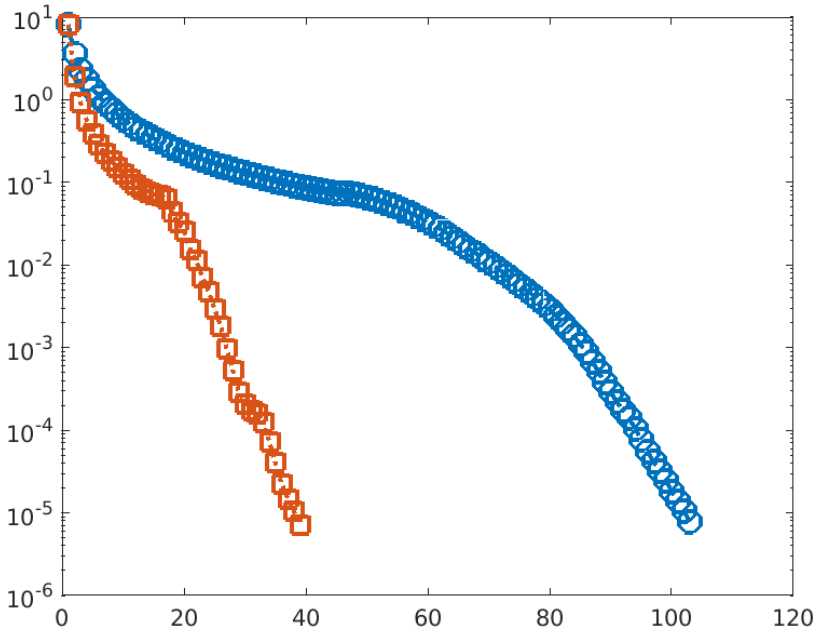
CS319: Scientific Computing (with MATLAB)

Direct and Iterative Solvers

Niall Madden

Week 10: **9am**, and **4pm**, 15 March 2023



This week...

1. 1. Projects (again)
2. 2: Linear Solvers in MATLAB
   - An example problem
3. 3: Direct solvers
4. 4. Iterative Solvers
   - minres
   - Conditioning
5. 5: Classes
   - Encapsulation

1. Projects (again)

The slides for this section are at https://www.niallmadden.ie/2223-CS319/2223-CS319-Projects.pdf

2: Linear Solvers in MATLAB

(This slide is from Week 9 notes). In this section, we study the details of solving linear systems of equations in MATLAB. Solvers can be classified as one of two types:

1. **Direct solvers**, which preform a fixed number of steps and give back the true answer (or, as close as possible, given that we have finite precision). Gaussian Elimination is the most famous example of this.
2. **Iterative solvers**, which take an initial guess and repeatedly try to improve it, until some tolerance is reached, or a maximum number of iterations is reached. The Jacobi method of Lab 5 is an example.

Both methods have their advantages and disadvantages:

