Advanced Data Analytics
Lecture week 3: Numerical Linear Algebra

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Overview

- Understand where stability issues may arise in numerical linear alegbra
- Understand how algorithms for solving simultaneous linear equations work
- Understand how algorithms for solving simultaneous linear equations work
- Able to use singular value decomposition (SVD) to robustly solve linear algebra tasks

The classical text for this material is Golub, Gene H., and Charles F. Van Loan. Matrix computations. Vol. 3. JHU press, 2013. (It currently has 71615 citations!).

Numerical Linear Algebra

- Linear algebra is one of the best understood parts of mathematics. We might hope that numerical algorithms for linear algebra would be simple and short.
- This is not the case because a general matrix can have very nasty properties.
- We will look at algorithms for two central problems of linear algebra:
  1. solving linear equations;
  2. solving the eigenproblem.

Solving Linear Algebraic Equations: Notation

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\
\cdots &= \cdots \\
a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m
\end{aligned}
$$

where there are n unknowns and m equations. In matrix form, this set of equations can be written

$$\mathbf{Ax} = \mathbf{b},$$

where $\mathbf{A}$ is $m \times n$, $\mathbf{x}$ is $n \times 1$ and $\mathbf{b}$ is $m \times 1$.

Numerical Problems in Solving Equations

If $m = n$ then there will be a unique solution provided that $\mathbf{A}$ is non-singular. However, two problems can arise in practice:

1. Some rows of $\mathbf{A}$ may be so close to being linearly dependent that roundoff errors make them linearly dependent during the solution process. The procedure will fail and can detect that it has failed.
2. Roundoff errors (often caused by a near singularity, particularly with large n) give an incorrect solution $\mathbf{x}$. It usually has a large multiple of some vector 'in the nearly-kernel of $\mathbf{A}$' added to a sensible answer. The only way to discover this is to substitute the supposed solution x back into the equations.

If problems do arise, then it is best to resort to singular value decomposition (SVD).

Wherever possible, use pre-packaged software (such as numpy, MATLAB or LINPACK) which has powerful and thoroughly tested routines for these problems.

LU Decomposition

- A common method for tackling problems in linear algebra is to decompose matrices as a product of other matrices.
- Suppose that $A = LU$, where L is lower triangular and U is upper triangular. Then

$$Ax = (L \cdot U)x = L \cdot (U \cdot x) = b.$$

- This is useful since it is easy to solve systems of linear equations for triangular matrices. So we can find a vector y such that $L \cdot y = b$ using forward substitution, and then find a vector x such that $U \cdot x = y$ using backward substitution.
- Each of these processes require (for a single r.h.s.) $n^2/2$ operations. Note that once we have the LU decomposition, we can solve efficiently for vectors b whenever we wish.

Computing Determinants

- The determinant of the LU decomposition is

$$\prod_{j=1}^{n} \beta_{jj}.$$

  Thus $\det(A)$ can be found in $n^3/3$ operations, rather than the $n!$ operations required by the naive approach.
- By keeping track of the parity of the number of row permutations s, the sign can be corrected by multiplying by $(-1)^s$. (This is because each time a pair of rows are swapped, the determinant is multiplied by -1.)
- For error bounds, see sections 4.4 to 4.6 of Stoer and Bulirsch.

Cholesky Decomposition

- Relevant to symmetric positive-definite matrices A. We write $A = LL^T$.
- Used for solving linear equations (`gtmem`) and for computing matrix inverses (`gmmactiv`).
- It is easy to show that all submatrices of a positive definite matrix are also positive definite. We can then prove the existence of the Cholesky decomposition by induction on the matrix size n.
- The Cholesky decomposition requires about $n^3/6$ operations and n square roots.
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Matrix Norms

Frobenius $\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2}$.

p-norms $\|A\|_p = \sup_{x \neq 0} \frac{\|Ax\|_p}{\|x\|_p}$.

