Lecture 10: Exploiting sparsity in the solution process

COMP5930M Scientific Computation

Today

- Recap
  - 1d model problem (Burger's equation)
  - Finite difference method
  - Time-stepping
- Sparsity
- Exploiting sparsity
  - Jacobian
  - Linear algebra
- Efficiency

Example: 1d viscous Burger's equation

Find $u(x, t)$ satisfying

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} \;=\; \varepsilon\,\frac{\partial^2 u}{\partial x^2}$$

on $x \in [X_1, X_2]$, and $t > 0$,
with boundary conditions $u(X_1, t) = u_1(t)$, $u(X_2, t) = u_2(t)$
and initial conditions $u(x, 0) = u_0(x)$.

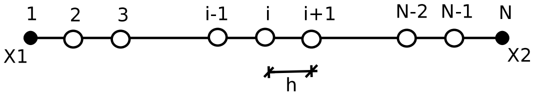
$\varepsilon > 0$ is a known constant

Approximations in 1d: Finite Difference Methods

Define a grid (mesh) for the spatial domain x

For FDM approximations define a uniform spacing h

$$x_i \;=\; X_1 + (i-1)h, \qquad i = 1, 2, ..., n$$



At point (node) i approximate all spatial terms of the PDE

Notation: $u(x_i, t) \equiv u_i(t), \quad u(x_i, t^n) \equiv u_i^n, \quad \frac{\partial u}{\partial t} \equiv \dot{u}$

Finite difference method for 1d Burger's Equation

Replace spatial derivatives with difference approximations:

$$\frac{\partial u}{\partial t}(x_i) + u(x_i)\,\frac{\partial u}{\partial x}(x_i) \quad = \quad \varepsilon\,\frac{\partial^2 u}{\partial x^2}(x_i)$$

to obtain the semi-discrete form (ordinary differential equation):

$$\dot{u}_i + u_i\left(\frac{u_i - u_{i-1}}{h}\right) \quad = \quad \varepsilon\,\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

for internal nodes $i = 2, 3, ..., n-1$

Approximating in time

The semi-discrete problem is a system of ODEs: $\dot{\mathbf{u}} = f(\mathbf{u})$

- Implicit Euler for time discretisation

$$\frac{\mathbf{u}^{k+1} - \mathbf{u}^{k}}{\Delta t} = f(\mathbf{u}^{k+1})$$

1d Burger's Equation

Equation $F_i(\mathbf{U})$ at node i of the grid:

$$F_i(\mathbf{U}) = \frac{u_i^{k+1} - u_i^k}{\Delta t} + u_i^{k+1}\frac{u_i^{k+1} - u_{i-1}^{k+1}}{h} \quad - \quad \varepsilon\,\frac{u_{i+1}^{k+1} - 2u_i^{k+1} + u_{i-1}^{k+1}}{h^2} = 0.$$

- Fully discrete nonlinear system $\mathbf{F}(\mathbf{U}) = \mathbf{0}$ for the unknowns $U_i = u_i^{k+1}, \;\; i = 2, ..., n-1$
- Depends on previous $\mathbf{u}^k$, time step Δt and grid size h
- Each equation F_i depends on three neighbouring nodes U_{i-1}, U_i, U_{i+1} through the FDM approximation

Time-stepping algorithm

- Initial conditions are specified at $t = t_0$ as $u = U(x, t_0)$
  - Sets the discrete solution $u_i^0 = U(x_i, t_0)$
- For each time step $k = 0, 1, 2, ...$
  we solve a nonlinear system to find $\mathbf{U} = \mathbf{u}^{k+1}$:
  - Solve $\mathbf{F}(\mathbf{U}) = \mathbf{0}$ by Newton's method, set
  - Advance u_i^k to u_i^{k+1} , $i = 2, 3, ..., n-1$
- Solving the tangent problem $\mathbf{J}\delta = -\mathbf{F}$ is expensive if n large.
  For an $n \times n$ Jacobian, the cost in general is $O(n^3)$.

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Sparsity

- Our 1-d PDE has a Jacobian matrix with sparse structure
- A general $n \times n$ matrix has n^2 entries
  - We term that matrix dense or full if all or most are nonzero
- A sparse matrix has only nnz non-zero entries, where $nnz \ll n^2$
  - nnz = "number of nonzeroes" (MATLAB: `nnz(A)`)
  - Typically we would think of $nnz = K \times n$ where $K \ll n$
  - Most matrix algorithms can be reformulated, more efficiently, to take advantage of sparsity (sparse linear algebra)

Sparse nonlinear systems

We can improve the efficiency of several aspects of our solution algorithm if we know the nonlinear system is sparse

- Construction of the Jacobian matrix at each Newton iteration
- Solution of the linear system $\mathbf{J}\boldsymbol{\delta} = -\mathbf{F}$
- Additionally, the nonlinear function evaluation is cheaper

