DS-GA.1013 Mathematical Tools for Data Science
Homework 1
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1. (Rotation) For a symmetric matrix $A$, can there be a nonzero vector $x$ such that $Ax$ is nonzero and orthogonal to $x$? Either prove that this is impossible, or explain under what condition on the eigenvalues of $A$ such a vector exists. Let $x \in V, x \neq 0$, an inner product space , by the spectral theorem there exists an orthonormal basis of $V$, consisting of eigenvectors of $A$, let $u_1, \dots, u_n$ be the eigenbasis of $A$, and $\lambda_1, \dots, \lambda_n$ the eigenvalues for each of these eigenvectors. $x \in \text{span}\{u_1, \dots, u_n\} \Rightarrow x = \sum_{i=1,n} \alpha_i u_i, \alpha_i \neq 0$. $x^T(Ax) = (\sum_{i=1,n} \alpha_i u_i)(\sum_{j=1,n} \alpha_j A u_j) = (\sum_{i=1,n} \alpha_i u_i)(\sum_{j=1,n} \alpha_j \lambda_j u_j) = \sum_{i=1,n} \alpha_i^2 \lambda_i$ since $u_i^T u_j = 0$ for $i \neq j$ and $u_i^T u_i = 1$. $Ax$ is orthogonal to $x$: $x^T(Ax) = 0 \Rightarrow \sum_{i=1,n} \alpha_i^2 \lambda_i = 0$.

2. (Matrix decomposition) The trace can be used to define an inner product between matrices:

$$\langle A, B \rangle := \text{tr}\left(A^T B\right), \quad A, B \in \mathbb{R}^{m \times n}, \tag{1}$$

where the corresponding norm is the Frobenius norm $||A||_{\text{F}} := \langle A, A \rangle$.

(a) Express the inner product in terms of vectorized matrices and use the result to prove that this is a valid inner product. $(AB)_{ij} = (\sum_k A_{ik} B_{kj})_{ij}$, and $(A^T B)_{ij} = (\sum_k A_{ki} B_{kj})_{ij}$. $\text{tr}\,(A) = \sum_i A_{ii} \Rightarrow \text{tr}\left(A^T B\right) = \sum_i \sum_k A_{ki} B_{ki} = \sum_i \sum_j A_{ij} B_{ij} = \text{vec}(A)^T \text{vect}(B) = \langle \text{vec}(A), \text{vec}(B) \rangle$. The trace is then the inner product between vectors in $\mathbb{R}^{mn}$ thus is a valid inner product.

(b) Prove that for any $A, B \in \mathbb{R}^{m \times n}$, $\text{tr}\left(A^T B\right) = \text{tr}\left(B A^T\right)$. $\text{tr}\left(B A^T\right) = \sum_i \sum_k B_{ik} A_{ik} = \sum_i \sum_j A_{ij} B_{ij} = \text{tr}\left(A^T B\right)$.

(c) Let $u_1, \dots, u_n$ be the eigenvectors of a symmetric matrix $A$. Compute the inner product between the rank-1 matrices $u_i u_i^T$ and $u_j u_j^T$ for $i \neq j$, and also the norm of $u_i u_i^T$ for $i = 1, \dots, n$. For $i \neq j$, $\left\langle u_i u_i^T, u_j u_j^T \right\rangle = \text{tr}\left(u_i u_i^T u_j u_j^T\right) = \text{tr}\left(u_i \; 0 \; u_j^T\right) = 0$, since $u_i, u_j$ are two eigenvectors of a symmetric matrix therefore orthogonal. if $i = j$ then $\left\langle u_i u_i^T, u_i u_i^T \right\rangle = \text{tr}\left(u_i u_i^T u_i u_i^T\right) = \text{tr}\left(u_i^T \; I \; u_i\right) = \text{tr}\left(u_i^T u_i\right) = 1$ if the eigenvectors are also orthonormal.

