

Numerical Linear Algebra

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Notation: $A \in \mathbb{R}^{m \times n}$: real matrix, m rows and n columns

$\mathbb{R}^{m \times 1} = \mathbb{R}^m$ are (column) vectors

Common Problems

- Eigenvalue Problem: given $A \in \mathbb{R}^{n \times n}$ find $\lambda \in \mathbb{R}$ or \mathbb{C}
and $x \in \mathbb{R}^n$ or \mathbb{C}^n such that $Ax = \lambda x$
- Linear System: given $A \in \mathbb{R}^{n \times n}$, $b \in \mathbb{R}^n$ find $x \in \mathbb{R}^n$
s.t. $Ax = b$
- Nonlinear system: almost always reduce to sequence
of linear systems eg. Newtons method for $F(U) = 0$

Guess U_0 and for $k = 1, 2, \dots$

solve $J\delta = -F(U_k)$ and set $U_{k+1} = U_k + \delta$

$$J = \{J_{i,j}\}, J_{i,j} = \frac{\partial F_i}{\partial x_j}(U_k), \quad \text{Jacobian}$$

- Least Squares (Regression): given $A \in \mathbb{R}^{m \times n}$, $m > n$,
 $b \in \mathbb{R}^m$ find $x \in \mathbb{R}^n$ such that $\|Ax - b\|$ is minimum

In different situations A can be:

- Full (dense) - most entries non-zero
- Banded: $\exists b < n$ with $a_{i,j} = 0$ if $|i - j| > b$
 - ▶ diagonal: $b = 0$
 - ▶ tridiagonal: $b = 1$
- Triangular: upper triangular: $a_{i,j} = 0$ if $i > j$, correspondingly lower
- Hessenberg: upper Hessenberg: $a_{i,j} = 0$ if $i > j + 1$, correspondingly lower
- in Block form: naturally expressed in terms of sub-matrices (matrix blocks)
- Sparse: many zero entries, often very few non-zeros per row

Block Matrices: If (m_1, \dots, m_p) and (n_1, \dots, n_q) are sets of positive integers with $\sum_i m_i = m$, $\sum_j n_j = n$, and $A_{ij} \in \mathbb{R}^{m_i \times n_j}$, $i = 1, \dots, p$, $j = 1, \dots, q$ then

$$A = [A_{ij}] = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1q} \\ A_{21} & A_{22} & \cdots & A_{2q} \\ \vdots & \vdots & \ddots & \vdots \\ A_{p1} & A_{p2} & \cdots & A_{pq} \end{bmatrix} \in \mathbb{R}^{m \times n}$$

is a $p \times q$ block matrix.

Names for ordinary matrices apply to block matrices, e.g.

$$T = \begin{bmatrix} A & B \\ O & C \end{bmatrix} \begin{matrix} r \\ s \end{matrix}$$

$r \quad s$

is 2×2 block upper triangular;

$$A \in \mathbb{R}^{r \times r}, C \in \mathbb{R}^{s \times s}, B \in \mathbb{R}^{r \times s}.$$

Matrix and vector multiplication work for block matrices: eg. if as above

$$T = \begin{bmatrix} A & B \\ O & C \end{bmatrix} \begin{matrix} r \\ s \end{matrix}, \quad U = \begin{bmatrix} D & E \\ O & F \end{bmatrix} \begin{matrix} r \\ s \end{matrix}, \quad x = \begin{bmatrix} y \\ z \end{bmatrix} \begin{matrix} r \\ s \end{matrix}$$