To tests some methods, we need a good test problem. We need the problem to be

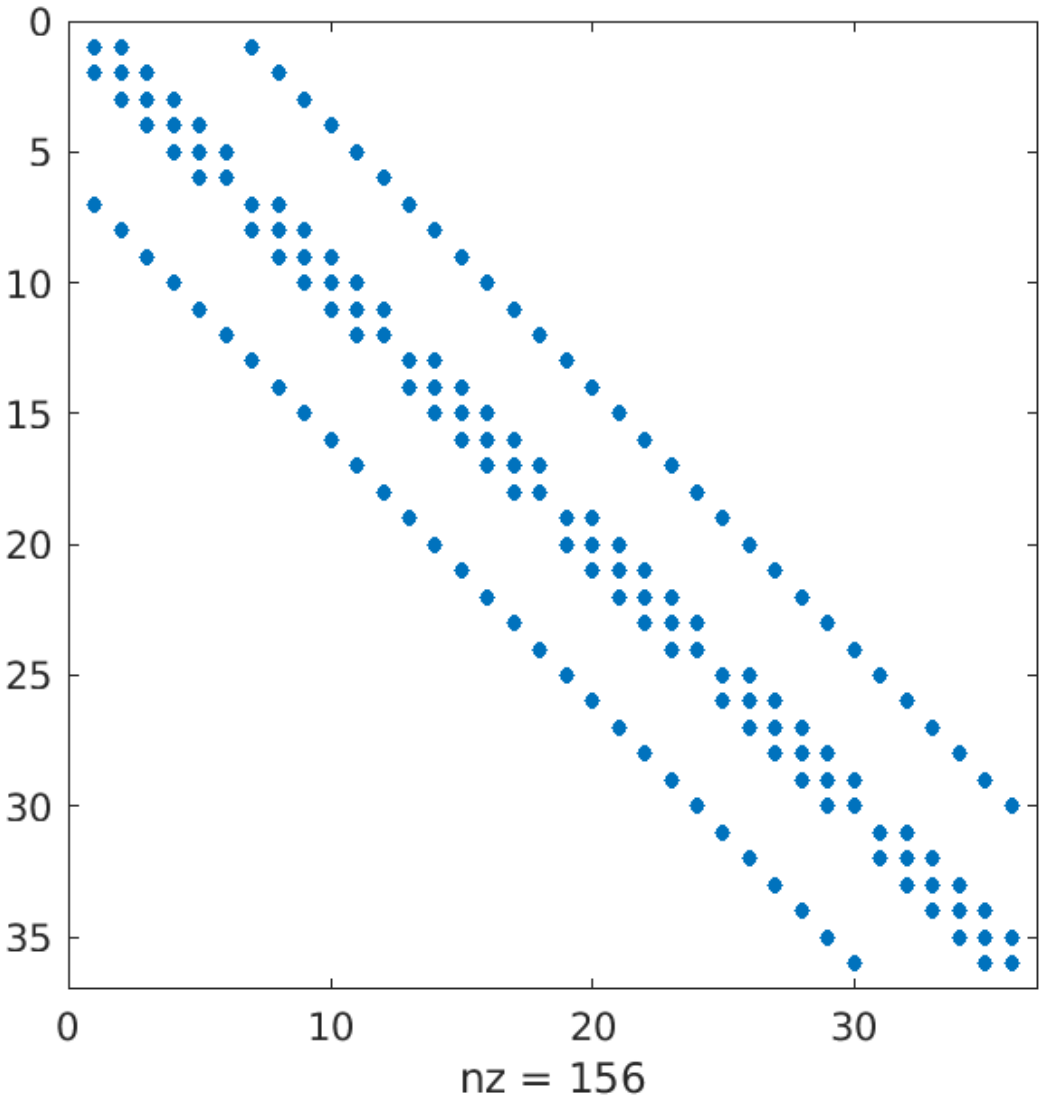
- Scalable: we can make up a version of any size we choose. In particular, we should be able to make it large.
- Not accidentally simple. For example, solving $Ax = b$ can be much easier when A is a tri-diagonal matrix, than when not.
- Sparse: most entries of A are zero.

For each matrix we choose some number n,

- The matrix will be $n^2 \times n^2$ (we usually say that there are n^2 "degrees of freedom", or "DoFs").
- It will be **banded**, with 5 non-zeros per row.
- The **band-width** is n.

MakeTestProblem.m

```
function [A,b]=MakeTestProblem(n)
A1 = sparse(1:n, 1:n, 1) ...
   + sparse(2:n, 1:n-1, -0.5, n,n) ...
   + sparse(1:n-1, 2:n, 1/4, n, n);
A = kron(A1,speye(n)) + kron(speye(n),A1) ;
x = ones(length(A),1);
b = A*x;
```


0
5
10
15
20
25
30
35
0
10
20
30
nz = 156

3: Direct solvers

The simplest way to solve a linear system in MATLAB is with the backslash operator:

```
>> x=A\b
```

To find out what is *really* happening we can turn on some diagnostics:

```
>> spparms('spumoni', 2)
>> x=A\b
sp\: bandwidth = 6+1+6.
sp\: is A diagonal? no.
sp\: is band density (0.366197) > bandden (0.500000)
    to try banded solver? no.
sp\: is A triangular? no.
sp\: is A morally triangular? no.
sp\: is A a candidate for Cholesky (symmetric, real
    positive or negative diagonal)? no.
sp\: use Unsymmetric MultiFrontal PACKagewith
    automatic reordering.
```

3: Direct solvers

In that example, we use the (somewhat obscure) function `spparms()` which sets parameters for sparse matrix routines.
The `spumoni` option turns on monitoring.
If we set it to Level 2, we get more output (usually way too much).
But with some effort, we can use the data to test the algorithms efficiency.

