Shift Matrices and Finite-Difference Matrices

A Short Introduction to Matrix-Based Numerical Differentiation

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1 Introduction

Finite-difference methods form one of the cornerstones of numerical analysis for ordinary and partial differential equations. Instead of viewing finite-difference formulas individually, it is often advantageous to interpret them as matrix operators acting on vectors of grid values.

An elegant observation is that many finite-difference matrices can be constructed from only three elementary matrices:

$$I, \qquad S_+, \qquad S_-,$$

where I denotes the identity matrix, S_+ the forward shift matrix, and S_- the backward shift matrix.

These matrices provide a compact algebraic framework for constructing finite-difference approximations of first and second derivatives, higher-order operators, and many discretizations used in numerical methods for differential equations.

The objective of these notes is to introduce these matrices, study their basic algebraic properties, derive the most common finite-difference matrices, and illustrate their use by means of several exercises.

2 Shift Matrices

Consider a uniform grid

$$x_i = ih, \qquad i = 1, \dots, n,$$

with grid spacing $h > 0$.

Suppose that a grid function is represented by the vector

$$u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}.$$

The forward and backward shift matrices move the components of this vector one grid point to the left or to the right.

The following sections introduce these matrices and investigate their fundamental properties.

2.1 Definition of the Shift Matrices

The most elementary matrices in finite-difference methods are the forward and backward shift matrices.

The *forward shift matrix* is defined by

$$S_+ = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ 0 & 0 & 0 & \ddots & \vdots \\ \vdots & & & \ddots & 1 \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

Similarly, the *backward shift matrix* is

$$S_- = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Both matrices are sparse and contain only zeros and ones.

2.2 Action on a Vector

Let

$$u = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_n \end{pmatrix}.$$

Multiplication by the forward shift matrix gives

$$S_+ u = \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ u_n \\ 0 \end{pmatrix}.$$

Thus every component is shifted one position upward.

Likewise,

$$S_- u = \begin{pmatrix} 0 \\ u_1 \\ u_2 \\ \vdots \\ u_{n-1} \end{pmatrix},$$

which shifts every component one position downward.
Hence,

S_+ shifts forward,	S_- shifts backward.

2.3 Example for Five Grid Points

For $n = 5$, the forward shift matrix becomes

$$S_+ = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

whereas the backward shift matrix is

$$S_- = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Applying these matrices to

$$u = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{pmatrix}$$

gives

$$S_+ u = \begin{pmatrix} 2 \\ 3 \\ 4 \\ 5 \\ 0 \end{pmatrix},$$

and

$$S_- u = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \\ 4 \end{pmatrix}.$$

These simple examples immediately illustrate the geometric meaning of both operators.

2.4 Interpretation on a Computational Grid

Suppose the vector u contains function values,

$$u_i = u(x_i),$$

at the grid points

$$x_i = ih.$$

Then

$$(S_+ u)_i = u_{i+1},$$

and

$$(S_- u)_i = u_{i-1}.$$

Therefore, the shift matrices move information from one grid point to a neighbouring grid point.

This interpretation forms the basis of almost all finite-difference operators encountered in numerical analysis.

2.5 First Observations

Several elementary properties are already apparent.

- Both matrices are sparse.
- Each row contains at most one nonzero entry.
- Each column contains at most one nonzero entry.
- Multiplication requires only copying neighbouring values.
- The matrices contain no approximations; they perform exact translations on the discrete grid.

Although extremely simple, these matrices will generate all standard finite-difference matrices studied later in these notes.

3 Basic Properties of Shift Matrices

The forward and backward shift matrices possess a remarkably rich algebraic structure. These properties form the basis for the construction and analysis of finite-difference matrices.

3.1 Transpose Relation

The first important observation is that the backward shift matrix is the transpose of the forward shift matrix:

$$\boxed{S_- = S_+^T.}$$

Indeed, taking the transpose of

$$S_+ = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

immediately gives

$$S_+^T = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} = S_-.$$

Consequently, every property of one shift matrix immediately yields a corresponding property of the other.