It is clear that $\|A\|_p$ is the p-norm of the largest vector obtained by applying A to a unit p-norm vector:

$$\|A\|_p = \sup_{x \neq 0} \left\| A \left(\frac{x}{\|x\|_p} \right) \right\|_p = \max_{\|x\|_p = 1} \|Ax\|_p.$$

It is easy to show that

$$\|AB\|_p \leq \|A\|_p \|B\|_p, \tag{1}$$

and it is also clear that

$$\|Ax\|_p \leq \|A\|_p \|x\|_p. \tag{2}$$

Computing l_1 and l_∞ Matrix Norms

It is easy to compute the 1 and ∞ norms:

$$\|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |a_{ij}| \quad (3)$$

$$\|A\|_\infty = \max_{1 \le i \le m} \sum_{j=1}^{n} |a_{ij}| \quad (4)$$

$$(5)$$

It can also be shown that

$$\frac{1}{\sqrt{n}}\|A\|_\infty \le \|A\|_2 \le \sqrt{m}\|A\|_\infty \quad (6)$$

$$\frac{1}{\sqrt{m}}\|A\|_1 \le \|A\|_2 \le \sqrt{n}\|A\|_1 \quad (7)$$

$$(8)$$

Computing the Matrix 2-norm

If $A \in \mathbb{R}^{m \times n}$, then there exists a unit 2-norm n-vector z such that $A^T Az = \mu^2 z$, where $\mu = \|A\|_2$.
Proof: Suppose that $z \in \mathbb{R}^n$ is a unit vector such that $\|Az\|_2 = \|A\|_2$. Since z maximises the function

$$g(x) = \frac{\|Ax\|_2^2}{2\|x\|_2^2} = \frac{x^T A^T Ax}{2x^T x}$$

it follows that it satisfies $\nabla g(z) = 0$. Differentiation gives

$$\frac{\partial g(z)}{\partial z_i} = \frac{(z^T z)\sum_{j=1}^n (A^T A)_{ij} z_j - (z^T A^T Az) z_i}{(z^T z)^2}.$$

In vector notation, this is

$$A^T Az = (z^T A^T Az) z = \|Az\|_2^2 z.$$

The Matrix 2-norm

- So $\|A\|_2^2$ is a zero of the polynomial $p(\lambda) = \det(A^T A - \lambda I)$. In particular, the 2-norm of A is the square root of the largest eigenvalue of $A^T A$. We will say more about this equation when we consider the singular value decomposition of A.
- We cannot directly compute the 2-norm from the matrix elements, which is a nuisance, since this corresponds to the Euclidean norm on the vector space, which is the most useful for us. A useful result for estimating the norm is

$$\|A\|_2 \leq \sqrt{\|A\|_1 \|A\|_\infty}.$$

- The condition of a matrix B, written $\kappa(B)$, is given by

$$\kappa(B) = \|B\|_2 \, \|B^{-1}\|_2,$$

which is equal to the ratio of the largest to smallest singular values. The condition is said to be infinite if B is singular.

Background to Eigenvalue Problems

- In principle, the eigenvalues of an $n \times n$ matrix A can be determined by finding the roots of the degree n polynomial $\det(A - \lambda I) = 0$.
- This is (usually) a very poor method, being both inefficient and inaccurate. Also, it does not help in the search for eigenvectors when these are required.
- Practical methods for computing the eigenvalues and eigenvectors of A are usually start with a reduction step, in which the matrix A is transformed to a similar (in the technical sense) matrix B with a simpler structure, either tridiagonal (so $b_{ij} = 0$ if $|i - j| > 1$) or Hessenberg (when $b_{ij} = 0$ for $i \geq j + 2$).
- For matrices in these special forms, standard methods for computing eigenvalues and eigenvectors are much faster.
- These algorithms are complicated, so whenever possible, use pre-packaged software (such as MATLAB, NAG or the public domain libraries LINPACK and EISPACK).

Restriction to Symmetric Matrices

We will only look at methods for computing eigenvalues and eigenvectors for symmetric matrices:

1. Most of the applications where eigenvectors are required involve covariance or correlation matrices, which are symmetric.
2. The calculation of eigenvalues for non-symmetric matrices is related to singular value decomposition, which will be covered later.
3. The eigenvalues of a non-symmetric matrix can be very sensitive to small changes in matrix elements (i.e. the problem is ill-conditioned).
4. Non-symmetric matrices may not have a complete set of eigenvectors. Algorithms may rely on the user to check if eigenvectors are parallel or 'almost parallel'.

