STAT 24310 Notes

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Contents

Abstract

Notes for STAT 24310 taught by Professor Yuehaw Khoo. Prior Linear Algebra knowledge will be assumed. MATLAB notation for matrices will be extensively used.

1 Lecture 1: Introduction

This class is heavily based on Trefethen and Bau's Textbook. Take a look at it if you have the time.
When we run an algorithm, we often are interested in how long it takes to run the algorithm. For example, if we have a matrix $A \in \mathbb{R}^{n \times n}$ an $x, b \in \mathbb{R}^n$, and we are interested in solving

$$Ax = b$$

and n is very large, say $n = 100,000$, a concern is that the algorithm takes forever to run. In this case, we may be worried about the worst case time complexity, denoted as *big O notation*. In this case, solving $x = A^{-1}b$ is $\mathcal{O}(n^3)$. But what is this notation?

Definition 1.1. If there exists a $C \in \mathbb{R}$ such that for fg, where $g \geq 0$, where for all sufficiently t large enough, such that $|f(t)| \leq C \cdot g(t)$, then $f(t)\mathcal{O}(g(t))$

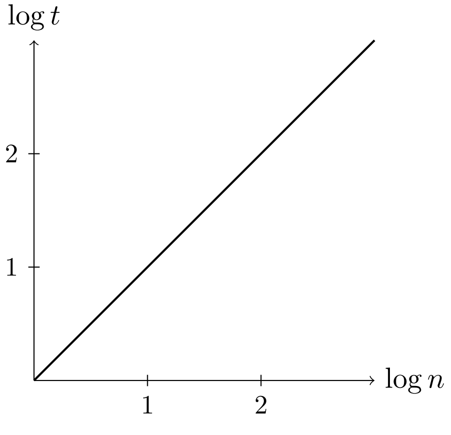
or equivantly:

Definition 1.2. If there exists a constant $C \in \mathbb{R}$ and a real number t_0 such that for all $t \geq t_0$, $|f(t)| \leq C \cdot g(t)$, where $g(t) \geq 0$, then we write $f(t) = \mathcal{O}(g(t))$ as $t \to \infty$.

Both are equivalent. For example, consider a problem that is $\mathcal{O}(n^3)$. If we were to increase the dimension of the problem, say a 100 times, then the algorithm would take 10000000 times longer to run. However, how do we visualize this? We do so by plotting the log-log plot, where we can note that:

$$t = \mathcal{O}(n^3)$$
$$\log t = 3 \log n + C$$

where C is some constant.



where we can see that the slope gives the exponent in time complexity.

1.1 Accuracy

When we are dealing with algorithms, we can also be concerned with how accurate it is. For example, consider $f : X \to Y$, where we are interested $f(x)$ for $x \in X$. However, pratically, we cannot calculate the exact values, take $\sqrt{x}$ for example, so a computer must make an approximation, usually denoted as $\tilde{f}(x)$. We can consider the relative accuracy, defined as follows:

Definition 1.3. Given an approximation of a function $\tilde{f}(x)$, we define relative accuracy as:

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|}$$

where $\|\cdot\|$ is the norm of choosing.

A natural extension of accuracy are the follwing topics: **Stability and Conditional Number**. Intuively, stability is usually related to the algorithm $(\tilde{f}(x))$ used to solve the problem and the condition number is related to the actual setup of the problem $(f(x))$. We can consider the following defintions:

Definition 1.4. Backwards Stability: if $x \in X$. $\tilde{f}(x) = f(\tilde{x})$ for some $\frac{\|\tilde{x}-x\|}{\|x\|} = \mathcal{O}(\epsilon)$

Intuively, this above definition says that the problem will give the good enough answer to a slight deviation in the input. This definition is usually easier to prove.

