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 the best linear approximation to f at x_0 is given by,

$$f(x_0) + J_f x$$

1.2 Gradients of Matrix Vector Forms

This can be useful for minimizing/maximizing expressions involving matrix vector quantities.

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

1.3 Taylor Expansions

$$f(t+k, x+h) = f + k f_t + h f_x + \frac{k^2}{2} f_{tt} + kh f_{tx} + \frac{h^2}{2} f_{xx} + \mathcal{O}(k^2 + h^2)$$

1.3.1 Computing Expansions in Mathematica

Compute Taylor expansion of $f(t+k, x+h)$ to d-th order.

```
Normal[Series[f[t + z k, x + z h], {z,0,d}]] /. {z->1}
```

This can be written into a function like,

```
F[n_,j_] := Normal[Series[f[t + z n k, x + z j h], {z,0,d}]] /. {z->1}
```

Then `F[n, j]` computes the Taylor expansion of $f(t+nk, x+jh)$ about (t, x). This is useful for compute local truncation errors. For instance, to compute the LTE of a second order centered difference approximation $f'(x) \approx (f(t+k,x) - f(t-k,x))/2k$ we set $d = 3$ and use,

```
FullSimplify[(F[1, 0] - F[-1, 0])/(2 k)]
```

This gives that the difference methods is like $f_t(t, x) + \mathcal{O}(k^2)$.

2 Basic Linear Algebra

2.1 Matrix and Vector Norms

The general definition of a matrix norm is,

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

Equivalent definition:

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

If A is self Hermitian, *Note:* double check this

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

2.2 Similar Matrices

Definition: Two matrices A and B are similar if $A = XBX^{-1}$ for some X.

Why it is useful: The eigenvalues of similar matrices are the same.

2.2.1 Diagonalizable

Definition: A matrix A is diagonalizable if it is similar to a diagonal matrix

3 Projectors

Definition: A matrix P is a projector if $P^2 = P$

Why it is useful: The eigenvalues of a diagonal matrix are the diagonal entries

3.1 Orthogonal Projectors

4 Rayleigh Quotients

Note: Anne seems to like these

Approximates eigenvalues

Can write every value in range of eigenvalues as rayleigh quotient for real symmetric matrices.

5 Classification of Matrices

Matrices are assumed to be complex and unless specified otherwise.

5.1 Upper Triangular

Definition: A matrix R is upper triangular if $r_{ij} = 0$ for $i > j$. If $r_{ii} = 0$ the matrix is called strictly upper triangular.

Properties:

$\Rightarrow$ Eigenvalues are diagonal entries
$\Rightarrow$ Inverse, product, and sum of upper triangular matrices are upper triangular
$\Rightarrow$ Can solve triangular linear systems in $\mathcal{O}(m^2)$ time with back substitution

5.2 Unitary

Definition: A matrix U is unitary if $U^*U = UU^* = I$.

Properties:

$\Leftrightarrow$ Columns are orthonormal and form a basis for $\mathbb{C}^n$
$\Rightarrow$ $\|AU\|_2 = \|UA\|_2 = \|A\|_2$

5.3 Hermitian

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

Properties:

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

5.4 Skew symmetric

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

Properties:

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

5.5 Normal

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

Properties:

- $\Leftrightarrow$ Unitarily diagonalizable (means eigenvectors are orthogonal)
- $\Rightarrow$ Hermitian if all eigenvalues are real

5.6 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

5.7 ???

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

Also things like

6 Matrix Decompositions

6.1 SVD

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

- U unitary
- Σ 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:

- Gives geometric interpretation for linear transforms on $\mathbb{C}^n$
- Rank revealing
- Numerical stability of algorithms using SVD

6.1.1 Reduced SVD

If A is rank deficient some singular values will be zero. We can drop these singular values and the corresponding singular vectors.

6.2 (P)LU

Existence:

Uniqueness:

Computing: Gaussian Elimination

6.2.1 Partial Pivoting

When is pivoting needed?

6.2.2 Cholesky

Existence: If A is Hermitian positive definite

Uniqueness: Unique up to sign

Why it is useful:

- Save storage space

6.3 QR

6.4 Eigen

6.5 Shur

6.6 Jordan Normal

7 Direct Methods for Linear Systems

7.1 QR

7.2 Gaussian Elimination

7.3 SVD

8 Iterative Methods for Linear Systems

8.1 Simple Iteration

8.2 Power Iteration

8.2.1 Simultaneous Power Iteration (QR)

8.3 Conjugate Gradient

8.4 GMRES

8.5 Other methods

9 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),

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

9.1 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

9.2 Solving Least Squares Numerically

10 Boundary Value Problems

10.1 Laplacian

11 Integrators and IVPs

11.1 Runge-Kutta Methods

11.2 LMMs

11.3 Stability

A method is stable, if when applied to the test equation with $\lambda < 0$, the solution doesn't blow up. That is, $\{U^n\}_{n=0}^{\infty}$ is bounded. *Note:* double check this

11.4 Zero Stable

11.5 Region of Absolute Stability

A stable L stable etc

12 PDEs

12.1 Method of Lines

12.1.1 Von Neumann Analysis

1. Replace U_j^n with $g(\xi)^n e^{i\xi j\Delta x}$
2. Solve for $g(\xi)$ and compute $|g(\xi)|$
3. Method is stable if and only if for all ξ, $|g(\xi)| \leq 1 + \mathcal{O}(\Delta x)$