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Reduction of Real Symmetric Matrices to Tridiagonal Form

- As symmetric matrices can be diagonalized, it is possible to reduce them to a diagonal matrix $P^T AP = D$ with P orthogonal.
- However, in general, a finite series of simple transformations cannot completely diagonalize a matrix. Instead we simplify A to be tridiagonal (and symmetric) and then use factorization methods to complete the process.
- An alternative is to iterate the finite reduction sequence until the deviation of the matrix from diagonal form is negligible: this is usually about 5 times less efficient.

Eigenvalues and Eigenvectors of Symmetric Tridiagonal Matrices

- The QR algorithm is commonly used to solve this problem because its convergence is generally cubic (i.e. $\epsilon_{i+1} = c\epsilon_i^3$) and is at worst quadratic for repeated eigenvalues.
- It is based on the decomposition of A as $A = QR$, where $Q^T Q = I$ and R is upper triangular. It follows that $Q^T A = R$.
- For a general matrix, such a decomposition can be constructed by applying Householder reflections to annihilate columns of A below the diagonal. For tridiagonal matrices, Givens transformations (which are rotations) are more efficient.

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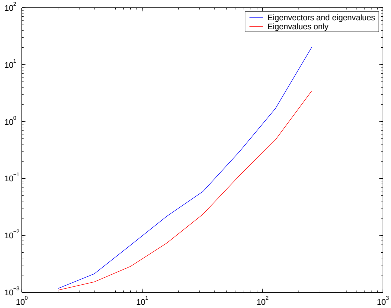
Computational Cost

- To find the eigenvalues requires about $30n^2$ operations (the count is approximate since an iterative algorithm is used).
- The eigenvectors require an additional $3n^3$ operations, which is a significant extra cost if n is reasonably large.



SVD: Definition

- Let A be a matrix of dimension $m \times n$. The matrix A^*A is Hermitian and positive semi-definite (i.e. it has non-negative eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n \geq 0$).
- Write $\lambda_k = \sigma_k^2$ where $\sigma_k \geq 0$. The values σ_k are called the singular values of A.
- There exists a unitary $m \times m$ matrix U and a unitary $n \times n$ matrix V such that $U^*AV = \Sigma$ is an $m \times n$ 'diagonal matrix':

$$\Sigma = \begin{pmatrix} D & 0 \\ 0 & 0 \end{pmatrix} \quad \text{where} \quad D = \mathrm{diag}(\sigma_1, \ldots, \sigma_r)$$

where $\sigma_1, \ldots \sigma_r$ are the non-zero singular values of A and r is the rank of A. We can then write

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

as the SVD of A.

Properties of the SVD

- Columns $r+1$ to m of U are not very interesting, since they are zeroed out by Σ; many algorithms for SVD don't even bother to calculate them (this is sometimes called the thin SVD).
- Columns of U represent m orthonormal eigenvectors of the $m \times m$ matrix AA^*, while those of V represent n orthonormal eigenvectors of the $n \times n$ matrix A^*A:

$$U^*AA^*U = \Sigma\Sigma^*$$

- The singular values of A are precisely the lengths of the semi-axes of the hyperellipsoid $E = \{Ax : \|x\|_2 = 1\}$.

- By the definition of the 2-norm, let $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^m$ be unit 2-norm vectors that satisfy $Ax = \sigma y$ with $\sigma = \|A\|_2$. By the Gram-Schmidt process, we can find $V_2 \in \mathbb{R}^{n\times(n-1)}$ and $U_2 \in \mathbb{R}^{m\times(m-1)}$ so that $V = [x, V_2] \in \mathbb{R}^{n\times n}$ and $U = [y, U_2] \in \mathbb{R}^{m\times m}$ are orthogonal.
- $$U^T AV = \begin{bmatrix} \sigma & w^T \\ 0 & B \end{bmatrix} \equiv A_1.$$

  Since
  $$\left\| A_1 \begin{bmatrix} \sigma \\ w \end{bmatrix} \right\|_2^2 \geq (\sigma^2 + w^T w)^2$$
  we have $\|A_1\|_2^2 \geq (\sigma^2 + w^T w)$. But $\|A_1\|_2^2 = \|A\|_2^2$, since U and V are orthogonal, and the latter is equal to σ^2. Hence $w = 0$ and we can finish off the proof by induction.