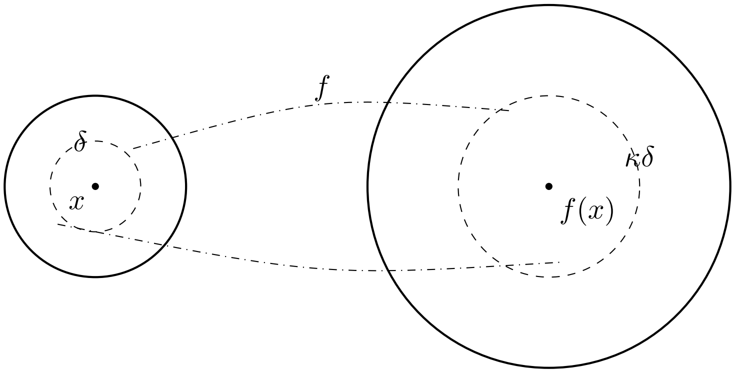
Definition 1.5. Absoulte Conditional Number: for (f, x)l we can consider the Absolute condition number as follows:

$$\hat{K}(f, x) = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|f(x + \delta x) - f(x)\|}{\|\delta x\|}$$

Definition 1.6. Relative Conditional Number: for (f, x), we define the relative condition number as:

$$\lim_{\delta \to 0} \sup_{\frac{\|\delta x\|}{\|x\|} \leq \delta} \frac{\frac{\|f(x+\delta) - f(x)\|}{\|f(x)\|}}{\frac{\|\delta x\|}{\|x\|}} = \frac{\|f(x + \delta x) - f(x)\|\|x\|}{\|f(x)\|\|\delta x\|}$$

We can consider the diagram as follows:



We can see that the condition number measures how senstive the actual problem is to a change in x, as seen above. The larger the problem is, the more sensitive the problem is. Think of the diameter of the circles as how values go between each set. If the condition number is large, then the diameter is larger and thus, there is chance that the small pertrepuabation lands in a different area than original output.

Remark 1.1. Note if f is a function from $\mathbb{R}^n - \mathbb{R}^m$, we can define the following:

$$K_{abs} = J_f \quad K_{rel} = J_f \cdot \frac{\|x\|}{\|f(x)\|}$$

We can observe the following. If $\tilde{f}$ is backwards stable with accuracy ϵ, and if f has a relative condition number k. then $\tilde{f}$ is accurate with the follwoing relation:

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} = \mathcal{O}(k\epsilon)$$

Proof. If $\tilde{f}$ is backward stable, then there exists a point $y \in (x - \delta, x + \delta)$, with $\|\delta\| = \mathcal{O}(\epsilon\|x\|)$, such that:

$$\tilde{f}(x) = f(y)$$

This means the computed value $\tilde{f}(x)$ is the exact value of f evaluated at a slightly perturbed input y.

Now, using the definition of the relative condition number κ of f, we know that for small perturbations:

$$\frac{\|f(y) - f(x)\|}{\|f(x)\|} \leq \kappa \cdot \frac{\|y - x\|}{\|x\|} + \mathcal{O}\left(\left(\frac{\|y - x\|}{\|x\|}\right)^2\right)$$

Since $\|y - x\|/\|x\| = \mathcal{O}(\epsilon)$, it follows that:

$$\frac{\|\tilde{f}(x) - f(x)\|}{\|f(x)\|} = \frac{\|f(y) - f(x)\|}{\|f(x)\|} = \mathcal{O}(\kappa\epsilon)$$

□

2 Lecture 2: Norms

We begin with following definition of a norm in a general vector space.

Definition 2.1. Let X denote a vector space. A norm $\|\cdot\| : X \to R$ sastisfies

- Positivity: $\|x\| \geq 0$, $\|x\| = 0$ iff $x = 0$
- Homogenuity: $\|\alpha x\| = |alpha|\|x\|$
- Triangle inquality: $\|x + y\| \leq \|x\| + \|y\|$

We can also define the l_p norm

Definition 2.2. The l_p is defined as:

- $\|x\|_p = (\sum_{i=1}^n |x_i|^p)^{\frac{1}{p}}$, where $0 < p < \infty$
- $\|x\|_0$ refers to number of non-zero elements of X.
- $\|x\|_\infty = \max_j\{|x_j|\}$

We also have the following definitions:

Definition 2.3. Inner product on $\mathbb{C}^n$: $\langle x, y\rangle = \sum_{i=1}^m \overline{x}_i y_i$

Definition 2.4. Cauchy Schwartz inequality: $|\langle x, y\rangle| \leq \|x\|\|y\|$

Definition 2.5. Holder's inequality: $|\langle x, y\rangle \leq \|x\|_p\|y\|_q$ is $\frac{1}{p} + \frac{1}{q} = 1$

We can also define the equivalence of norms:

Definition 2.6. $\|\cdot\|_a, \|\cdot\|_b$ are equivalent if for $c_2 \geq c_1 \geq 0$:

$$C_1\|x\|_b \leq \|x\|_a \leq C_2\|x\|_b$$

We can prove that all norms are equivalent. This will be left as an exercise to the reader.

2.1 Matrix Norms

We can also introduce the notion of norms on matrices.

Definition 2.7. Frobenious norm: $\|A\|_F = \left(\sum_{i=1,j=1}^{m,n} |A_{ij}|^2\right)^{\frac{1}{2}}$

Definition 2.8. Induced norm: Given $A \in \mathbb{C}^{m\times n}, x \in \mathbb{C}^n$. We define the induced norm as follows:

$$\|A\|_{a\to b} = \sup_{x\neq 0} \frac{\|Ax\|_a}{\|x\|_b} = \sup_{\|x\|_b=1} \|Ax\|_a$$

Remark 2.1. By definition, we can see that:

$$\|Ax\|_a \leq \|A\|_{a\to b}\|x\|_b \quad \|A\|_a = \|A\|_{a\to a}$$

We also have the follwing properties:

Definition 2.9. We can also denote the following p norms.

- $\|A\|_1 = \max_{1\leq j\leq n} \|A(:,j)\|_1$, which is just the maximum column sum.
- $\|A\|_\infty = \max_{1\leq i\leq m} \|A(i,:)\|_1$ Which is the max of the row sum.

We also have the Cauchy Schwartz inequality for the matrix norm:

Definition 2.10. $\|AB\|_2 \leq \|A\|_2\|B\|_2$ and $\|AB\|_f \leq \|A\|_F\|B\|_f$ and $\|AB\|_f \leq \|A\|_2\|B\|_F$

We can prove the fact $\|AB\|_2 \leq \|A\|_2\|B\|_2$, which is as follows:

Proof. $\|AB\|_2 \leq \|A\|_2\|B\|_2$. To show this note,

$$\sup_{\|x\|=1} \|ABx\|_2 \leq \|Ay\|_2 \leq \|A\|_2\|y\|_2 \leq \|A\|_2$$

□

3 3: linear Transform

In numerical linear algebra, most problems and algorithms consist of linear maps.

Definition 3.1. Linear Transform is a function from $T : X \to Y$ where

- $T(\alpha x + \beta y) = \alpha T(x) + \beta T(y)$
- $T(v) = Av$ where $A \in \mathbb{C}^{m\times n}, v \in \mathbb{C}^n$

For example consider the following example.
Example
Let $P_k(x) = x^k$, where it is monomial, where $k \in \mathbb{N} \cup \{0\}$, where $X = span\{P_0, P_1, P_2\}$ and $Y = span\{P_0, P_1, P_2, P_3$. Note that if $q \in X$. this means that q is equivalent to a linear combination of the polynomials, where we can see that $Tq = (q+1)q$ It is trivial to show that T is a linear transform. Thus, we aim to find the matrix for this. Consider the following

$$Tp_1 = p_2 + p_1 \quad Tp_2 = p_3 + p_2$$

where we can construct the matrix as follows[1]

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}$$

where columns vector is $\{p_0, p_1, p_2, p_3\}$ and row vectors are $\{p_0, p_1, p_2\}$.

3.1 Inner Products

We can introduce the inner product as follos.

