DS-GA.1013 Mathematical Tools for Data Science Homework 1 Yves Greatti - yg390

- 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, \ldots, u_n be the eigenbasis of A, and $\lambda_1, \ldots, \lambda_n$ the eigenvalues for each of these eigenvectors. $x \in \text{span}\{u_1, \ldots, u_n\} \Rightarrow x = \sum_{i=1,n} \alpha_i u_i, \alpha_i \neq 0$. $x^T(Ax) = (\sum_{i=1,n} \alpha_i u_i)(\sum_{j=1,n} \alpha_j Au_j) = (\sum_{i=1,n} \alpha_i u_i)(\sum_{j=1,n} \alpha_j \lambda_j u_j) = \sum_{i=1,n} \alpha_i^2 \lambda_i$ 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:

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

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

- (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 $(A^TB)_{ij} = (\sum_k A_{ki} B_{kj})_{ij}$. $\operatorname{tr}(A) = \sum_i A_{ii} \Rightarrow \operatorname{tr}(A^TB) = \sum_i \sum_k A_{ki} B_{ki} = \sum_i \sum_j A_{ij} B_{ij} = \operatorname{vec}(A)^T \operatorname{vect}(B) = \langle \operatorname{vec}(A), \operatorname{vec}(B) \rangle$. The trace is then the inner product between vectors in \mathbb{R}^{mn} thus is a valid inner product.
- (b) Prove that for any $A, B \in \mathbb{R}^{m \times n}$, $\operatorname{tr}(A^T B) = \operatorname{tr}(B A^T)$. $\operatorname{tr}(B A^T) = \sum_i \sum_k B_{ik} A_{ik} = \sum_i \sum_j A_{ij} B_{ij} = \operatorname{tr}(A^T B)$.
- (c) Let u_1, \ldots, u_n be the eigenvectors of a symmetric matrix A. Compute the inner product between the rank-1 matrices $u_iu_i^T$ and $u_ju_j^T$ for $i \neq j$, and also the norm of $u_iu_i^T$ for $i = 1, \ldots, n$. For $i \neq j$, $\left\langle u_iu_i^T, u_ju_j^T \right\rangle = \operatorname{tr}\left(u_iu_i^Tu_ju_j^T\right) = \operatorname{tr}\left(u_i\ 0\ u_j^T\right) = 0$, since u_i, u_j are two eigenvectors of a symmetric matrix therefore orthogonal. if i = j then $\left\langle u_iu_i^T, u_iu_i^T \right\rangle = \operatorname{tr}\left(u_iu_i^Tu_iu_i^T\right) = \operatorname{tr}\left(u_i^T\ I\ u_i\right) = \operatorname{tr}\left(u_i^Tu_i\right) = 1$ if the eigenvectors are also orthonormal.
- (d) What is the projection of A onto $u_iu_i^T$? If A is a symmetric matrix, by the spectral theorem, $A = UDU^T$ where D is the diagonal matrix having $\lambda_i, i = 1, \ldots, n$ the eigenvalues of A on the diagonal. Then $A = \sum_i \lambda_i u_i u_i^T$, where u_1, \ldots, u_n are the eigenvectors of A. The projection of A onto $u_iu_i^T$ is $\langle A, u_iu_i^T \rangle$ thus

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

$$= \sum_{j=1}^n \left\langle \lambda_j u_j u_j^T, u_i u_i^T \right\rangle$$

$$= \sum_{j=1}^n \lambda_j \left\langle u_j u_j^T, u_i u_i^T \right\rangle$$

$$= \lambda_i \left\langle u_i u_i^T, u_i u_i^T \right\rangle$$

$$= \lambda_i$$

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 ℓ_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, $A = U \operatorname{diag}(\lambda) U^T$ 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 λ_1 and is in the direction of the corresponding eigenvector u_1 . The smallest curvature is given by the smallest eigenvalue λ_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.

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

The kth update of projected gradient ascent equals

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

where α 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 f on f on f on f or f o

$$||y - x||_{2}^{2} = ||y||_{2}^{2} - 2y^{T}x + ||x||_{2}^{2}$$

$$y^{T}x = ((1 - \lambda)x^{T} + x_{\perp}^{T})x$$

$$= (1 - \lambda)x^{T}x \Rightarrow$$

$$||y - x||_{2}^{2} = ||y||_{2}^{2} - 2(1 - \lambda)||x||_{2}^{2} + ||x||_{2}^{2}$$

$$= (1 - \lambda)^{2}||x||^{2} + ||x_{\perp}||^{2} - 2(1 - \lambda)||x||_{2}^{2} + ||x||_{2}^{2}$$

$$= \lambda^{2}||x||_{2}^{2} + ||x_{\perp}||^{2}$$

$$> ||x - y_{p}||_{2}^{2}$$

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:

$$x^{'[k-1]} = x^{[k-1]} + \alpha \nabla f(x^{[k-1]})$$

$$= x^{[k-1]} - 2\alpha A x^{[k-1]}$$

$$x^{[k]} = \frac{x^{'[k-1]}}{\|x^{'[k-1]}\|_2}$$

$$= \frac{(I - 2\alpha A)x^{[k-1]}}{\|(I - 2\alpha A)x^{[k-1]}\|_2} k = 1, \dots$$

where α is a positive constant and $x^{[0]}$ is an arbitrary initial point. We run this algorithm until either the number maximum of iterations is reached or $|x^{[k]} - x^{[k-1]}| < \epsilon$.