Our example fully-discrete problem

Finite differences + Implicit Euler. At node i of the grid:

$$F_i = \frac{U_i - u_i^k}{\Delta t} + U_i \frac{U_i - U_{i-1}}{h} - \epsilon \frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} \;=\; 0$$

- The full system is defined by writing out the equations for every internal node $i = 2, ..., n-1$
- Function F_i involves only U_i and its neighbours U_{i-1}, U_{i+1}
- Function evaluation of F_i requires only those 3 values
- Jacobian evaluation of F_i requires only those 3 values

Analytical Jacobian

For this problem we can analytically evaluate the Jacobian matrix:

$$\begin{aligned}
\frac{\partial F_i}{\partial U_{i-1}} &= -\frac{U_i}{h} - \frac{\varepsilon}{h^2} \\
\frac{\partial F_i}{\partial U_i} &= \frac{1}{\Delta t} + \frac{2U_i - U_{i-1}}{h} + \frac{2\varepsilon}{h^2} \\
\frac{\partial F_i}{\partial U_{i+1}} &= -\frac{\varepsilon}{h^2}
\end{aligned}$$

are the only nonzero elements of the *i*'th row

- Tridiagonal structure allows us to only perform computations for which we know the result will be nonzero
- $3n$ arithmetic operations to compute the nonzero part of **J**

Numerical Jacobian

- The standard algorithm requires $n + 1$ function evaluations

$$\frac{\partial \mathbf{F}}{\partial u_j} \approx \frac{\mathbf{F}(u_1, ..., u_j + \delta, ..., x_n) - \mathbf{F}(u_1, ..., u_n)}{\delta}$$

  - Apply perturbation to each variable u_j in turn, $j = 1, \ldots, n$
  - Only option when Jacobian is dense

- For a tridiagonal system we only require 3 function evaluations
  - Independent of problem size n
  - Exploits tridiagonal (sparse) structure
  - Perturb sets of variables simultaneously

Solving the linear system

- The Thomas algorithm – a special case of Gaussian elimination without pivoting for tridiagonal systems
- The algorithm has two stages:
  - Forward elimination
  - Back substitution

The Thomas algorithm

Assume our tridiagonal linear system is written as

$$a_i u_{i-1} + b_i u_i + c_i u_{i+1} \;=\; d_i, \qquad i = 1, \ldots, n$$

$$\begin{bmatrix} b_1 & c_1 & & & 0 \\ a_2 & b_2 & c_2 & & \\ & a_3 & b_3 & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ 0 & & & a_n & b_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ \vdots \\ d_n \end{bmatrix}.$$

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Multiply with a_2/b_1 and subtract

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Continue elimination row per row

$$\begin{bmatrix} b_1 & c_1 & & & 0 \\ 0 & & \ddots & & \\ & a_3 & b_3 & \ddots & \\ & & \ddots & \ddots & c_{n-1} \\ 0 & & & a_n & b_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} d_1 \\ \vdots \\ d_3 \\ \\ d_n \end{bmatrix}.$$

The Thomas algorithm

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$$a_i u_{i-1} + b_i u_i + c_i u_{i+1} \;=\; d_i, \qquad i = 1, \ldots, n$$

- Forward Gaussian elimination: $j = 2, \ldots, n$

$$b_j \leftarrow b_j - c_{j-1}\frac{a_j}{b_{j-1}}, \quad d_j \leftarrow d_j - d_{j-1}\frac{a_j}{b_{j-1}}$$

  reduces the problem to an upper-triangular form $Tu = d$

- Note: If $b_{j-1} = 0$, we need to use different algorithm that allows pivoting without breaking the tridiagonal structure[1]

[1] see e.g. Erway et al. Generalized diagonal pivoting methods for tridiagonal systems without interchanges. IAENG Int. J. Appl. Math. 40(4), 269275 (2010)

The Thomas algorithm

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The Thomas algorithm

- The upper-triangular problem $Tu = d$ can be solved by back substitution: $j = n-1, ..., 1$

$$\begin{aligned} u_n &= \frac{d_n}{b_n} \\ u_j &= \frac{d_j - c_j u_{j+1}}{b_j} \end{aligned}$$

- Algorithm performs $2n-1$ divisions, $3n-3$ multiplications and $3n-3$ subtractions $\Rightarrow$ complexity is $\mathcal{O}(n)$

Computational expense (tridiagonal system)

For a single Newton iteration of our algorithm for the 1d viscous Burger's Equation (or any tridiagonal system)

	Function calls	Algorithmic
Evaluate $\mathbf{J}$	3	n
Solve $\mathbf{J}\delta = -\mathbf{F}$	1	n
Update $\mathbf{u}^{k+1}$	0	n

Note:

- Overall $\mathcal{O}(n)$ algorithmic expense
- Fixed number of function evaluations per iteration