Definition 3.2. Given a inner product $\langle \cdot, \cdot \rangle$ where $v \in \mathbb{C}^n$, we can see that

- It sastifies bilinearity
- $\langle v, w \rangle = \langle w, v \rangle$
- $\langle v, v \rangle \geq 0$ if and only if $v = 0$

Note that $\langle v, v \rangle = \|v\|^2$. We can also define $\langle v, v \rangle_M = v^T MV$ where M is a positive definite matrix.

Definition 3.3. A matrix is positive definite if and only if all the eigenvalues are positive.

Definition 3.4. A matrix is negative definite if and only if all the eigenvalues are negative.

Definition 3.5. Hermitian matrix is the complex analgue to the transpose of a matrix. Symmmetric matrix is $A^T = A$ and Hermitian matrix is $A = A^*$ [2]

3.2 Different kinds of multiplication

Refer to my STAT 24300 notes. Covers all the definition in Lectures 1 and 5. The only extension we have to be concerned about is the complexity of each operation. We can characterize it as follows:

- Inner product $\mathcal{O}(n)$, as we are multiplying ad summing n times
- Matrix vector product is $\mathcal{O}(mn)$ as we are doing the dot product over m rows.
- Matrix Matrix product is $\mathcal{O}(mnp)$, where $A \in \mathbb{C}^{m \times n}, B \in \mathbb{C}^{n \times p}$, as we are doing matrix vector product p times.

[1] Professor Khoo did some weird proof about the change of basis here, and frankly I don't think its worth putting here as an FYI

[2] The * superscript denotes the complex conjugate, where every entry of the matrix is conjugated.

4 4: Conditioning of the Linear Transform

Let us consider $T(x) = Ax$. To analyze behavior of the matrix, we decompose is $A = F_1F_2 \dots F_n$. We have the following key decompositions.

- For a square matrix, we have Eigenvalue Decomposition (EVD), where if we have a diagnolzaible matrix A where[3]

$$A = V\Lambda V^{-1} \quad \Lambda = diag(\lambda_1, \lambda_2, \dots, \lambda_n)$$

  where V have columns are linearly independent vectors. Let v_i be a column of the eigenbasis, then we see that $Av_i = \lambda_i v_i$ as

$$\det(A - \lambda I) = 0 \implies \quad \exists \quad v \text{s.t} \quad (A - \lambda I)v = 0 \iff Av = \lambda v$$

- SVD, where we have $A \in \mathbb{C}^{m\times n}$ where $A = U\Sigma V^*$, where $U \in \mathbb{C}^{m\times m}$ and $\Sigma \in \mathbb{C}^{m\times n}$ and $V \in \mathbb{C}^{n\times n}$ and where $\Sigma = diag(\sigma_1, \sigma_2, \dots, \sigma_n)$.

The SVD is something that we discuss heavily in this class. For the time being, assume that U and V is unitary, which means that $U^TU = V^TV = I_n$. This will be covered later. For both cases, the number of eigenvaues or singular values equals the rank of the matrix.

4.1 Spectral Radius

Given a matrix $A \in \mathbb{C}^{n\times n}$, we can define the spectral norm

Definition 4.1. We define the spectral norm as

$$\rho(A) := \max_{j\in\{1,2,\dots,m\}} |\lambda_j(A)|$$

Remark 4.1. Note that $\|A\|_p \geq \rho(A)$. As let v be an eigenvector of A,

$$\|Av\|_p = \|\lambda v\|_p \leq \|A\|_p \|v\|_p$$
$$|\lambda| \leq \|A\|_p$$

We can prove that $\|A\|_2^2 = \sigma_1$.

Proof. Let $A \in \mathbb{C}^{m\times n}$, and let the singular value decomposition (SVD) of A be:

$$A = U\Sigma V^*$$

where:

[3] Diag is shorthand for a diagnol matrix

- $U \in \mathbb{C}^{m \times m}$, $U^*U = I_m$ (unitary),
- $V \in \mathbb{C}^{n \times n}$, $V^*V = I_n$ (unitary),
- $\Sigma \in \mathbb{R}^{m \times n}$ is diagonal with nonnegative entries $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$, the singular values of A.

