
 1.09062362e-03 3.37118692e-02 1.66407466e-03 3.12541400e-02
 2.60020335e-03 2.95934525e-02 3.02880193e-02 2.42984255e-02
 1.82551911e-02 1.55450608e-02 1.97011893e-02 2.74784013e-02
 2.33426363e-02 1.27271703e-02 3.56435043e-03 2.30966408e-03
 5.65711639e-03 1.16310125e-02 8.16743098e-03 4.19193147e-03
 6.99755477e-03 3.97279291e-03 1.05690109e-02 9.60206485e-03
 2.08285097e-02 2.24585553e-02 6.49598072e-03]

Eigenvalues with Offset:
[3.67262729e+10 2.74598861e+10 2.01021408e+10 1.18988675e+03
 8.19186338e+02 6.37976296e+02 4.15141472e+02 2.57573529e+02
 2.32433769e+02 1.54193573e+02 1.20354334e+02 8.42387548e+01
```

```
7.40990719e+01 6.38200735e+01 4.99577311e+01 4.60905256e+01
3.76242604e+01 3.27085613e+01 2.92662755e+01 2.58563444e+01
2.30444546e+01 1.99106574e+01 1.84298614e+01 1.67655648e+01
1.55598978e+01 1.54101304e+01 1.42343374e+01 1.33817355e+01
1.27272843e+01 1.19691858e+01 1.15840233e+01 1.10391750e+01
1.04296916e+01 1.00717779e+01 9.86631858e+00 9.46764119e+00
9.29417765e+00 8.78319684e+00 8.49413288e+00 8.35081178e+00
8.23322348e+00 8.02296993e+00 7.88759719e+00 7.70377520e+00
7.67961279e+00 7.51390189e+00 7.32836397e+00 7.34795560e+00
7.27165369e+00 7.14170251e+00 7.02541585e+00 6.95334856e+00
6.87940406e+00 6.84960157e+00 6.74581098e+00 6.69889163e+00
6.64857782e+00 6.53886938e+00 6.59668394e+00 6.44258565e+00
6.40044712e+00 6.34574920e+00 6.31899275e+00 6.28213568e+00
6.22354622e+00 6.20323353e+00 6.14518726e+00 6.11732903e+00
6.07691070e+00 6.05956795e+00 6.02539447e+00 6.01277932e+00
5.98595410e+00 5.93535223e+00 5.90179414e+00 5.89753314e+00
5.83873594e+00 5.82120794e+00 5.80731092e+00 5.80220768e+00
5.78416476e+00 5.77850458e+00 5.75685037e+00 5.72998995e+00
5.71077301e+00 5.68316802e+00 5.67789708e+00 5.64354613e+00
5.62551262e+00 5.61379870e+00 5.59118492e+00 5.58522027e+00
5.56037482e+00 5.55057299e+00 5.54270795e+00 5.52852270e+00
5.49773478e+00 5.49417887e+00 5.48438248e+00 5.44398534e+00
5.43734658e+00 5.42761163e+00 5.41716709e+00 5.41348945e+00
5.39161808e+00 5.38570319e+00 5.37017073e+00 5.38131354e+00
5.35595364e+00 5.36013067e+00 5.35039663e+00 5.34054023e+00
5.33665015e+00 5.31325276e+00 5.32132328e+00 5.30062912e+00
5.22997070e+00 5.29131727e+00 5.28343387e+00 5.24299984e+00
5.24578709e+00 5.25276802e+00 5.26050070e+00 5.26348303e+00
5.27007786e+00 5.22698965e+00 5.21228823e+00 5.21325990e+00
5.20005879e+00 5.18603107e+00 5.18258164e+00 5.17381513e+00
5.16861802e+00 5.16571210e+00 5.15676293e+00 5.15218402e+00
5.14685906e+00 5.13879561e+00 5.13735495e+00 5.13316798e+00
5.12201108e+00 5.11969457e+00 5.11512079e+00 5.11601199e+00
5.10937028e+00 5.10513899e+00 5.09941629e+00 5.09018551e+00
5.09210903e+00 5.09703013e+00 5.09560233e+00 5.08039899e+00
5.07754017e+00 5.07236784e+00 5.07074871e+00 5.06946637e+00
5.06424107e+00 5.05995980e+00 5.05395148e+00 5.06278578e+00
5.05021657e+00 5.05110825e+00 5.04604599e+00 5.05672001e+00
5.03914323e+00 5.04088352e+00 5.04132714e+00 5.00001991e+00
5.00011885e+00 5.00026635e+00 5.00042251e+00 5.00053584e+00
5.00109066e+00 5.03371200e+00 5.00166396e+00 5.00260005e+00
5.00356445e+00 5.00230954e+00 5.01554472e+00 5.01825513e+00
5.01272739e+00 5.00565714e+00 5.00816745e+00 5.00419193e+00
5.00699728e+00 5.01163112e+00 5.00397275e+00 5.00960187e+00
5.01056902e+00 5.01970142e+00 5.02429832e+00 5.03125436e+00
5.02959341e+00 5.02334245e+00 5.03028796e+00 5.02747852e+00
5.02082859e+00 5.02245854e+00 5.00649602e+00]
```

Exercise4: ‘Krein spaces’ (10 points) 1. Provide some python code to illustrate that the claimed statement indeed holds for indefinite (non-psd) kernel matrices (use the eigen-decomposition)

[5]:
```
import numpy as np
import pandas as pd

