Sparse matrices

where A only has elements on – or right next to – the diagonal (and is called a “tridiagonal” matrix)

$$\begin{pmatrix}
X & X & O & O & O & O & O & O \\
X & X & X & O & O & O & O & O \\
O & X & X & X & O & O & O & O \\
O & O & X & X & X & O & O & O \\
O & O & O & X & X & X & O & O \\
O & O & O & O & X & X & X & O \\
O & O & O & O & O & X & X & X \\
O & O & O & O & O & O & X & X
\end{pmatrix}$$

The LU decomposition of A (and the forward and backsubstitution steps) only involve O(N) computations!

- The solution to **A x** = **b** can go much faster if the matrix is “sparse”, i.e. has few non-zero elements.

- Example: consider the numerical solution to $d^2x/dt^2 + f(t)x = g(t)$

Driven 1-D harmonic oscillator with time-varying spring constant

Sparse matrices

- Let's represent x on a uniform grid of discrete times, $t_i = i\,\Delta t$,

  ….and define $x_i \equiv x(t_i)$, $f_i \equiv f(t_i)$, and $g_i \equiv x(t_i)$,

- The second derivative can be approximated

  $d^2x/dt^2 \sim (x_{i+1} - 2x_i + x_{i-1}) / \Delta t^2$

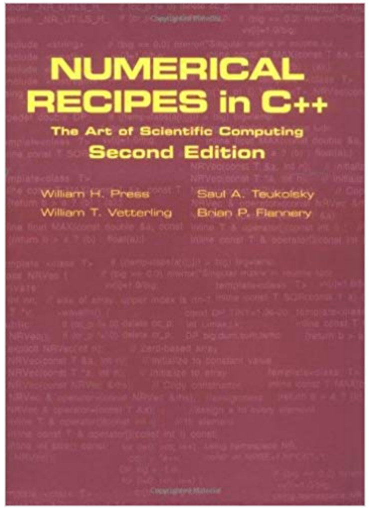
  and the equation can be written as a linear system $\mathbf{A}.\ \mathbf{x} = \mathbf{g}$

Singular systems

- When linear systems fail, many things can be going on

Consider the singular system

$$\begin{aligned} x_1 + x_2 &= b_1 \\ 2x_1 + 2x_2 &= b_2 \end{aligned}$$

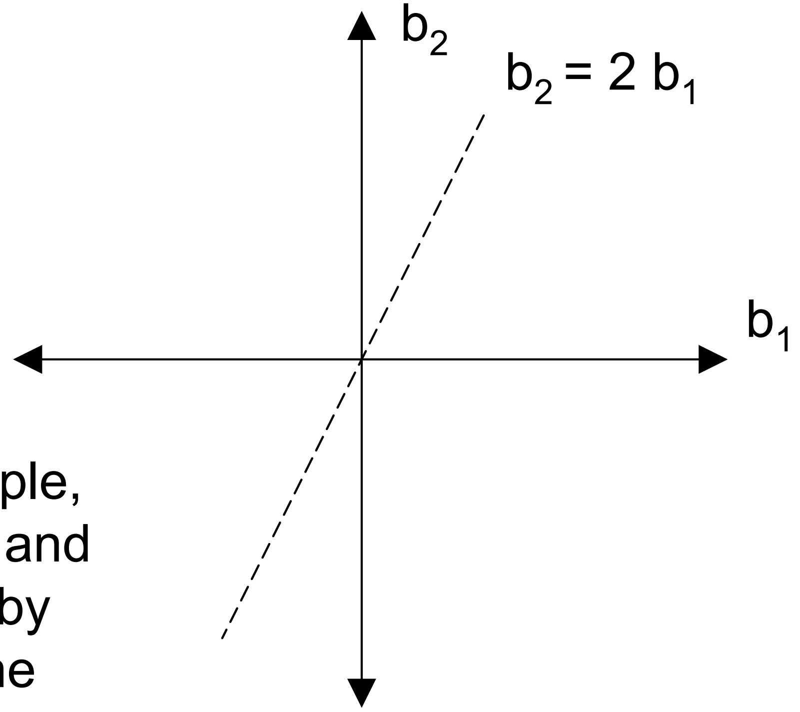


- In general, the equation has no solution
- But if $b_2 = 2b_1$, it has the (non-unique) solution