Recall that the operator 2-norm (spectral norm) of A is defined by:

$$\|A\|_2 := \sup_{\|x\|_2=1} \|Ax\|_2$$

Using the SVD $A = U\Sigma V^*$, and noting that U and V are unitary (thus preserve the 2-norm), we compute:

$$\|A\|_2 = \sup_{\|x\|_2=1} \|Ax\|_2 = \sup_{\|x\|_2=1} \|U\Sigma V^* x\|_2 = \sup_{\|x\|_2=1} \|\Sigma V^* x\|_2$$

Let $y = V^*x$. Since V is unitary, $\|y\|_2 = \|x\|_2 = 1$. So:

$$\|A\|_2 = \sup_{\|y\|_2=1} \|\Sigma y\|_2$$

Now, Σ is a diagonal matrix with singular values $\sigma_1, \ldots, \sigma_r$, so for any unit vector $y = (y_1, \ldots, y_n)$, we have:

$$\|\Sigma y\|_2^2 = \sum_{i=1}^{r} \sigma_i^2 |y_i|^2 \leq \sigma_1^2 \sum_{i=1}^{r} |y_i|^2 \leq \sigma_1^2$$

The supremum is achieved when $y = e_1$, so:

$$\|A\|_2^2 = \sup_{\|y\|_2=1} \|\Sigma y\|_2^2 = \sigma_1^2$$

□

Using a very similar logic, we can see that $\|A^{-1}\|_2 = \frac{1}{\sigma_n}$

5 Lecture 5: Unitary Matrix

We begin with the proof of the unitary matrix.

Proof. Consider the definition of the relative condition number, where we see that

$$K = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|x\|}{\|Ax\|} \frac{\|A\delta x\|}{\|\delta x\|}$$

and we see that the above is equivalent to:

$$k(A) = \|A^{-1}\|\|A\|$$

Note that if $\|\cdot\| = \|\cdot\|_2$ □

6 Lecture 9: Introduction to Optimization

Last class, we showed that there existed a solution to the Least Squares problem, or rather $\min \|Ax - b\|_2^2$ through a combination of the QR and LU decomposition. We can consider the following general optimization problem, where we define $f : \Omega \to \mathbb{R}$:

$$x^* = \arg\min_{x \in \Omega} f(x)$$

where we say that Ω is the objective domain. The intuition is that we want to find the input that would minimize the value of the function.

6.1 Examples

Consider the nonlinear inverse problem used within physics.

Explain this better

6.2 Classes of Optimization Problems

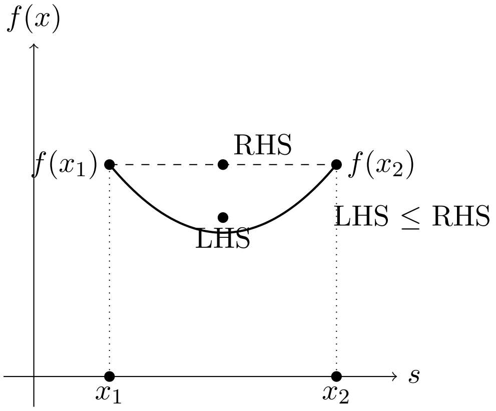
Given a domain Ω that we want to optimize over, we have the following scenarios:

- a set of discrete points, which is discrete optimization
- $\Omega \subseteq \mathbb{R}^n, \subseteq \mathbb{R}^n$, a constrained optimization problem. An example of this would be induced norms.
- $\Omega = \mathbb{R}^n$, a unconstrained optimization problem. An example of this would be the Least Squares Regression Problem.

We can often times utilize properties of the function, which is where we can introduce the idea of convexity.