3.2 Higher Powers

Repeated multiplication corresponds to repeated shifting.

For example,

$$S_+^2 u = \begin{pmatrix} u_3 \\ u_4 \\ \vdots \\ 0 \\ 0 \end{pmatrix},$$

while

$$S_-^2 u = \begin{pmatrix} 0 \\ 0 \\ u_1 \\ u_2 \\ \vdots \end{pmatrix}.$$

More generally,

$$\boxed{S_+^k = \text{forward shift over } k \text{ grid points},}$$

and

$$\boxed{S_-^k = \text{backward shift over } k \text{ grid points}.}$$

3.3 Nilpotency

After sufficiently many shifts, every component leaves the computational domain.

Therefore,

$$\boxed{S_+^n = 0,}$$

and similarly,

$$\boxed{S_-^n = 0.}$$

Matrices with this property are called *nilpotent*.
Since all sufficiently high powers vanish, every eigenvalue satisfies

$$\lambda^n = 0,$$

which immediately implies

$$\boxed{\lambda = 0.}$$

Hence all eigenvalues of both shift matrices are equal to zero.

3.4 Rank

Only one row of the forward shift matrix is completely zero.
Consequently,

$$\boxed{\operatorname{rank}(S_+) = n - 1.}$$

The same argument gives

$$\boxed{\operatorname{rank}(S_-) = n - 1.}$$

Thus the matrices are singular.

3.5 Products of Shift Matrices

The products

$$S_+ S_-$$

and

$$S_- S_+$$

are almost equal to the identity matrix.
Indeed,

$$S_+ S_- = \operatorname{diag}(1, \ldots, 1, 0),$$

whereas

$$S_- S_+ = \operatorname{diag}(0, 1, \ldots, 1).$$

Hence,

$$\boxed{S_+ S_- \neq I, \qquad S_- S_+ \neq I.}$$

The discrepancy is entirely caused by the boundary points.
Away from the boundaries the shift operators behave like inverse translations.

3.6 Norms

Since each row contains at most one nonzero entry,

$$\|S_+\|_\infty = 1,$$

and

$$\|S_-\|_\infty = 1.$$

Likewise,

$$\|S_+\|_2 = 1, \qquad \|S_-\|_2 = 1.$$

Thus shifting does not amplify the magnitude of a vector.

3.7 Interpretation

The shift matrices may be viewed as discrete translation operators.

Instead of moving a continuous function,

$$u(x) \longrightarrow u(x+h),$$

they move a vector of sampled values,

$$u_i \longrightarrow u_{i+1}.$$

Therefore they provide the discrete analogue of the translation operator from continuous analysis.

3.8 Summary

The most important properties established so far are

$$\boxed{S_- = S_+^T,}$$

$$\boxed{S_\pm^n = 0,}$$

$$\boxed{\operatorname{rank}(S_\pm) = n-1,}$$

and

$$\boxed{\sigma(S_\pm) = \{0\},}$$

where $\sigma(\cdot)$ denotes the spectrum of a matrix.

These simple algebraic properties will allow us to derive all standard finite-difference matrices in the next section by taking suitable linear combinations of

$$I, \qquad S_+, \qquad S_-.$$

4 Construction of Finite-Difference Matrices

One of the main advantages of introducing the shift matrices is that the most common finite-difference matrices can be written as simple linear combinations of

$$I, \qquad S_+, \qquad S_-.$$

Consequently, many algebraic properties of finite-difference operators follow immediately from the properties of the shift matrices.

4.1 Forward Difference Matrix

The classical forward difference approximation of the first derivative is

$$u'(x_i) \approx \frac{u_{i+1} - u_i}{h}.$$

Since

$$(S_+ u)_i = u_{i+1},$$

this approximation can be written in matrix form as

$$\boxed{D_{1,+} = \frac{1}{h}(S_+ - I).}$$

For $n = 5$,

$$D_{1,+} = \frac{1}{h}\begin{pmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix}.$$

Each row computes a forward difference using one neighbouring grid point.