$$x_2 = b_1 - x_1$$

Singular systems

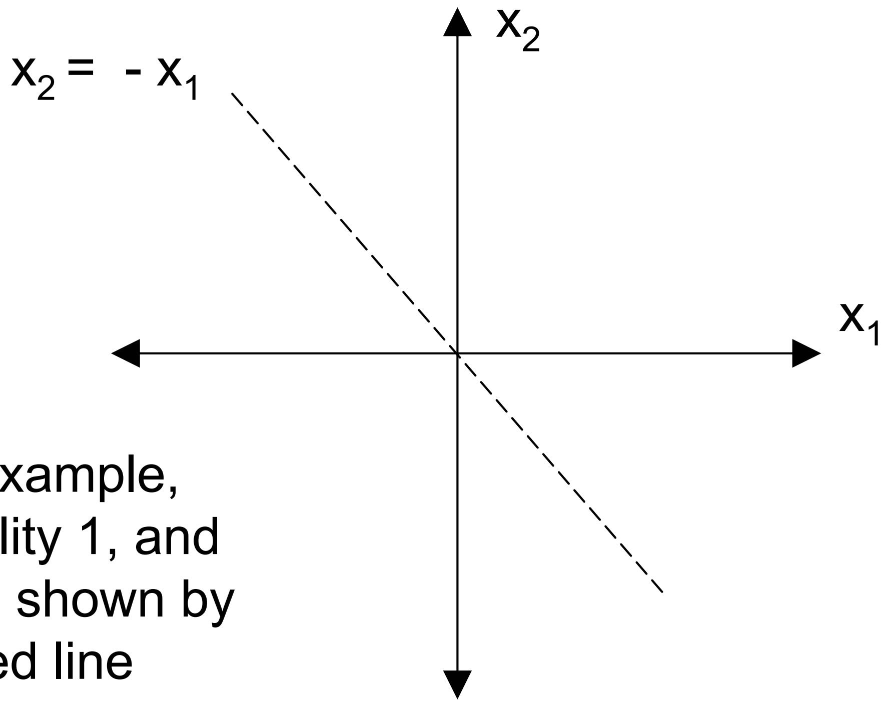
- The subspace within which **b** yields a solution to **A** . **x** = **b** is called the range of **A**
- The dimensionality of this range is called the rank of A



For this example, A has rank 1, and range shown by the dashed line

Singular systems

- If **A** is singular, and **b** lies within the range of A, the solution to **A**. **x** = **b** is always non-unique. In particular, the solution to **A**. **x** = **O** is called the nullspace of **A** and its dimensionality is called the nullity of **A**



For this example,
A has nullity 1, and
nullspace shown by
the dashed line

Singular systems

- The nullity and rank of an N x N matrix are related by rank + nullity = N
- If A is non-singular:

  rank = N ➔ the range of **A** covers the entire N x N space and there is a unique solution for any **b**

  nullity = 0 ➔ the nullspace of **A** is a single point, **x** = **0**, which is the only solution to **A** . **x** = 0

Singular systems

- The nullity and rank of an N x N matrix are related by rank + nullity = N
- If **A** is singular:

  rank < N ➔ the range of **A** covers only a subspace within the N x N space. There is only a solution to **A** . **x** = **b** when **b** lies within this subspace (and then the solution is non-unique)

  nullity > 0 ➔ the nullspace of **A** consists of more than a single point (i.e a line, a plane, a 3-space….)

Singular value decomposition

- SVD (Singular value decomposition) is a powerful technique for diagnosing and solving singular systems: essentially, it tells you the range and nullspace of **A**

- It can also be used to understand (and sometimes fix) nearly-singular problems

Singular value decomposition

- The singular value decomposition of **A** is written

$$\underset{[M\times N]}{\mathbf{A}} = \underset{[M\times N]}{\mathbf{U}}\ \underset{[N\times N]}{\mathbf{W}}\ \underset{[N\times N]}{\mathbf{V}^T}$$

  where W is diagonal and U and V are orthonormal
  i.e. $\mathbf{U}^T \mathbf{U} = \mathbf{V}^T \mathbf{V} = \mathbf{I}$

  This can always be done, and the decomposition is nearly unique (except for some transpositions)
  - important theorem that we will not prove
  - we will also not discuss the computational method for obtaining the SVD; the algorithm used in Numerical Recipes is very robust

Singular value decomposition

- The matrix W is diagonal

$$\begin{pmatrix} w_1 & & & & & \\ & w_2 & & & & \\ & & w_3 & & & \\ & & & \cdots & & \\ & & & & w_{N-1} & \\ & & & & & w_N \end{pmatrix} \equiv \mathrm{diag}\,(w_i)$$

The w_i are called the singular values of matrix **A**.
All the w_i are non-negative: if $M < N$, the last $N - M$ singular values are zero

Singular value decomposition of a square matrix

- The SVD is $\mathbf{A} = \mathbf{U} \; \mathbf{W} \; \mathbf{V}^T$,
  with $\mathbf{U}$, $\mathbf{V}^T$ and $\mathbf{W}$ all square N x N matrices

- The inverse of $\mathbf{A}$ (if it exists) is therefore

$$\mathbf{A}^{-1} = (\mathbf{V}^T)^{-1} \mathbf{W}^{-1} \mathbf{U}^{-1} = \mathbf{V} \mathbf{W}^{-1} \mathbf{U}^T$$

with $\mathbf{W}^{-1} = \mathrm{diag}\,(1/w_i)$

Clearly, $\mathbf{A}^{-1}$ exists iff $\mathbf{W}^{-1}$ exists,
and $\mathbf{W}^{-1}$ exists iff all the w_i are non-zero

Next …

Singular value decomposition of a singular matrix