Unfortunately, it is not easy to record this data in a systematic way. But we will look at the solve times...

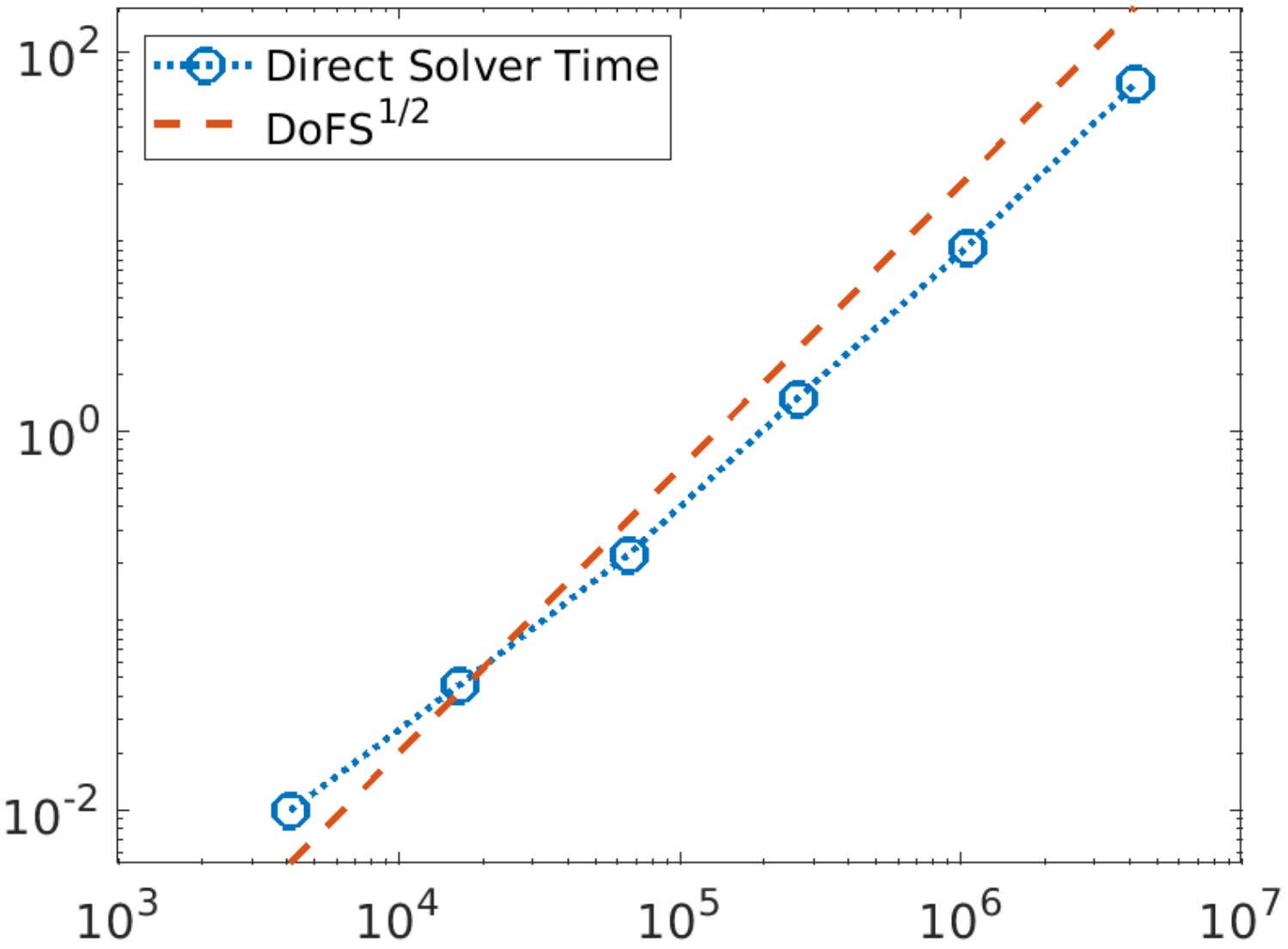
3: Direct solvers

TimeDirectSolver.m

```
k=0;
for n=2.^(6:10)
    k=k+1;
    A = MakeTestProblem(n);
    b = randn(length(A),1);
    DoFs(k)=length(b);
    tic; x=A\b; SolveTime(k)=toc;
    fprintf("n=%4d, DoFs=%8d, Time(s)=%8.3f\n", ...
        n, DoFs(k), SolveTime(k));
end
loglog(DoFs, SolveTime, ':o', DoFs,2e-8*DoFs.^1.5,...
```

```
n=  64, DoFs=    4096, Time(s)=   0.010
n= 128, DoFs=   16384, Time(s)=   0.046