(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, α , and $\beta_1^{[0]}, \ldots, \beta_n^{[0]}$ (and also the eigenvalues). Under what conditions on α and the initial point does the algorithm converge to the eigenvector u_1 corresponding to the largest eigenvalue? What happens if α is extremely large (i.e. when $\alpha \to \infty$)?

Let $x^{[0]} = \sum_{i=1}^n \beta_i^{[0]} u_i$, and $\lambda_1, \dots, \lambda_n$ the eigenvalues of A, from the previous question, we have:

$$x^{[k]} = \frac{(I - 2\alpha A)x^{[k-1]}}{\|(I - 2\alpha A)x^{[k-1]}\|_{2}}$$

$$= \frac{(I - 2\alpha A)^{k}x^{[0]}}{\|(I - 2\alpha A)^{k}x^{[0]}\|_{2}}$$

$$= \frac{(I - 2\alpha A)^{k}\sum_{i=1}^{n}\beta_{i}^{[0]}u_{i}}{\|(I - 2\alpha A)^{k}\sum_{i=1}^{n}\beta_{i}^{[0]}u_{i}\|_{2}}$$

$$= \frac{\sum_{i=1}^{n}\beta_{i}^{[0]}(1 - 2\alpha \lambda_{i})^{k}u_{i}}{\|\sum_{i=1}^{n}\beta_{i}^{[0]}(1 - 2\alpha \lambda_{i})^{k}u_{i}\|_{2}}$$

$$= \frac{\sum_{i=1}^{n}\beta_{i}^{[0]}(1 - 2\alpha \lambda_{i})^{k}u_{i}}{(\sum_{i=1}^{n}(\beta_{i}^{[0]})^{2}(1 - 2\alpha \lambda_{i})^{2k})^{\frac{1}{2}}}$$

This give us:

$$u_j^T x^{[k]} = \frac{\beta_j^{[0]} (1 - 2\alpha \lambda_j)^k}{(\sum_{i=1}^n (\beta_i^{[0]})^2 (1 - 2\alpha \lambda_i)^{2k})^{\frac{1}{2}}}$$
$$u_1^T x^{[k]} = \frac{\beta_1^{[0]} (1 - 2\alpha \lambda_1)^k}{(\sum_{i=1}^n (\beta_i^{[0]})^2 (1 - 2\alpha \lambda_i)^{2k})^{\frac{1}{2}}}$$

We want $|u_1^T x^{[k]}| \to 1$. By the spectral theorem, $\lambda_n \le \cdots \le \lambda_i \le \ldots \le \lambda_1 \Rightarrow (1 - 1)$

$$(2\alpha\lambda_n)^{2k} \ge \ldots \ge (1-2\alpha\lambda_i)^{2k} \ldots \ge (1-2\alpha\lambda_1)^{2k}$$
, so we have

$$\begin{split} &|(\frac{1-2\alpha\lambda_1}{1-2\alpha\lambda_n})^k\frac{\beta_1^{[0]}}{(\sum_{i=1}^n(\beta_i^{[0]})^2)^{\frac{1}{2}}}|\leq |\frac{\beta_1^{[0]}(1-2\alpha\lambda_1)^k}{(\sum_{i=1}^n(\beta_i^{[0]})^2(1-2\alpha\lambda_i)^{2k})^{\frac{1}{2}}}|\leq |(\frac{1-2\alpha\lambda_1}{1-2\alpha\lambda_1})^k\frac{\beta_1^{[0]}}{(\sum_{i=1}^n(\beta_i^{[0]})^2)^{\frac{1}{2}}}|\\ &|\frac{1-2\alpha\lambda_1}{1-2\alpha\lambda_n}|^k|\frac{\beta_1^{[0]}}{(\sum_{i=1}^n(\beta_j^{[0]})^2)^{\frac{1}{2}}}|\leq |\frac{\beta_1^{[0]}(1-2\alpha\lambda_1)^k}{(\sum_{i=1}^n(\beta_i^{[0]})^2(1-2\alpha\lambda_i)^{2k})^{\frac{1}{2}}}|\leq |\frac{\beta_1^{[0]}}{(\sum_{i=1}^n(\beta_j^{[0]})^2)^{\frac{1}{2}}}| \end{split}$$

One condition for convergence of the previous inequality will be $2\alpha |\lambda_1| - 1 < |1 - 2\alpha \lambda_1| < 1$ so $|1 - 2\alpha \lambda_1|^k \to 0$ which gives us $0 < \alpha < \frac{1}{|\lambda_1|}$ and for upper bound we need $|\beta_1^{[0]}| = |(\sum_{i=1}^n (\beta_i^{[0]})^2)^{\frac{1}{2}}|$, then $u_1^T x^{[k]} \to +1$ or -1, and $x^{[k]^T} A x^{[k]} \to +\lambda_1$ or $-\lambda_1$.