# Load data from the provided CSV file
file_path = '/content/sample_data/krein.cvs'
data = pd.read_csv(file_path, header=None)
matrix = data.values

if matrix.shape[0] != matrix.shape[1]:
    matrix = matrix.T

# Perform eigen-decomposition of the matrix
eigenvalues, eigenvectors = np.linalg.eig(matrix)

# Extract positive and negative eigenvalues
positive_indices = eigenvalues > 0
negative_indices = eigenvalues < 0

# Create submatrices A+ and A- with positive and negative eigenvalues␣
↪respectively
A_positive = np.dot(eigenvectors[:, positive_indices], np.dot(np.
↪diag(eigenvalues[positive_indices]), eigenvectors[:, positive_indices].T))
A_negative = np.dot(eigenvectors[:, negative_indices], np.dot(np.
↪diag(eigenvalues[negative_indices]), eigenvectors[:, negative_indices].T))

# Combine A+ and A- to reconstruct the original matrix
reconstructed_matrix = A_positive + A_negative

# Check if the original matrix and the reconstructed matrix are similar
is_same_matrix = np.allclose(matrix, reconstructed_matrix)

print("Original Matrix:")
print(matrix)
print("\nReconstructed Matrix (A+ + A-):")
print(reconstructed_matrix)
print("\nAre the original and reconstructed matrices the same?", is_same_matrix)
```

```
Original Matrix:
[[ 3171.1    -421.35   1320.3    … -2228.5      27.078  1890.1  ]
 [ -421.35   2170.3    1929.3    …  -159.86   -988.92    334.18 ]
 [ 1320.3    1929.3    2643.8    … -1364.5    -938.2    1338.8  ]
 …
 [-2228.5    -159.86  -1364.5    …  1897.      635.8   -1879.9  ]
 [   27.078  -988.92   -938.2    …   635.8    1286.1   -1055.4  ]
 [ 1890.1     334.18   1338.8    … -1879.9   -1055.4    2055.4  ]]
```

```
Reconstructed Matrix (A+ + A-):
[[ 3171.1    -421.35   1320.3   … -2228.5      27.078  1890.1  ]
 [ -421.35   2170.3    1929.3   …  -159.86   -988.92    334.18 ]
 [ 1320.3    1929.3    2643.8   … -1364.5    -938.2    1338.8  ]
 …
 [-2228.5    -159.86  -1364.5   …  1897.      635.8   -1879.9  ]
 [   27.078  -988.92   -938.2   …   635.8    1286.1   -1055.4  ]
 [ 1890.1     334.18   1338.8   … -1879.9   -1055.4    2055.4  ]]

Are the original and reconstructed matrices the same? True
```