n= 256, DoFs=   65536, Time(s)=   0.222
n= 512, DoFs=  262144, Time(s)=   1.484
n=1024, DoFs= 1048576, Time(s)=   9.276
n=2048, DoFs= 4194304, Time(s)=  68.213
```

3: Direct solvers



3: Direct solvers

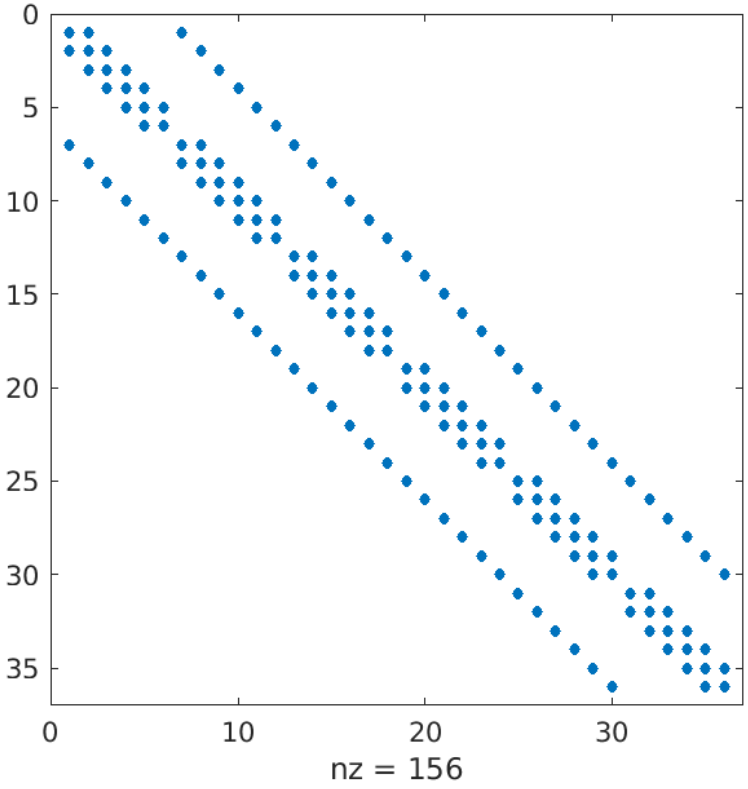
However, these timing are not a completely reliable guide to the effort required to solve these systems of equations.

In particular, they were computed on a laptop with 8 cores. As the system gets larger, more and more of these are used by the solver (for smaller systems, it is not worth using more than one core).

