

Numerical Analysis 1

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Stability

Let $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ be a function. Let $f(x) = y$ and let $\hat{f}(x) = \hat{y}$ be the computed value of $f(x)$, and assume that for some $\hat{x} \in \mathbb{R}^n$, $f(\hat{x}) = \hat{y}$.

- Forward error: $\|y - \hat{y}\|$
- Backward error: $\|x - \hat{x}\|$
- Condition number is the smallest M such that for all x , $\frac{\|y - \hat{y}\|}{\|y\|} \leq M \frac{\|x - \hat{x}\|}{\|x\|}$

As a linear operator, a matrix has a condition number. For a norm $\|\cdot\|$, the condition number of A is given by $\text{cond}(A) = \|A^{-1}\| \|A\|$ and can be interpreted as closeness to singularity.

Linear Solves

Solve $\mathbf{Ax} = \mathbf{b}$ using gaussian elimination. This can also be expressed as finding the LU decomposition $\mathbf{A} = \mathbf{LU}$ and solving

$$\mathbf{Ux} = \mathbf{L}^{-1}\mathbf{b}$$

where \mathbf{L} and \mathbf{U} are lower and upper triangular respectively.

If \mathbf{A} is poorly conditioned, we may need to swap some of its rows to ensure stability. These row swaps can be captured by adding a permutation matrix \mathbf{P} :

$$\mathbf{A} = \mathbf{P}^{-1}\mathbf{LU}.$$

Note that \mathbf{P} will be the identity matrix with its columns shuffled. If \mathbf{A} is sparse, we can instead pivot to avoid fill-in.

If \mathbf{A} is SPD, then there exists a nonsingular lower triangular matrix \mathbf{L} and diagonal matrix \mathbf{D} such that

$$\mathbf{A} = \mathbf{LDL}^T.$$

This is called the Cholesky decomposition and is faster than the LU decomposition. Then we can solve $\mathbf{Ax} = \mathbf{b}$ by

$$\mathbf{DL}^T\mathbf{x} = \mathbf{L}^{-1}\mathbf{b}.$$

Least Squares

Find solution \mathbf{x}^* to minimize $\|\mathbf{Ax} - \mathbf{b}\|_2$ over \mathbf{x} . Note that a necessary and sufficient condition is that the residual vector $\mathbf{b} - \mathbf{Ax}^*$ must be orthogonal to the range of \mathbf{A} . It follows that \mathbf{x}^* is the projection of \mathbf{b} onto the range of \mathbf{A} .

One solution (Normal Equations) is to solve:

$$\mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b}.$$

Another solution (Gram-Schmidt) is to compute an orthonormal basis for the range of \mathbf{A} and use it to locate the projection of \mathbf{b} then take this solution as \mathbf{x}^* . This is equivalent to decomposing \mathbf{A} into an orthonormal matrix \mathbf{Q} and an upper triangular \mathbf{R} such that $\mathbf{A} = \mathbf{QR}$ then solving $\mathbf{Rx} = \mathbf{Q}^T \mathbf{b}$, for all the nonzero rows of \mathbf{R} . The \mathbf{QR} decomposition can also be done with householder reflectors (which is computationally equivalent to Gram-Schmidt) or Givens rotations.

If \mathbf{A} is rank-deficient, then there are infinitely many solutions. To obtain a minimum norm solution, take the SVD of \mathbf{A} :

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T,$$

and solve

$$\mathbf{x}^* = \mathbf{V}_r \mathbf{\Sigma}_r^{-1} \mathbf{U}^T \mathbf{b},$$

where \mathbf{V}_r and $\mathbf{\Sigma}_r$ denote the first r columns of \mathbf{V} and rows of $\mathbf{\Sigma}$ respectively, and where r is the rank of $\mathbf{\Sigma}$.

Eigenvalue Problems

Find all eigenpairs of \mathbf{A} : (λ, x) satisfying $\mathbf{Ax} = \lambda \mathbf{x}$. Note that any matrix \mathbf{B} such that $\mathbf{B} = \mathbf{S}^{-1} \mathbf{AS}$ is similar to \mathbf{A} in that it has the same eigenpairs as \mathbf{A} . We will say that \mathbf{A} is diagonalizable if it is similar to a diagonal matrix. Note that if we know the eigenvalues of \mathbf{A} , we can find the eigenvectors by solving a linear system.

Schur Decomposition:

$\mathbf{U}^* \mathbf{AU} = \mathbf{T}$ where \mathbf{U} is unitary, \mathbf{U}^* denotes conjugate transpose, and \mathbf{T} is upper triangular with the eigenvalues of \mathbf{A} on its diagonal.

Gershgoran Disk Thm:

If $\mathbf{A} \in \mathbb{C}^{n \times n}$, then there are n disks in the complex plane centered at each of the diagonals of \mathbf{A} with radius equal to the sum of the nondiagonal elements in each column. All the eigenvalues of \mathbf{A} are contained in these disks.

Using the fact that \mathbf{A} and $\mathbf{S}^* \mathbf{AS}$ have the same number of positive/negative/zero eigenvalues, we can use bisection to search for them by scaling a diagonal matrix \mathbf{S} .

We can also use vector iterations: pick a vector \mathbf{x} and multiply by \mathbf{A} until it converges to something (the largest eigenvalued eigenvector).

Also see subspace iteration, QR iteration, inverse iteration, Rayleigh quotient iteration.

Iterative Methods

Again, we want to solve $\mathbf{Ax} = \mathbf{b}$, but this time we want to solve with an iterative method. Split \mathbf{A} into $\mathbf{A} = \mathbf{M} - \mathbf{N}$ where \mathbf{M} is something easily invertible (to get the Jacobi iterative, just take \mathbf{M} to be the diagonal of \mathbf{A}). Then $\mathbf{x} = \mathbf{M}^{-1}\mathbf{Nx} + \mathbf{M}^{-1}\mathbf{b}$. Iterate by

$$\mathbf{x}_{k+1} = \mathbf{M}^{-1}\mathbf{Nx}_k + \mathbf{M}^{-1}\mathbf{b}.$$

One can also perform overrelaxation by over stepping in the direction of each iterate by a constant factor of $\tau > 1$. In some cases, this may accelerate convergence since $x_k \rightarrow x_{k+1}$ may advance slowly. One can use vector acceleration by writing the step as

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{M}^{-1}\mathbf{r}_k$$

where $\mathbf{r}_k = \mathbf{b} - \mathbf{Ax}_k$, then modifying to

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \tau_k \mathbf{M}^{-1}\mathbf{r}_k$$

where τ_k is chosen variably at each step to maximize convergence by some metric.

Note that the above accelerated methods always produce solutions $\mathbf{x}_k \in \text{span}\{\mathbf{b}, \hat{\mathbf{A}}\mathbf{b}, \hat{\mathbf{A}}^2\mathbf{b}, \dots\}$ where $\hat{\mathbf{A}} = \mathbf{M}^{-1}\mathbf{A}$. This is called the Krylov space, and Krylov methods reduce complexity by restricting the search for \mathbf{x} to the Krylov space: $\text{span}\{\mathbf{b}, \hat{\mathbf{A}}\mathbf{b}, \hat{\mathbf{A}}^2\mathbf{b}, \dots\}$. The Arnoldi iteration is one such method and is used to solve least squares problems in Lapack `GMRES`.