How not to Compute the SVD

- Solving for the eigenvalues of A^*A is not the best approach, as this is subject to loss of accuracy. Let $|\epsilon| < \sqrt{\text{eps}}$ and

$$A = \begin{pmatrix} 1 & 1 \\ \epsilon & 0 \\ 0 & \epsilon \end{pmatrix}$$

- Then in exact arithmetic,

$$A^*A = \begin{pmatrix} 1+\epsilon^2 & 1 \\ 1 & 1+\epsilon^2 \end{pmatrix}$$

so the singular values are $\sigma_1(A) = \sqrt{2+\epsilon^2}$ and $\sigma_2(A) = |\epsilon|$.

- If computed with precision eps,

$$A^*A = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

which has eigenvalues $\lambda_1 = 2$ and $\lambda_2 = 0$. Thus the second singular value is not accurate to machine precision.

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How It Should Be Done

- The SVD algorithm is closely related to the QR method.
- Reduce A to bidiagonal form using Householder transformations. Find a matrix P_1 of dimension $m \times m$ such that $P_1 A = A'$ has the first column zero (apart from the first element). Then choose a matrix Q_1 which is $n \times n$ of the form

$$Q_1 = \begin{pmatrix} 1 & 0 \\ 0 & \tilde{Q} \end{pmatrix}$$

so that $A' Q_1 = A''$ has zeroes in the first row, apart from the first two elements. Continuing iteratively, we obtain a matrix

$$J = \begin{pmatrix} J^{(0)} \\ 0 \end{pmatrix} \quad J^{(0)} = \begin{pmatrix} q_1 & e_2 & 0 & \cdots & 0 \\ 0 & q_2 & e_3 & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & q_{n-1} & e_n \\ 0 & \ddots & \ddots & 0 & q_n \end{pmatrix}$$

- We then use Givens reflections and shift strategies to get (generally) cubic convergence as in the QR algorithm.

Uses of SVD

For a real matrix A, we can write $A = U\Sigma V^T$. In our applications, m will usually be greater than n, so removing unnecessary columns from U, we write U as an $m \times n$ matrix. Then $U^T U = V^T V = VV^T = I$, but UU^T is not necessarily equal to the identity.

- Matrix Inversion
- Rank Deficiency
- Solution of Linear Equations
- Constructing an Orthonormal Basis

Matrix Inversion

Consider the case when $m = n$.

- The inverses of U and V are trivial to compute: we simply take their transposes. So $A^{-1} = V\,\mathrm{diag}(1/\sigma_i)U^T$.
- This can only go wrong if at least one σ_i is zero, or its value is so small that it is comparable to the rounding error.
- We define the condition number of A to be

$$\kappa(A) = \frac{\max_i \sigma_i}{\min_i \sigma_i}.$$

Then A is singular if $\kappa(A) = \infty$, and is ill-conditioned if

$$\frac{1}{\kappa(A)} \approx \text{eps}.$$

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Rank Deficiency

- The SVD allows us to deal more sensibly with the concept of numerical matrix rank.
- While theorems in linear algebra may depend on a matrix having full rank, in practice, matrices often have full rank in theory, but are close to being rank deficient, perhaps because of rounding errors or noise in data.
- For small ϵ we define the ϵ-rank of a matrix by

$$\operatorname{rank}(A, \epsilon) = \min_{\|A-B\|_2 \leq \epsilon} \operatorname{rank}(B)$$

  as the smallest rank of nearby matrices B.
- For example, if A is measured with each a_{ij} accurate to within ± 0.01, it may make sense to consider $\operatorname{rank}(A, 0.01)$.