(d) What is the projection of $A$ onto $u_i u_i^T$? If $A$ is a symmetric matrix, by the spectral theorem, $A = UDU^T$ where $D$ is the diagonal matrix having $\lambda_i, i = 1, \dots, n$ the eigenvalues of $A$ on the diagonal. Then $A = \sum_i \lambda_i u_i u_i^T$, where $u_1, \dots, u_n$ are the eigenvectors of A. The projection of $A$ onto $u_i u_i^T$ is $\langle A, u_i u_i^T \rangle$ thus

$$\begin{aligned}
\langle A, u_i u_i^T \rangle &= \left\langle \sum_{j=1}^{n} \lambda_j u_j u_j^T, u_i u_i^T \right\rangle \\
&= \sum_{j=1}^{n} \langle \lambda_j u_j u_j^T, u_i u_i^T \rangle \\
&= \sum_{j=1}^{n} \lambda_j \langle u_j u_j^T, u_i u_i^T \rangle \\
&= \lambda_i \langle u_i u_i^T, u_i u_i^T \rangle \\
&= \lambda_i
\end{aligned}$$

Where we applied linearity of the inner product for equations 2 and 3 and reuse the results of the inner product between eigenvectors from the previous question (assuming we chose eigenvectors orthonormal).

(e) Provide a geometric interpretation of the matrix $A' := A - \lambda_1 u_1 u_1^T$, which we defined in the proof of the spectral theorem, based on your previous answers. From the previous question the orthogonal projection of A in $u_i u_i^T$ is $\lambda_i u_i u_i^T$ so $A' = \sum_i \lambda_i u_i u_i^T, i \neq 1$ has row or column subspaces contained in $(u_1)^\perp$.

3. (Quadratic forms) Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix, and let $f(x) := x^T A x$ be the corresponding quadratic form. We consider the 1D function $g_v(t) = f(tv)$ obtained by restricting the quadratic form to lie in the direction of a vector $v$ with unit $\ell_2$ norm.

   (a) Is $g_v(t)$ a polynomial? If so, what kind? $g_v(t) = f(tv) = (tv)^T A(tv) = t^2 v^T A v = v^T A v\, t^2$, $v^T A v$ is a scalar, and $g_v(t)$ is a second-order polynomial in $t$.

   (b) What is the curvature (i.e. the second derivative) of $g_v(t) = f(tv)$ at an arbitrary point $t$? $g_v'(t) = 2v^T A v\, t$ and the curvature is $g_v''(t) = 2v^T A v$

   (c) What are the directions of maximum and minimum curvature of the quadratic form? What are the corresponding curvatures equal to? By the spectral theorem, $A = U\mathbf{diag}(\lambda)U^T$ where **diag** is the diagonal matrix with on the diagonal: $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_n$, which are the eigenvalues and $u_1, \ldots, u_n$ the corresponding eigenvectors. The largest eigenvalue is $\lambda_1 = \max_{\|v\|_2=1} v^T A v$ with eigenvector $u_1 = \arg\max_{\|v\|_2=1} v^T A v$, and the smaller eigenvalue is given by $\lambda_n = \max_{\|v\|_2=1} v^T A v, u_n = \arg\max_{\|v\|_2=1} v^T A v$. Thus the maximum curvature is given by the largest eigenvalue $\lambda_1$ and is in the direction of the corresponding eigenvector $u_1$. The smallest curvature is given by the smallest eigenvalue $\lambda_n$ and is in the direction of the corresponding eigenvector $u_n$.

4. (Projected gradient ascent) Projected gradient descent is a method designed to find the maximum of a differentiable function $f : \mathbb{R}^n \to \mathbb{R}$ in a constraint set $\mathcal{S}$. Let $\mathcal{P}_\mathcal{S}$ denote the projection onto $\mathcal{S}$, i.e.

$$\mathcal{P}_\mathcal{S}(x) := \arg\min_{y \in \mathcal{S}} ||x - y||_2^2 \,. \tag{2}$$

The $k$th update of projected gradient ascent equals

$$x^{[k]} := \mathcal{P}_{\mathcal{S}}(x^{[k-1]} + \alpha \nabla f(x^{[k-1]})), \qquad k = 1, 2, \ldots, \tag{3}$$

where $\alpha$ is a positive constant and $x^{[0]}$ is an arbitrary initial point.