4.2 Backward Difference Matrix

Similarly,

$$u'(x_i) \approx \frac{u_i - u_{i-1}}{h}.$$

Since

$$(S_- u)_i = u_{i-1},$$

we obtain

$$\boxed{D_{1,-} = \frac{1}{h}(I - S_-).}$$

For $n = 5$,

$$D_{1,-} = \frac{1}{h}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 1 \end{pmatrix}.$$

The forward and backward difference matrices are transposes of each other up to a minus sign,

$$D_{1,-} = -D_{1,+}^T,$$

apart from the treatment of the boundary points.

4.3 Central Difference Matrix

A more accurate approximation of the first derivative is obtained by using neighbouring grid points on both sides:

$$u'(x_i) \approx \frac{u_{i+1} - u_{i-1}}{2h}.$$

Using the shift matrices,

$$(S_+ u)_i = u_{i+1}, \qquad (S_- u)_i = u_{i-1},$$

we immediately obtain

$$\boxed{D_{1,c} = \frac{1}{2h}(S_+ - S_-).}$$

For $n = 5$,

$$D_{1,c} = \frac{1}{2h}\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \end{pmatrix}.$$

Unlike the forward and backward differences, this operator uses information from both neighbouring grid points.

4.4 Second-Derivative Matrix

The standard central approximation of the second derivative is

$$u''(x_i) \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}.$$

Since

$$(S_+ u)_i = u_{i+1},$$

and

$$(S_- u)_i = u_{i-1},$$

the corresponding matrix is

$$\boxed{D_2 = \frac{1}{h^2}(S_+ - 2I + S_-).}$$

For $n = 5$,

$$D_2 = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix}.$$

This tridiagonal matrix is one of the most frequently occurring matrices in numerical analysis.

4.5 Stencil Interpretation

The previous matrices correspond to the following finite-difference stencils:

$$D_{1,+} \quad \leftrightarrow \quad [-1,\ 1],$$

$$D_{1,-} \quad \leftrightarrow \quad [-1,\ 1],$$

where the stencil is shifted one grid point to the left,

$$D_{1,c} \quad \leftrightarrow \quad \left[-\frac{1}{2},\ 0,\ \frac{1}{2}\right],$$

and

$$D_2 \quad \leftrightarrow \quad [1,\ -2,\ 1].$$

Thus every stencil corresponds to a linear combination of the matrices

$$I, \qquad S_+, \qquad S_-.$$

4.6 General Three-Point Difference Operators

More generally, every three-point finite-difference operator can be written as

$$\boxed{A = a_{-1}S_- + a_0 I + a_1 S_+,}$$

where the coefficients a_{-1}, a_0, and a_1 determine the stencil.
For example,

$$A = \frac{1}{h^2}(S_+ - 2I + S_-) + \frac{3}{2h}(S_+ - S_-)$$

is the standard finite-difference approximation of the differential operator

$$u'' + 3u'.$$

4.7 Summary

The four most important finite-difference matrices are

$$\boxed{D_{1,+} = \frac{1}{h}(S_+ - I),}$$

$$\boxed{D_{1,-} = \frac{1}{h}(I - S_-),}$$

$$\boxed{D_{1,c} = \frac{1}{2h}(S_+ - S_-),}$$

and

$$\boxed{D_2 = \frac{1}{h^2}(S_+ - 2I + S_-).}$$

All these operators are constructed from only three elementary matrices,

$$\boxed{I, \qquad S_+, \qquad S_-,}$$

which explains why shift matrices play such a central role in finite- difference methods.

5 Algebraic Properties of Finite-Difference Matrices

The finite-difference matrices introduced in the previous section inherit many of their properties from the shift matrices. These algebraic properties are useful for the analysis of numerical methods for ordinary and partial differential equations.

5.1 Transpose Relations

Since

$$S_- = S_+^T,$$

we immediately obtain

$$D_{1,c}^T = \frac{1}{2h}(S_- - S_+) = -D_{1,c}.$$

Hence

$$\boxed{D_{1,c}^T = -D_{1,c},}$$

so the central difference matrix is *skew-symmetric.*
Similarly,

$$D_2^T = D_2,$$

which shows that the second-derivative matrix is symmetric.