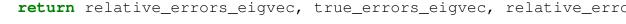
(d) Implement the algorithm derived in part (b). Support code is provided in main.py within Q4.zip. Observe what happens for different sizes of α . Report the plots generated by the script. As we increase α , the algorithm converges faster to the maximum eigenvalue and corresponding eigenvector, for $\alpha=0.1<1$, there is no convergence. We also observe that the initial point plays a role to the rate of convergence:

```
import os
import matplotlib.pyplot as plt
import numpy as np
def unit_vector(vector):
    """ Returns the unit vector of the vector.
    return vector / np.linalg.norm(vector)
def angle_between(v1, v2):
    """ Returns the angle in radians between vectors 'v1' and 'v2'::
    n n n
    v1_u = unit_vector(v1)
    v2_u = unit_vector(v2)
    return np.arccos(np.clip(np.dot(v1_u, v2_u), -1.0, 1.0))
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 en
    return 1 - abs(np.cos(angle_between(x1, x2)))
    # return np.linalg.norm(np.abs(x1) - np.abs(x2))
```

def eigen_iteration(A, x0, alpha, max_iter=50, thresh=1e-5):

```
'''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 |lambda[k] - lambda[k-1]| \le t
   return:
   relative_error_eigvec: array with ||x[k] - x[k-1]||_2
   true_error_eigvec: array with ||x[k] - u_1 ||_2 where u_1 is fi
   relative_error_eiqval: array with |lambda[k] - lambda[k-1] |
   true_error_eigval: array with |lambda[k] - lambda_1|
   x[k] is your estimated max eigenvec at iteration k and lambda[]
   lambda_1 is the max eigenvalue of A and u_1 is the corresponding
   I I I
assert ((A.transpose() == A).all()) # asserting A is symmetric
assert (A.shape[0] == len(x0))
w_{\bullet} v = np.linalg.eigh(A)
true_lam = w[w.size - 1] # fill in your code to find max eigenval
true_u1 = v[:, v.shape[1] - 1] # np array with the first eigenved
relative_errors_eigvec = list()
true_errors_eigvec = list()
relative_errors_eigval = list()
true_errors_eigval = list()
curr\_eiqvec = x0.copy()
iteration = 1
while True:
    next_eigv = curr_eigvec + alpha * np.matmul(-2 * A, curr_eigve
    next_eigv = unit_vector(next_eigv)
    rel_eigvec_error = np.linalg.norm(next_eigv - curr_eigvec)
    relative_errors_eigvec.append(rel_eigvec_error)
    true_eigvec_error = calc_true_error(true_u1, next_eigv)
    true_errors_eigvec.append(true_eigvec_error)
    eigval_prev = curr_eigvec.T.dot(np.matmul(A, curr_eigvec))
    eigval_next = next_eigv.T.dot(np.matmul(A, next_eigv))
    rel_eigval_error = abs(eigval_next - eigval_prev)
    relative_errors_eigval.append(rel_eigval_error)
    true_eigval_error = abs(true_lam - eigval_next)
    true_errors_eigval.append(true_eigval_error)
```

```
if rel_eigval_error <= thresh:</pre>
        print("Convergence in {} iterations, alpha:{},\
         init_point_norm={}".format(iteration, alpha, np.linalg.
        print("True u1:{}, computed u1:{}, rel_error:{}, true_er
              .format(true_u1, next_eigv, rel_eigvec_error, true
        print("True max.eigenval:{}, computed max_eigval:{}, rel
              .format(true_lam, eigval_next, rel_eigval_error, t
        break
    iteration += 1
    if iteration >= max_iter:
        print("Maximum iteration exceeded!")
        print("True u1:{}, computed u1:{}, rel_error:{}, true_er
              .format(true_u1, next_eigv, rel_eigvec_error, true
        print("True max.eigenval:{}, computed max_eigval:{}, rel
              .format(true_lam, eigval_next, rel_eigval_error, t
        break
    curr_eigvec = next_eigv
## fill in code to do do your projected gradient ascent
## append both the list with the errors
```



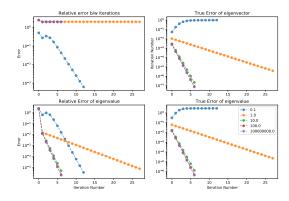


Figure 1: First matrix: relative errors on the left, absolute errors on the right for largest eigenvalue and corresponding eigenvector.

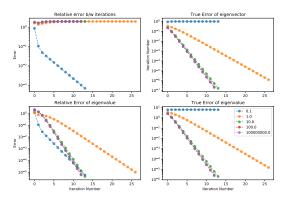


Figure 2: Second matrix: relative errors on the left, absolute errors on the right for largest eigenvalue and corresponding eigenvector.

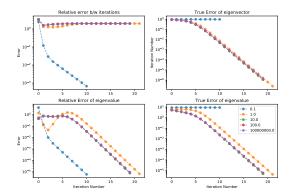


Figure 3: Third matrix: relative errors on the left, absolute errors on the right for largest eigenvalue and corresponding eigenvector.