(a) Use the same arguments we used to prove Lemmas 5.1 and 5.2 in the notes on PCA to derive the projection of a vector $x$ onto the unit sphere in $n$ dimensions. Let define $f(x) = ||x - y||_2^2, y \in \mathcal{S}$, the directional derivative cannot be different than zero $f'_v(x) = \langle \nabla x, v \rangle = 0$ for any $v$ such that $x + \epsilon v$ is on the sphere $\mathcal{S}$. Let $g(x) = x^T x, \|y\|_2 = 1$, $g$ describes points on the surface of the unit sphere. $x + \epsilon v$ is in the tangent plane of $g$ at $x$ if $\nabla g(x)^T v = 0$, and for $\epsilon \approx 0$, $g(x + \epsilon v) \approx g(x)$. We are then looking for global minimizer points (global because $f$ is convex), where the level curves of $f$ are tangent to the curve $g$, or where the gradients are colinear. $\nabla_x f(x) = \nabla_x(x^T x - 2x^T y + y^T y) = 2(x - y)$ and $\nabla_x g(x) = 2x$, thus the projection of $x$ on $\mathcal{S}$, $y_p$, verifies $x - y_p = \lambda x$ or $y_p = (1 - \lambda)x$. for any vector $y \in \mathcal{S}$, we have $y = (1-\lambda)x + x_\perp$ where $x_\perp$ is in the hyperplane orthogonal to $x$. We want to show that the projection point is the closest to $x$. By Pythagoras' theorem, $\|y\|_2^2 = (1-\lambda)^2 \|x\|^2 + \|x_\perp\|^2$ and:

$$\begin{aligned}
\|y - x\|_2^2 &= \|y\|_2^2 - 2y^T x + \|x\|_2^2 \\
y^T x &= ((1-\lambda)x^T + x_\perp^T)x \\
&= (1-\lambda)x^T x \Rightarrow \\
\|y - x\|_2^2 &= \|y\|_2^2 - 2(1-\lambda)\|x\|_2^2 + \|x\|_2^2 \\
&= (1-\lambda)^2\|x\|^2 + \|x_\perp\|^2 - 2(1-\lambda)\|x\|_2^2 + \|x\|_2^2 \\
&= \lambda^2 \|x\|_2^2 + \|x_\perp\|^2 \\
&> \|x - y_p\|_2^2
\end{aligned}$$

Thus $\arg\min_{y \in \mathcal{S}} ||x - y||_2^2 = \arg\min (1-\lambda)^2 \|x\|_2^2, \lambda x \in \mathcal{S}$. If $x \in \mathcal{S}$ then $\lambda = 1$, if $x \neq \mathcal{S}$ and $\lambda x \in \mathcal{S} \Rightarrow \|\lambda x\|_2 = 1 \Rightarrow \lambda = \frac{1}{\|x\|_2}$, thus $\lambda = \min(1, \frac{1}{\|x\|_2})$, that is $\mathcal{P}_{\mathcal{S}}(x) = \min(x, \frac{x}{\|x\|_2})$.

(b) Derive an algorithm based on projected gradient ascent to find the maximum eigenvalue of a symmetric matrix $A \in \mathbb{R}^{n \times n}$. Let $f(x) = x^T A x$, the largest eigenvalue can be found by solving the optimization problem $\lambda_1 = \max_{\|x\|_2 = 1} x^T A x$ or equivalently $\lambda_1 = \min_{\|x\|_2=1} -f(x)$. We have $\nabla f(x) = 2Ax$, by assumption and using the previous result, the algorithm to find the largest eigenvalue of a symmetric matrix $A \in \mathbb{R}^{n \times n}$ is:

$$\begin{aligned}
x'^{[k-1]} &= x^{[k-1]} + \alpha \nabla f(x^{[k-1]}) \\
&= x^{[k-1]} - 2\alpha A x^{[k-1]} \\
x^{[k]} &= \frac{x'^{[k-1]}}{\|x'^{[k-1]}\|_2} \\
&= \frac{(I - 2\alpha A)x^{[k-1]}}{\|(I - 2\alpha A)x^{[k-1]}\|_2} \; k = 0, 1, \ldots
\end{aligned}$$

(c) Let us express the iterations in the basis of eigenvectors of $A$: $x^{[k]} := \sum_{i=1}^{n} \beta_i^{[k]} u_i$. Compute the ratio between the coefficient corresponding to the largest eigenvalue and the rest $\frac{\beta_1^{[k]}}{\beta_i^{[k]}}$ as a function of $k$, $\alpha$, and $\beta_1^{[0]}, \ldots, \beta_n^{[0]}$. Under what conditions on $\alpha$ and the initial point does the algorithm converge to the eigenvector $u_1$ corresponding to the largest eigenvalue? What happens if $\alpha$ is extremely large (i.e. when $\alpha \to \infty$)?