Definition 6.1. f is convex over S if for any $x_1, x_2 \in S$ and $t \in [0, 1]$, $f(tx_1 + (1-t)x_2) \leq tf(x_1) + (1-t)f(x_2)$

This concept can be illustrated in the following diagram:



We can then expand the definition of convexity as follows:

Definition 6.2. f is strongly convex over S if for any $x_1, x_2 \in S$ and $t \in [0,1]$, $f(tx_1 + (1-t)x_2) < tf(x_1) + (1-t)f(x_2)$

A natural expansion of this is when f is convex, then $f\left(\sum_{i=1}^{n} t_i x_i\right) \leq \sum_{i=1}^{n} t_i f(x_i)$ where $\sum_{i=1}^{n} t_i = 1$ such that $t_i \geq 0$. We can also consider the following definition of convexity:

Definition 6.3. Locally Convex: $f : \Omega \to \mathbb{R}$, where f is convex over some $S \subseteq \Omega$

6.3 Taylor's Theorem

We begin with an introduction of smoothness.

Definition 6.4. A function is said to be C^n if it is contionus and differentiable n number of times.

Also a refresher on what the Taylor's Theorem in 1D is.

Definition 6.5. if $f : \mathbb{R} \to \mathbb{R}$ is $(k+1)$ times differentiable at $x = a$, then

$$f(x) = f(a) + \frac{\partial f(a)}{\partial x}(x-a) + \cdots + \frac{1}{k!}\frac{\partial^k f(x)}{\partial x^k}(x-a)^k + \frac{L}{(k+1)!}(x-a)^{k+1}$$

where

$$L = \sup_{\xi \in [x,a]} \left| \frac{\partial^{k+1} f(x)}{\partial x^k} \right|$$

note that if $|x-a|$ is sufficiently small, we can discard the remainder the term (the one with the L in it). Note that also that if the $(k+1)$ derivative is bounded, then we can approximate f with the kth order polynomial. We can also consider the case of the special case of the third order taylor polynomial expansion.

Definition 6.6. For $f : \mathbb{R}^n \to \mathbb{R}$, and f has a bounded 3rd deriative, the expansion is as follows

$$f(x) = f(a) + \frac{\partial f(a)}{\partial x}(x-a) + \frac{1}{2}(x-a^T)H(a)(x-a) + \mathcal{O}(\|x-a\|^3)$$

where we define

$$H(a)_{ij} = \frac{\partial f(a)}{\partial x_i \partial x_j}$$

where $H(a)$ is $n \times n$

To illustrate the nature of the Hessian Matrix, we can visualize f locally to see that we can use a contour map. The Hessian usually shows the directions of the biggest changes in direction, given by the Eigenvalues.

Need to fix

However, we can see that if our function is convex and smooth, then *optimality is guarantted based on the local deriative.* We can see this in the following proof:

Proof. if f is convex and differentiable, we can see that if we let a, b be in the domain of f. we can see that we are left with the following inequality.

$$f(b) \geq f(a) + \frac{\partial f(a)}{\partial x}(b-a)$$

by the definition of convexity. If we choose a such that $f'(a) = 0$, we see that we have guarnteed an optimal solution. □

However, we can see that if we are working with a strongly convex differentiable solution, we can use the same assumptions as above to see in the following proof.

Proof. We are given that f is strongly convex and differentiable. Thus, we can see that for the following taylor expansions

$$f(b) \geq f(a) + \frac{\partial f(a)}{\partial x}(b-a) + \frac{a}{2}\|b-a\|_2^2$$

We see that we can choose a point such that $\frac{\partial f(a)}{\partial x} = 0$, which implies that

$$\begin{gathered} f(b) \geq f(a) + \frac{a}{2}\|b-a\|^2 \\ \implies f(b) > f(a), \forall b, b \neq a \end{gathered}$$

Since we know that the function is strongly convex and thus, we know that for any point b and a. the last inequality holds, we can see that we have indeed foound the unique optimizer. □

Remark 6.1. Strongly convex implies strictly convex, but not the other way around.

6.4 Applications of convexity

Consider the following:

$$f(x) = \frac{1}{2}ax^2 - bx, a > 0$$

and consider the following:

$$\begin{aligned} f(x) &= \frac{1}{2}ax^2 - bx \\ f(y) - f(x) &= \frac{1}{2}a(y^2 - x^2) - b(y - x) \end{aligned}$$