5.2 Bandwidth

All finite-difference matrices considered so far are sparse.
The first-derivative matrices contain only two nonzero diagonals, whereas

$$D_2$$

contains three nonzero diagonals.
Hence

$$D_{1,+},\ D_{1,-}$$

are bidiagonal matrices, while

$$D_{1,c},\ D_2$$

are tridiagonal matrices.
Their storage requirements therefore grow only linearly with the number of grid points.

5.3 Symmetry Properties

The symmetry of the second-derivative matrix follows immediately:

$$D_2 = \frac{1}{h^2}(S_+ + S_- - 2I).$$

Taking the transpose gives

$$D_2^T = \frac{1}{h^2}(S_- + S_+ - 2I) = D_2.$$

Therefore

$$\boxed{D_2 \text{ is symmetric.}}$$

5.4 Quadratic Form

For homogeneous Dirichlet boundary conditions,

$$u^T D_2 u = -\sum_i \left(\frac{u_{i+1} - u_i}{h}\right)^2 \leq 0.$$

Hence

$$\boxed{D_2 \text{ is negative semidefinite.}}$$

This discrete identity is the analogue of

$$\int u\, u_{xx}\, dx = -\int (u_x)^2\, dx.$$

5.5 Consistency

Taylor expansion immediately yields

$$D_{1,+}u = u' + \mathcal{O}(h),$$

$$D_{1,-}u = u' + \mathcal{O}(h),$$

$$D_{1,c}u = u' + \mathcal{O}(h^2),$$

and

$$D_2 u = u'' + \mathcal{O}(h^2).$$

Thus the central schemes are second-order accurate, while the one-sided schemes are first-order accurate.

5.6 Discrete Differential Operators

Many differential operators are obtained simply by combining the basic difference matrices.

For example,

$$u'' + 3u'$$

is approximated by

$$D_2 + 3D_{1,c},$$

while

$$-u'' + 5u$$

corresponds to

$$-D_2 + 5I.$$

Thus matrix algebra replaces differential calculus.

5.7 Commuting Operators

Because every finite-difference matrix is a polynomial in

$$I,\ S_+,\ S_-,$$

many operators commute.

For example,

$$D_2 D_{1,c} = D_{1,c} D_2.$$

This property considerably simplifies the analysis of numerical PDE schemes and matrix exponentials.

5.8 Summary

The most important algebraic properties are

$$\boxed{D_{1,c}^T = -D_{1,c},}$$

$$\boxed{D_2^T = D_2,}$$

$$\boxed{D_2 \text{ is negative semidefinite,}}$$

and

$$\boxed{D_{1,+},\ D_{1,-},\ D_{1,c},\ D_2 \text{ are sparse band matrices.}}$$

These properties explain why finite-difference matrices are efficient, stable, and easy to analyze.

6 General Matrix Representation of Finite-Difference Operators

The finite-difference matrices introduced in the previous sections are all special cases of a much more general construction.

Indeed, every linear finite-difference operator with a finite stencil can be written as a polynomial in the shift matrices.

This observation provides a unified matrix framework for the construction of numerical differentiation formulas.

6.1 General Three-Point Stencil

Consider the finite-difference approximation

$$(Au)_i = a_{-1}u_{i-1} + a_0 u_i + a_1 u_{i+1},$$

where the coefficients

$$a_{-1}, \qquad a_0, \qquad a_1$$

are constants.