(d) Implement the algorithm derived in part (b). Support code is provided in `main.py` within `Q4.zip`. Observe what happens for different sizes of $\alpha$. Report the plots generated by the script.

```python
import os

import matplotlib.pyplot as plt
import numpy as np


def calc_true_error(x1, x2):
    ''' eigenvecs could converge to u or -u - both are valid eigvecs
    The function should output the L2 norm of (x1 - x2)
    If x1 = u and x2 = -u, we still want the function to output 0 er

    return np.linalg.norm(x1 - x2)

def eigen_iteration(A, x0, alpha, max_iter=50, thresh=1e-3):
    '''A - nxn symmetric matrix
       x0 - np.array of dimension n which is the starting point
       alpha - learning rate parameter
       max_iter - number of iterations to perform
       thresh - threshold for stopping iteration

       stopping criteria: can stop when ||x[k] - x[k-1]||_2 <= thres

       return:
       relative_error: array with ||x[k] - x[k-1]||_2
       true_error: array with ||x[k] - u_1 ||_2 where u_1 is first e
       '''

    assert ((A.transpose() == A).all())  # asserting A is symmetric
    assert (A.shape[0] == len(x0))

    w, v = np.linalg.eigh(A)
    true_u1 = v[:, 0]  # np array with the first eigenvector of A
    relative_error = []
    true_error = []
    x_cur = x0.copy()
    iteration = 0
```

```
while True:
    x_next = x_cur + alpha * np.matmul(-2 * A, x_cur)
    x_next = np.divide(x_next, np.linalg.norm(x_next))

    if calc_true_error(x_cur, x_next) <= thresh:
        print("Convergence in {} iterations, alpha:{},\
         init_point_norm={}".format(iteration, alpha, np.linalg.no
        print("True u1:{}, computed u1:{}, rel_error:{}".format(tr
        break
    iteration += 1
    if iteration >= max_iter:
        print("Maximum iteration exceeded!")
        print("True u1:{}, computed u1:{}, rel_error:{}, alpha:{}"
              .format(true_u1, x_next, calc_true_error(x_cur, x_ne
        break
    relative_error.append(calc_true_error(x_cur, x_next))
    true_error.append(calc_true_error(x_cur, true_u1))
    x_cur = x_next

## fill in code to do do your projected gradient ascent
## append both the list with the errors

return relative_error, true_error
```

For $\alpha \geq 1$ the gradient steps are very similar, the relative errors do not change, the algorithm does not progress from one iteration to the other, the true error decreases for $\alpha < 1$ to zero, while it is constant and non zero for $\alpha \geq 1$: the algorithm does not converge to the first eigenvector when $\alpha \geq 1$:.

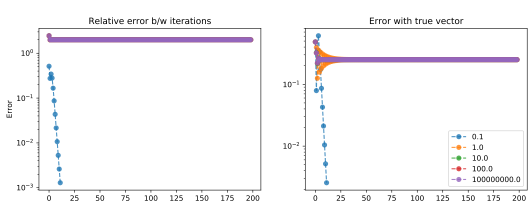


Figure 1: First matrix: relative and absolute errors $\|x_k - x_{k+1}\|_2$ on the left, $\||x_k| - |u_1|\|_2$ on the right

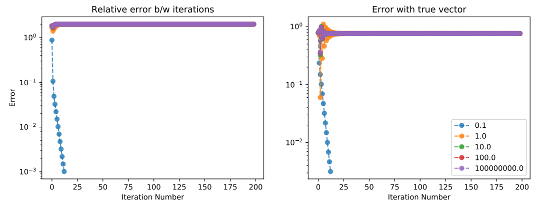


Figure 2: Second matrix: relative and absolute errors $\|x_k - x_{k+1}\|_2$ on the left, $\||x_k| - |u_1|\|_2$ on the right

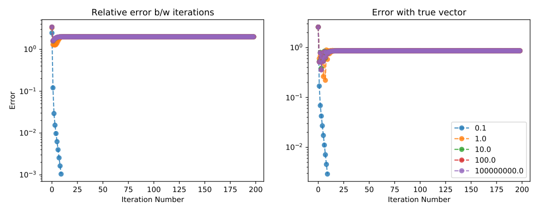


Figure 3: Third matrix: relative and absolute errors $\|x_k - x_{k+1}\|_2$ on the left, $\||x_k| - |u_1|\|_2$ on the right