Lectures on Scientific Computing

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1 Building a basis of eigenvectors

(Variational Principles for the Symmetric Eigenvalue Problem)

1.1 Step 1

Since $x \in C^m, ||x|| = 1$ is compact, ω with $||\omega = 1$ such $Q(\omega) = maxQ(x)$, $||x|| = 1$.
$\rightarrow \nabla Q(r) = 0$
$Ar = Q(\omega)\omega$

Iteration:
Remark: If $\omega_j^* = 0$ then $\omega_j^*(Ax) = (A^*\omega_j)^*x$
$= (A\omega_j)^*x$ since $A^+ = A$ Suppose $\omega_1, ..., \omega_m$ are orthogonal eigenvectors of A. If

2 Least Square Method

For this method we are only going to be looking at real matrices ($\in \mathbb{R}$). Assume that $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, where $Ax = b$.
Definition:
If $n < m$, the linear system $Ax = b$ is **overdetermined**. The idea is that we have too many constraints to find the unknown, so there might not be an x that satisfies exactly $Ax = b$. We define the **Residual** as what remains when we look at the difference $\omega := Ax - b$. i.e. we might not be able to find an exact solution but we can find something that has a small residual ω. The **Least Square Problem** is to minimize the residual. Formally, we are looking for $min_x||Ax - b||_{l^2}$ (the l^2 norm of the residual).

Remark: $||\omega||_{l^2}^2 = \sum_{i=1}^m \omega_i^2$. This is used in linear regression in statistics. $||\omega||_{l^2}^2 = (Ax - b)^*(Ax - b) = x^*A^*Ax - 2x^*A^*b + b^*b(2)$.

Definition: The **normal equations** are $A^*Ax = A^*b$. A^*A is called either the **moment matrix** or the **Gram matrix**.

Remark: A^*A is symmetric, if A is of rank n ($rnk(A) = n$), which is the maximum rank it can have, then A^*A is positive definite so the Choshi decomposition is a good way to solve $A^*Ax = A^*b$.

Definition: We define the pseudo-inverse of A as $(A^*A)^{-1}A^*$. This is only possible when $rnk(A) = m$. Finally, one important thing to note is that there are problems with conditioning in $Ax = b$ and $A^*Ax = A^*b$ This 'normal equation' approach is the fastest way to solve tense least-square problems but it is often not suitable in practice because of ill conditioning. It only works well if the initial problem $Ax = b$ is well-condition.

3 Alternatives to LSM

3.1 Singular Values and Principle Components

Theorem: If you have a matrix you can break it down in the following way. Let $A \in \mathbb{R}^{m\times n}$. The **Singular Value Decomposition** of A is a factorization of the form $A = U\Sigma V^*$ where U is an $m \times n$ orthogonal matrix ($U^TU = I$), Σ is an $m \times n$ diagonal matrix ($\sum_{ij} = 0$) iff $i \neq j$, and V is an $n \times m$ orthogonal matrix ($V^TV = I$).

Definition: The diagonal values of $\Sigma\{\sigma_j\}_{1\leq j\leq min(m,n)}$ are called the singular values of A. The columns $\{u_j\}_{1\leq j\leq m}$ of U are the left singular vectors of A. By convention $\sigma_j \geq \sigma_2, ... \geq 0$, $\sigma_k = 0$ if $k > min(m, n)$.

Construction of U and V: Suppose $A \neq 0$.

3.1.1 Step 1

We want to find σ_1, v_1, and u_1. $\sigma 1$ is the largest singular value of A. We define this as $\sigma_1 := max_{x\neq 0}\frac{||Ax||}{||x||} = max_{||x||=1}||A_x|| > 0$

We can now define the vector v_1. $\exists v_1$ such that $||v_1|| = 1$ and $||Av_1|| = \sigma_1 >$ 0

We can now define $u_1 := \frac{Av_1}{||Av_1||} \rightarrow Av_1 = \sigma_1 u_1$

Remarks: The **Optimality Condition** $\sigma_1^2 = max_{x\neq 0}\frac{x^*A^*Ax}{x^*x}$. The denominator is the Rayleigh Quotient of the matrix A^*A. Therefore with $\sigma_1^2 = v_1^*A^*Av_1$, $||v_1|| = 1$ so what remains is that $\sigma_1 = v_1^*A^*u_1$. We want to obtain $\sigma_1 v_1 = A^*u_1$ (prove this is true).

The Orthogonality Principle: $(Ax)^*u_1 = x^*(A^*u_1) = \sigma_1 x^* v_1$ so $x^*v_1 = 0 \rightarrow (Ax)^*u_1 = 0$

3.1.2 Step 2

$V_1 := \{x \in \mathbb{R}^n, x^* v_1 = 0\}$
$V_1 := \{x \in \mathbb{R}^m, x^* u_1 = 0\}$

If A_1 is not identically 0, we can define $\sigma_2 := \max_{x \in v_1, x \neq 0} \frac{||Ax||}{||x||} = max_x$