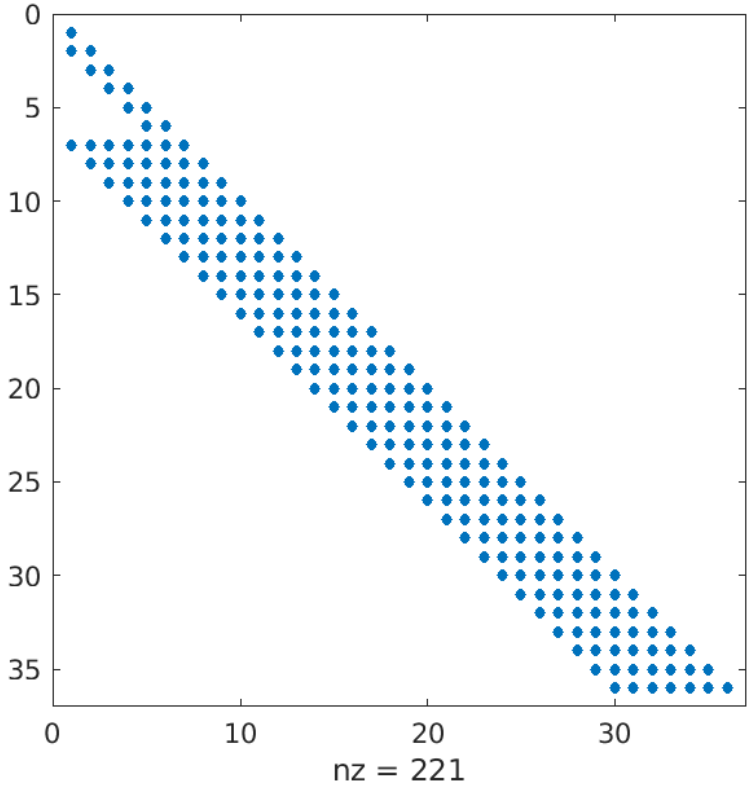
Nonetheless, for this (very typical) problem, we estimate that the time is proportional to n^3. Here is why that is correct...

- We solve a system with n^2 rows;
- Each row has a band-width of n;
- When we apply Gaussian Elimination to the system, we "fill-in" the bands. That is, everything between the diagonals and the bands becomes (potentially) non-zero.

Before row reduction



After row reduction



3: Direct solvers

Under the hood, the algorithm does its best to minimise this fill-in (using some very interesting methods from graph theory). However, although this can often reduce the computational time by a significant factor, the rate of growth remains the same.

However, there is an even bigger problem...

Suppose $n = 1000$. So A has 1,000,000 rows, and each row as (up to) 5 non-zero entries. That will take about 15Mb to store.

But when we apply Gaussian Elimination, we will need to store n non-zeros per row: so about 15Gb.

These calculations are very rough, but the conclusion is correct: such methods have significant limitations when it comes to solving large problems.

4. Iterative Solvers

For large scale sparse problems, direct solvers are of little use. The alternative is to use iterative solvers. The very simplest are the Jacobi and Gauss-Seidel methods from Labs 5 and 6, but there are methods that are much more modern and efficient.

How they work is beyond the scope of this module (but roughly, think about the effectiveness of Newton's method compare the bisection method).

For this example, we'll use the "Minimum Residual" method, (`minres`, for short).

It is not hard to code: have a look at the Wiki Page: `https://en.wikipedia.org/wiki/Minimal_residual_method`.

However, `minres()` in only designed for symmetric matrices. In `MakeSymTestProblem.m` you'll find code that builds a **symmetric** banded matrix.

Like all iterative methods, `minres` computes a sequence of approximations to the solution of $Ax = b$.

You can apply it, in MATLAB, using `x = minres(A,b)`.

But when using any of these iterative method, you have to choose:

- A convergence tolerance, `tol`
- Maximum number of iterations, `maxit`

At each iteration (hopefully) the quality of the approximation improves. That is, if the kth iteration is $x(k)$ then we "hope" that $\|x - x^{(k)}\| < \|x - x^{(k-1)}\|$.

In practical settings, we don't know x, so we can't just iterate until $\|x - x^{(k)}\| \leq tol$. Instead we use the residual as a proxy for the error.

That is, if in fact $x^{(k)} = x$, then $Ax^{(k)} = b$. Put another way, $\|b - Ax^{(k)}\| = 0$. That is unlikely to happen unless k is very small. So instead we stop when the **residual** $\|b - Ax^{(k)}\|$ is less than `tol`.

However, sometimes the method can be very slow, so we also need to specify the maximum value of k. This is `maxit`.

So now we know that we should choose values of `tol` and `maxits`, and then call `x = minres(A, b, tol, maxit);`

However, since convergence is precarious, we should also take some diagnostic information from `minres`.