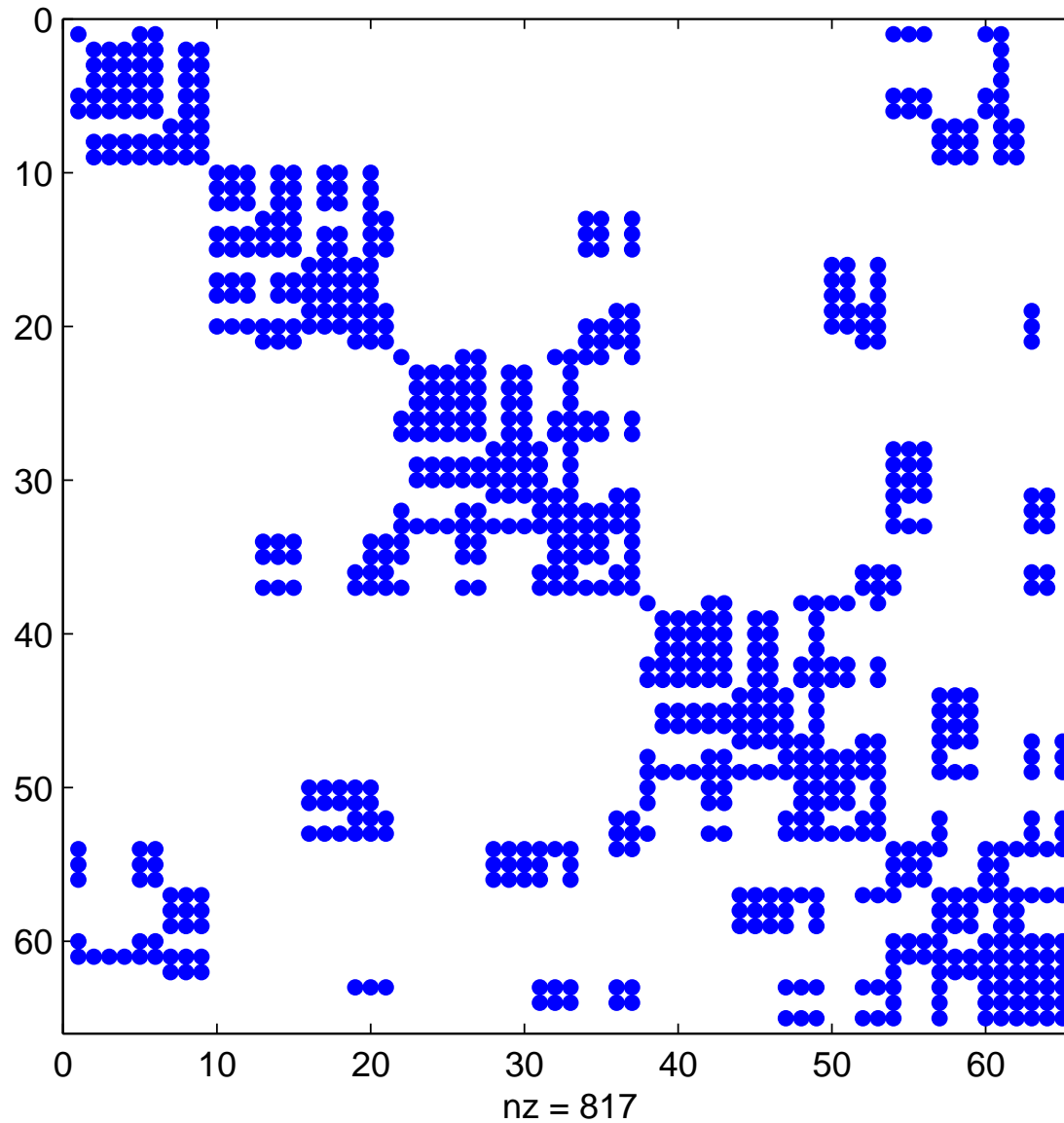
then

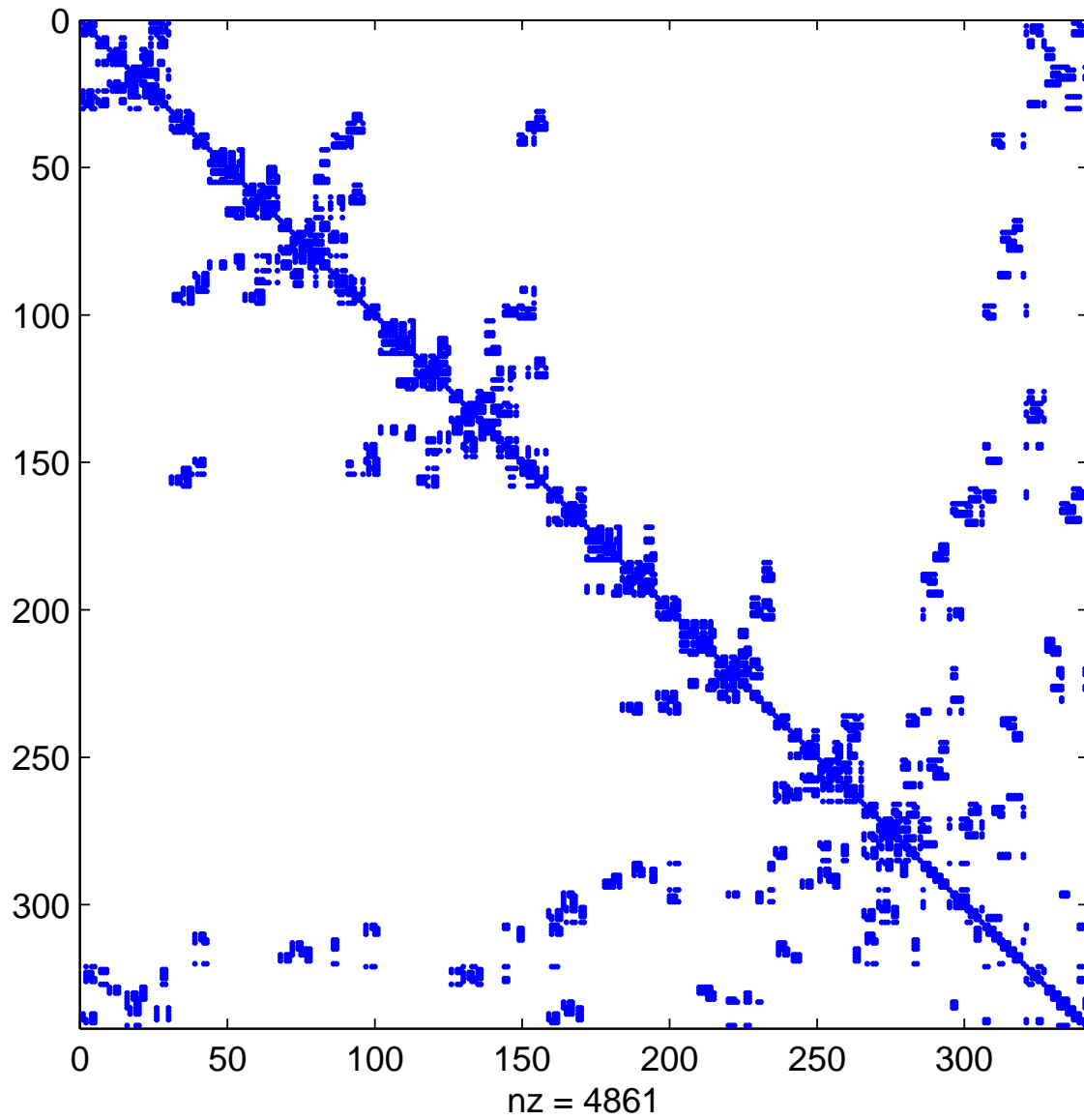
$$TU = \begin{bmatrix} AD & AE + BF \\ O & CF \end{bmatrix}, \quad Tx = \begin{bmatrix} Ay + Bz \\ Cz \end{bmatrix}.$$

Exercise: Deduce that T^{-1} exists if and only if A^{-1} and C^{-1} do, and equals

$$\begin{bmatrix} A^{-1} & -A^{-1}BC^{-1} \\ O & C^{-1} \end{bmatrix}$$

Sparse Matrices





and in any of these structures a square matrix $A \in \mathbb{R}^{n \times n}$ may be

- symmetric: $A^T = A$ ($a_{i,j} = a_{j,i}$)
- skew-symmetric: $A^T = -A$
- positive definite: $x^T Ax > 0$ for all non-zero $x \in \mathbb{R}^n$
- positive semi-definite: $x^T Ax \geq 0$ for all non-zero $x \in \mathbb{R}^n$
- indefinite: $(x^T Ax)(y^T Ay) < 0$ for some $x, y \in \mathbb{R}^n$
- ...

