

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:

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

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 $(A^T B)_{ij} = (\sum_k A_{ki} B_{kj})_{ij}$. $\text{tr}(A) = \sum_i A_{ii} \Rightarrow \text{tr}(A^T B) = \sum_i \sum_k A_{ki} B_{ki} = \sum_i \sum_j A_{ij} B_{ij} = \text{vec}(A)^T \text{vec}(B) = \langle \text{vec}(A), \text{vec}(B) \rangle$. The trace is then the inner product between vectors in \mathbb{R}^{mn} thus is a valid inner product.
- (b) Prove that for any $A, B \in \mathbb{R}^{m \times n}$, $\text{tr}(A^T B) = \text{tr}(BA^T)$. $\text{tr}(BA^T) = \sum_i \sum_k B_{ik} A_{ik} = \sum_i \sum_j A_{ij} B_{ij} = \text{tr}(A^T B)$.
- (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 $i \neq j$, $\langle u_i u_i^T, u_j u_j^T \rangle = \text{tr}(u_i u_i^T u_j u_j^T) = 0$, if u_i, u_j are two eigenvectors for different eigenvalues. if $i = j$ then $\langle u_i u_i^T, u_i u_i^T \rangle = \text{tr}(u_i u_i^T u_i u_i^T) = \text{tr}((u_i^T u_i)^2) = (u_i^T u_i)^2 \Rightarrow \|u_i u_i^T\|_F = u_i^T u_i$ and $\|u_i u_i^T\|_F = 1$ if the eigenvectors are also orthonormal.
- (d) What is the projection of A onto $u_i u_i^T$? The projection of A onto $u_i u_i^T$ is $\langle A, u_i u_i^T \rangle u_i u_i^T$. If A is a symmetric matrix, by the spectral theorem, $A = U D U^T = \sum_i \lambda_i u_i u_i^T$ where $\lambda_i, i = 1, \dots, n$ are the eigenvalues of A . If u_1, \dots, u_n form an eigenbasis then $\langle A, u_i u_i^T \rangle = \lambda_i$. $u_i u_i^T$ is the matrix for the orthogonal projection onto $\text{span}(u_i)$.
- (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, $A = U \mathbf{diag}(\lambda) U^T$ where \mathbf{diag} is the diagonal matrix with on the diagonal: $\lambda_1 \geq \lambda_2 \geq \dots \lambda_n$, which are the eigenvalues and u_1, \dots, 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 $f : \mathbb{R}^n \rightarrow \mathbb{R}$ in a constraint set \mathcal{S} . Let $\mathcal{P}_{\mathcal{S}}$ denote the projection onto \mathcal{S} , i.e.

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

The k th update of projected gradient ascent equals

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

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 $f'_v(x) = \langle \nabla_x f, v \rangle = 0$ 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. $x + v$ is in the tangent plane of g at x if $\nabla g(x)^T v = 0$, and for $\epsilon \approx 0$, $g(x + \epsilon v) \approx g(x)$. So we are looking for global minimizer points 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 $\nabla_x g(x) = 2x$, so 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 , 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 $x \notin \mathcal{S}$ thus $\lambda x \in \mathcal{S} \Rightarrow \|\lambda x\|_2 = 1 \Rightarrow \lambda = \frac{1}{\|x\|_2}$, and $\lambda = \min(1, \frac{1}{\|x\|_2})$, 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:

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

- (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 , α , and $\beta_1^{[0]}, \dots, \beta_n^{[0]}$. 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 $\alpha \rightarrow \infty$)?
- (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 α . Report the plots generated by the script.