That is we call

```
[x,flag,res, its, resvec] = minres(A,b, tol, maxits);
```

- `x` is the solution, i.e., $x^{(k)}$.
- `flag` is an integer that gives reasons why if failed (if it did). If `flag==0` the method "converged".
- `res` is $\|b - Ax^{(k)}\|$ for the final k.
- `its` is the number of iterations computed.
- `resvec` is a vector for all iterations, except the last one.

Example

Suppose we take $n = 16$ and make the symmetric test problem w. Then setting $tol = 10^{-4}$ we'll find that `minres()` needs 22 iterations. Each iteration is quick, but that is still suboptimal: if we double n then the number of iterations doubles too.

TimeIterativeSolver.m

```
Minres  n=   16, DoFs=     256, Time(s)=   0.003, Its=  26
Minres  n=   32, DoFs=    1024, Time(s)=   0.001, Its=  53
Minres  n=   64, DoFs=    4096, Time(s)=   0.007, Its= 102
Minres  n=  128, DoFs=   16384, Time(s)=   0.058, Its= 198
Minres  n=  256, DoFs=   65536, Time(s)=   0.323, Its= 382
Minres  n=  512, DoFs=  262144, Time(s)=   3.031, Its= 736
Minres  n=1024, DoFs= 1048576, Time(s)=  19.449, Its=1000
```

At a glance, that seems like the method is not very good, but in fact we we just need to understand:

- What determines the convergence;
- How it can be improved.

The speed of methods like `minres` depends on the **condition number** of the matrix, which is defined as

$$\kappa(A) := \|A\|\|A^{-1}\|.$$

Then (roughly) at each iteration the residual changes by a factor or

$$\sqrt{\frac{\kappa(A)-1}{\kappa(A)+1}}$$

Certainly, this factor is less than one (which is good), but not by much...

```
Minres  n=  16, DoFs=     256, Time(s)=   0.003, Its=  26
Minres  n=  32, DoFs=    1024, Time(s)=   0.001, Its=  53
Minres  n=  64, DoFs=    4096, Time(s)=   0.007, Its= 102
Minres  n= 128, DoFs=   16384, Time(s)=   0.058, Its= 198
Minres  n= 256, DoFs=   65536, Time(s)=   0.323, Its= 382
Minres  n= 512, DoFs=  262144, Time(s)=   3.031, Its= 736
Minres  n=1024, DoFs= 1048576, Time(s)=  19.449, Its=1000
```

There is a strategy, called **preconditioning** that tries to improve this situation.

Unfortunately, it is beyond the scope of what we can do today but, roughly...

- Find a matrix M that approximates A, but for which M^{-1} is easily computed.
- Also need that $\kappa(M^{-1}A) < \kappa(A)$.
- Instead of solving $Ax = b$ we solve $M^{-1}Ax = M^{-1}b$.

The simplest method use to take `M=diag(diag(A))`. (However, that is so easy, minres automatically does it).

