# **Numerics** Methods and Useful Facts

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# Contents

# 1 Calculus

## 1.1 Gradient and Jacobian

For $f : \mathbb{R}^n \to \mathbb{R}$ we define the gradient as,

$$\nabla f = \left[\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_n}\right]$$

For $f : \mathbb{R}^n \to \mathbb{R}^m$ we define the Jacobian as,

$$J_f = \begin{bmatrix} \nabla f_1 \\ \nabla f_2 \\ \vdots \\ \nabla f_m \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

Note that a liner approximation to $f$ at $x_0$ is given by,

$$f(x_0) + J_f x$$

## 1.2 Gradients of Matrix Vector Forms

$$\nabla b^T A x = A^T b$$
$$\nabla x^T A x = (A + A^T) x$$

## 1.3 Taylor Expansions

2d case.

### 1.3.1 Computing Expansions in Mathematica

# 2 Matrices

## 2.1 Classification of Matrices

Matrices are assumed to be complex unless specified otherwise.

### 2.1.1 Hermetian

*Definition*: A matrix $A$ is Hermetian if $A^* = A$

*Properties*:

$\Rightarrow$ Real eigenvalues
$\Rightarrow$ Normal
$\Rightarrow$ Unitarily diagonalizable
$\Rightarrow$ $\|A\|_2 = \rho(A)$

### 2.1.2 Skew symmetric

*Definition*: A real matrix $A$ is skew symmetric if $A^T = -A$

*Properties*:

$\Rightarrow$ pure imaginary eigenvalues
$\Rightarrow$ $I + A$ is invertible

### 2.1.3 Normal

*Definition*: A matrix $A$ is normal if $A^*A = AA^*$

*Properties*:

$\Leftrightarrow$ Unitarily diagonalizable

### 2.1.4 Positive definite

*Definition*: A matrix $A$ is positive definite if all eigenvalues are positive.

*Properties*:

$\Leftrightarrow$ $v^*Av > 0$ for all $v$
$\Leftrightarrow$ Has Cholesky factorization

## 2.2 ???

Where should I put things like similarity transform, unitarily diagonalizable, etc.

Also things like

## 2.3 Matrix Decompositions

### 2.3.1 SVD

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

- $U$ unitary
- $\Sigma$ diagonal, with real positive entries in non-increasing order
- $V$ unitary

*Existence*: Always

*Uniqueness*: *Note:* double check Unique up to complex sign of columns of $U$ and $V$

*Computing*:

*Why it is useful*:

- Rank revealing
- Numerical stability of algorithms using SVD

### 2.3.2 (P)LU

*Existence*:

*Uniqueness*:

*Computing*: Gaussian Elimination

When is pivoting needed?

### 2.3.3 Cholesky

*Existence*: If $A$ is Hermetian positive definite

*Uniqueness*: Unique up to sign

*Why it is useful*:

- Save storage space

### 2.3.4 QR

### 2.3.5 Eigen

### 2.3.6 Shur

### 2.3.7 Jordan Normal

## 2.4 Matrix and Vector Norms

$$\|A\| = \sup_{u \neq 0} \frac{\|Au\|}{\|u\|} = \sup_{\|u\|=1} \|Au\|$$

$$\|A\| = \sup_{u,v \neq 0} \frac{\langle Au, v\rangle}{\|u\| \, \|v\|} = \sup_{\|u\|=\|v\|=1} \langle Au, v\rangle$$

If $A$ is self Hermetian, *Note:* double check this

$$\|A\| = \sup_{u \neq 0} \frac{\langle Au, u\rangle}{\|u\|^2} = \sup_{\|u\|=1} \langle Au, u\rangle$$

## 2.5 Rayleigh Quotients

*Note:* Anne seems to like these

# 3 Linear Systems

## 3.1 Direct Methods

### 3.1.1 QR

### 3.1.2 Gaussian Elimination

### 3.1.3 SVD

## 3.2 Iterative Metods

### 3.2.1 Simple Iteration

### 3.2.2 Conjugate Gradient

### 3.2.3 GMRES

## 3.3 Solving Least Squares

The linear least squares problem is,

$$\min_x \|b - Ax\|_2$$

This is solved when $x$ solve the linear system (called the normal equations),

$$A^T Ax = A^T b$$

### 3.3.1 Derivations of Normal Equations

*Using Projectors*:

*Using Calculus*:

Note that

$$\|b - Ax\| = (b - Ax)^T(b - Ax) = b^T b + -2b^T Ax + x^T(A^T A)x$$

Therefore, taking the gradient of $\|b - Ax\|$, we know it is minimized when $2A^T Ax - 2A^T b = 0$.

*Note:* How do we do derivative of things like x*Ax

### 3.3.2 Solving Least Squares Numerically

# 4 Boundary Value Problems

## 4.1 Laplacian

# 5 Initial Value Problems

*Note:* need better section names

## 5.1 Runge-Kutta Methods

## 5.2 LMMs

## 5.3 Stability

zero stable

region of abs stability

A stable L stable etc

MOL

Von Neumann