Different structures call for different numerical techniques

Goal of a numerical method is often to convert a given problem to a simpler form (where the solution may be obvious)

Orthogonal Matrices

$Q \in \mathbb{R}^{n \times n}$ is orthogonal if

(i) $Q^T Q = I$ ie. $Q^T = Q^{-1}$

equivalently

(ii) $Q Q^T = I$

(iii) columns of Q are an orthonormal basis for \mathbb{R}^n

(iv) rows of Q when transposed are an orthonormal basis for \mathbb{R}^n

Exercise: **(i) \Leftrightarrow (ii) \Leftrightarrow (iii) \Leftrightarrow (iv)**

2 important orthogonal matrices for computation:

(a) Householder matrices (elementary reflections)

for $w \in \mathbb{R}^n$, $w \neq 0$ defined by

$$H(w) = I - 2 \frac{ww^T}{w^T w} \in \mathbb{R}^{n \times n}$$

Note

- $w^T w \in \mathbb{R}$: inner product
 $ww^T \in \mathbb{R}^{n \times n}$: outer product
- $H(w) = H(w)^T = H(w)^{-1}$ Exercise: prove this
- Geometrically $H(w)x$ is the reflection of x in the hyperplane $\{y : w^T y = 0\}$

Norms (ways of measuring size)

for vectors:

$$\mathbf{x} \in \mathbb{R}^n, \quad \|\mathbf{x}\|_2 = \left(\sum_{i=1}^n x_i^2 \right)^{\frac{1}{2}} = (\mathbf{x}^T \mathbf{x})^{\frac{1}{2}}$$

or more generally $\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}$

Special/useful cases: $\|\mathbf{x}\|_1 = \sum |x_i|$, $\|\mathbf{x}\|_\infty = \max_i |x_i|$

All satisfy the axioms for a norm:

- $\|\alpha \mathbf{x}\| = |\alpha| \|\mathbf{x}\|$, $\alpha \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^n$
- $\|\mathbf{x}\| \geq 0$ and $\|\mathbf{x}\| = 0 \Leftrightarrow \mathbf{x} = \mathbf{0}$
- $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$, triangle inequality

Exercise: check

Norms for matrices: operator norm:

$$\|A\|_p = \sup_{x \in \mathbb{R}^n, x \neq 0} \frac{\|Ax\|_p}{\|x\|_p} = \sup_{x \in \mathbb{R}^n, \|x\|=1} \|Ax\|_p$$

satisfies matrix norm axioms:

- $\|\alpha A\| = |\alpha| \|A\|$, $\alpha \in \mathbb{R}$, $A \in \mathbb{R}^{m \times n}$
- $\|A\| \geq 0$ and $\|A\| = 0 \Leftrightarrow A = 0$ ($a_{i,j} = 0$ for all i, j)
- $\|A + B\| \leq \|A\| + \|B\|$, triangle inequality for matrices

Special cases:

$$\|A\|_1 = \max_j \sum_i |a_{i,j}| \quad (\text{max absolute column sum})$$

$$\|A\|_\infty = \max_i \sum_j |a_{i,j}| \quad (\text{max absolute row sum})$$

Also: Frobenius norm:

$$\|A\|_F = \left(\sum_i \sum_j a_{i,j}^2 \right)^{\frac{1}{2}}$$

satisfies norm axioms.

Fact: because of compactness (finite dimensionality)

$$\exists x \in \mathbb{R}^n \text{ with } \|x\| = 1 \text{ and } \|A\| = \|Ax\|$$

Orthogonal Matrices and Norms:

If Q, Z orthogonal of appropriate dimensions

$$\|Qx\|_2 = \|x\|_2, \quad \forall x$$

because $\|Qx\|_2^2 = x^T Q^T Q x = x^T x = \|x\|_2^2$

and so also

$$\|QAZ\|_2 = \|A\|_2, \quad \forall A$$

because

$$\frac{\|QAZx\|_2}{\|x\|_2} = \frac{\|AZx\|_2}{\|x\|_2} = \frac{\|A(Zx)\|_2}{\|Zx\|_2} = \frac{\|Ay\|_2}{\|y\|_2}, \quad y = Zx$$

and take supremum over x .

Also $\|QAZ\|_F = \|A\|_F$ (see exercises)

Basic/Important point:

orthogonal matrices do not change 'size' (in $\|\cdot\|_2$ and $\|\cdot\|_F$) so have good numerical properties in finite precision arithmetic