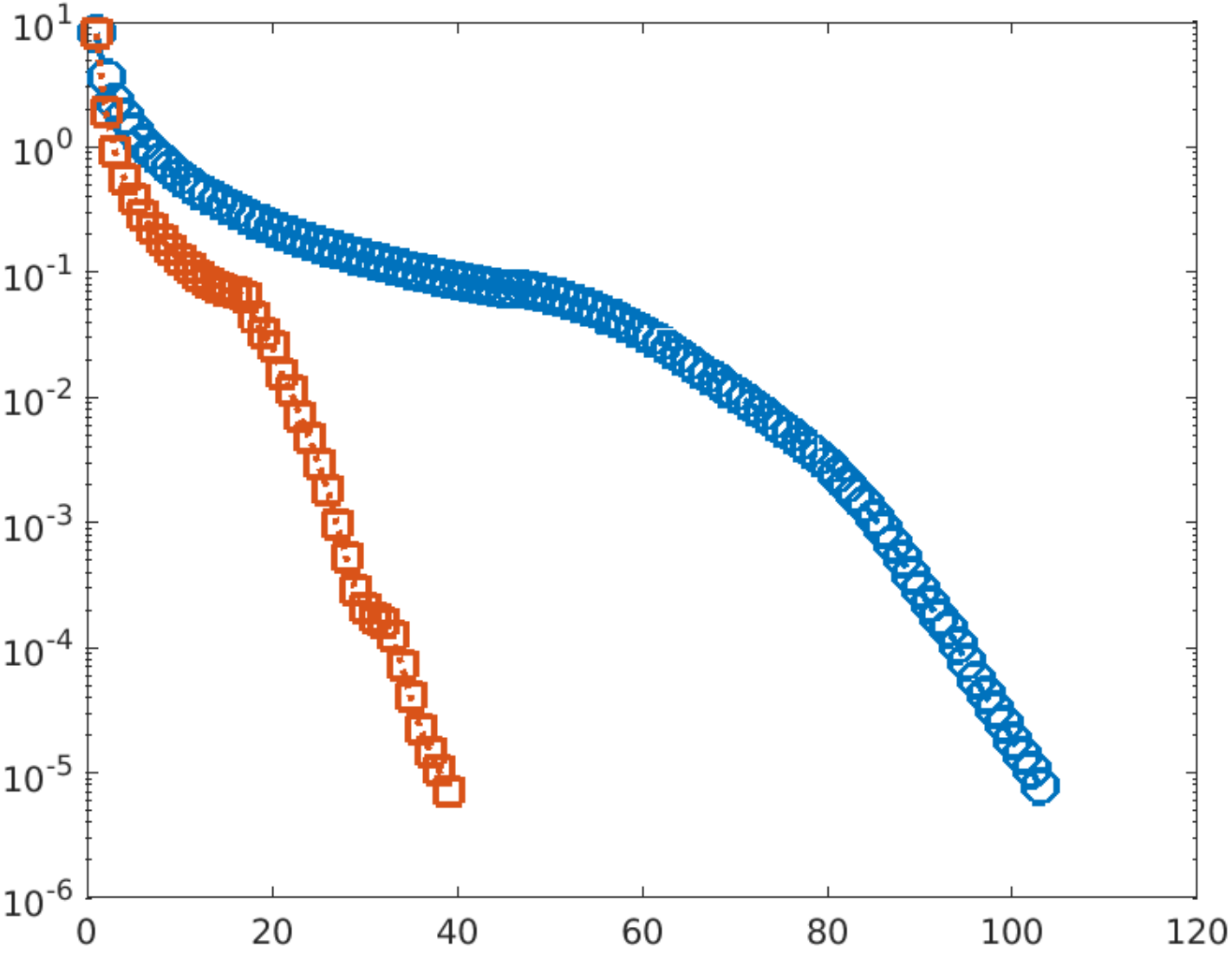
The second simplest is called **Incomplete LU factorisation**

Min res: No preconditioning

```
n=   16, DoFs=     256, Time(s)=    0.003, Its=  26
n=   32, DoFs=    1024, Time(s)=    0.001, Its=  53
n=   64, DoFs=    4096, Time(s)=    0.007, Its= 102
n=  128, DoFs=   16384, Time(s)=    0.058, Its= 198
n=  256, DoFs=   65536, Time(s)=    0.323, Its= 382
n=  512, DoFs=  262144, Time(s)=    3.031, Its= 736
n=1024, DoFs= 1048576, Time(s)=   19.449, Its=1000
```

Min res with ILU

```
n=   16, DoFs=     256, Time(s)=    0.055, Its=  14
n=   32, DoFs=    1024, Time(s)=    0.008, Its=  24
n=   64, DoFs=    4096, Time(s)=    0.015, Its=  38
n=  128, DoFs=   16384, Time(s)=    0.059, Its=  67
n=  256, DoFs=   65536, Time(s)=    0.307, Its= 115
n=  512, DoFs=  262144, Time(s)=    2.514, Its= 220
n=1024, DoFs= 1048576, Time(s)=   19.601, Its= 420
```


10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
0
20
40
60
80
100
120

To date, the programming we have done in MATLAB has been *procedural*: it has been driven by algorithms and involved on very simple data structures.

Encapsulation

Idea: create a single entity in a program that combines data with the program code (i.e., functions) that manipulate that data.
In MATLAB, a description/definition of such entities is called a **class**, and an instance of such an entity is called an **object**.