Calculating ϵ-rank

Consider the SVD of $A \in \mathbb{R}^{m \times n}$. If $k < r = \text{rank}(A)$ and

$$A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T,$$

then

$$\min_{\text{rank}(B)=k} \|A - B\|_2 = \|A - A_k\|_2 = \sigma_{k+1}$$

So, if $r_\epsilon = \text{rank}(A, \epsilon)$ then

$$\sigma_1 \geq \cdots \geq \sigma_{r_\epsilon} > \epsilon \geq \sigma_{r_\epsilon+1} \geq \cdots \geq \sigma_p.$$

SVD and Solutions of Linear Equations

The SVD of A enables us to find solutions to the linear equations. In fact we can do better than this:

1. If there is a solution, we can find the one with minimal norm.
2. If there is no exact solution, we can find a vector x with minimal residual $r = \|Ax - b\|$.

Solving Degenerate Equations with SVD

- Suppose that $U^T AV = \Sigma$ is the SVD of A and that the rank of A is equal to r.
- If $b \in \mathbb{R}^m$, then

$$x_{LS} = \sum_{i=1}^{r} \frac{u_i^T b}{\sigma_i} v_i \tag{9}$$

  minimises $\|Ax - b\|_2$ and has the smallest 2-norm of all minimisers.
- Moreover, the minimum residual is given by

$$\rho_{LS}^2 = \|Ax_{LS} - b\|_2^2 = \sum_{i=r+1}^{m} (u_i^T b)^2. \tag{10}$$

Properties of the Pseudo-Inverse

Let A be an $m \times n$ matrix. The pseudo-inverse $A^\dagger$ is an $n \times m$ matrix satisfying:

1. $A^\dagger A = P$ is the orthogonal projector $P = P^* = P^2$ onto the orthogonal complement of $\ker(A)$ and $AA^\dagger = \bar{P}$ is the orthogonal projector onto the orthogonal complement of $\mathrm{im}(A)$.
2. The following formulas hold:

- $A^\dagger A = (A^\dagger A)^*$,
- $AA^\dagger = (AA^\dagger)^*$,
- $AA^\dagger A = A$,
- $A^\dagger AA^\dagger = A^\dagger$.

If Z is a matrix that satisfies these conditions, then it must be the pseudo-inverse of A. (i.e. the pseudo-inverse, like the normal inverse, is unique.) We can also show that

$$A^{\dagger\dagger} = A \quad \text{and} \quad (A^\dagger)^* = (A^*)^\dagger.$$

Note that, if A^*A is invertible, then $A^\dagger = (A^*A)^{-1}A^*$.

Conditioning of Least Squares Solution

Unfortunately, the news is bad: x_{LS} is not even a continuous function of the data, and small changes in A and b can induce arbitrarily large changes in $x_{LS} = A^\dagger b$. If A and δA are in $\mathbb{R}^{m \times n}$, then it can be shown that

$$\|(A+\delta A)^\dagger - A^\dagger\|_F \leq 2\|\delta A\|_F \max\{\|A^\dagger\|_2^2, \|(A+\delta A)^\dagger\|_2^2\}$$

Unlike the square nonsingular case, the upper bound does not necessarily tend to zero as δA tends to zero. If

$$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \qquad \text{and} \qquad \delta A = \begin{pmatrix} 0 & 0 \\ 0 & \epsilon \\ 0 & 0 \end{pmatrix}$$

then

$$A^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{and} \qquad (A+\delta A)^\dagger = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1/\epsilon & 0 \end{pmatrix}$$

and $\|A^\dagger - (A+\delta A)^\dagger\|_2 = 1/\epsilon$.

Conditioning II

- If σ_j is 'small' (i.e. A is ill-conditioned), then it is likely that although direct solution methods will succeed in finding an answer x, the image Ax will be far from b.
- In such cases, using SVD and $\tilde{\Sigma}$ as above will probably give a smaller residual. In effect, we throw away a linear combination of equations that are corrupted by rounding error.
- To quantify the 'small', we may require $\kappa(A) \leq 10^{12}$ for double precision. If $m \geq n$ (the over-determined case) we may wish to zero additional σ. When solving the least squares equation $\chi^2 = \|Ax - b\|^2$, such σ_j correspond to linear combinations of variables that have little effect on χ^2.

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