Since

$$(S_- u)_i = u_{i-1},$$

and

$$(S_+ u)_i = u_{i+1},$$

it follows immediately that

$$\boxed{A = a_{-1}S_- + a_0 I + a_1 S_+.}$$

Thus every three-point finite-difference operator is simply a linear combination of the three elementary matrices

$$I, \qquad S_+, \qquad S_-.$$

6.2 Example 1: First Derivative

The central approximation

$$u'(x_i) \approx \frac{u_{i+1} - u_{i-1}}{2h}$$

corresponds to the coefficients

$$a_{-1} = -\frac{1}{2h},$$

$$a_0 = 0,$$

$$a_1 = \frac{1}{2h}.$$

Hence

$$D_{1,c} = \frac{1}{2h}(S_+ - S_-).$$

6.3 Example 2: Second Derivative

The classical approximation

$$u''(x_i) \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

gives

$$a_{-1} = \frac{1}{h^2},$$

$$a_0 = -\frac{2}{h^2},$$

$$a_1 = \frac{1}{h^2},$$

which leads to

$$D_2 = \frac{1}{h^2}(S_+ - 2I + S_-).$$

6.4 Five-Point Stencils

More accurate approximations require larger stencils.

For example,

$$(Au)_i = a_{-2}u_{i-2} + a_{-1}u_{i-1} + a_0u_i + a_1u_{i+1} + a_2u_{i+2}.$$

Since

$$S_+^2 u = (u_{i+2}),$$

and

$$S_-^2 u = (u_{i-2}),$$

the corresponding matrix is

$$\boxed{A = a_{-2}S_-^2 + a_{-1}S_- + a_0I + a_1S_+ + a_2S_+^2.}$$

Thus higher-order finite-difference methods are obtained simply by including higher powers of the shift matrices.

6.5 General Finite Stencils

Suppose a finite-difference approximation involves the stencil

$$u_{i-m}, \ldots, u_i, \ldots, u_{i+m}.$$

Then the corresponding matrix is

$$\boxed{A = \sum_{k=-m}^{m} a_k S^{(k)},}$$

where

$$S^{(k)} = \begin{cases} S_+^k, & k > 0, \\ I, & k = 0, \\ S_-^{-k}, & k < 0. \end{cases}$$

Consequently, every finite-band difference operator is generated by the shift matrices.

6.6 Connection with Toeplitz Matrices

Ignoring the boundary rows, every finite-difference matrix has constant diagonals.

Such matrices are called *Toeplitz matrices*.

For example,

$$D_2 = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \cdots \\ 0 & 0 & 1 & -2 & \cdots \\ \vdots & & & & \ddots \end{pmatrix},$$

is a tridiagonal Toeplitz matrix.

Toeplitz matrices play a central role in numerical linear algebra because they admit efficient algorithms and possess well-understood spectral properties.

6.7 A Matrix View of Differential Operators

The previous sections show that differential operators may be regarded as matrix polynomials.

Typical examples are

$$u' \quad \longleftrightarrow \quad D_{1,c},$$

$$u'' \quad \longleftrightarrow \quad D_2,$$

and

$$u'' + 3u' \quad \longleftrightarrow \quad D_2 + 3D_{1,c}.$$

Likewise,

$$-u'' + \alpha u$$

is approximated by

$$-D_2 + \alpha I.$$

Therefore, solving a differential equation numerically is equivalent to solving a matrix equation.

6.8 Summary

The central idea of this section is that every finite-difference operator with a finite stencil can be written as a polynomial in the shift matrices.

Symbolically,

$$\boxed{\text{Shift matrices} \Longrightarrow \text{Difference matrices} \Longrightarrow \text{Discrete differential operators.}}$$

This algebraic viewpoint provides a unified framework for the construction, analysis, and implementation of finite-difference methods for ordinary and partial differential equations.

6.9 Construction of Shift Matrices

The following MATLAB function constructs the forward and backward shift matrices.

```
function [Sp,Sm] = shift_matrices(n)

Sp = zeros(n);

for i=1:n-1
    Sp(i,i+1)=1;
end

Sm = Sp';

end
```

For example:

```
n = 6;

[Sp,Sm] = shift_matrices(n)
```

produces

$$S_+ = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & & & \end{pmatrix}.$$

6.10 Construction of Finite-Difference Matrices

The four standard difference matrices are constructed directly from the shift matrices.

```
n = 100;
h = 1/(n-1);

[Sp,Sm] = shift_matrices(n);

I = eye(n);

D1p = (Sp-I)/h;

D1m = (I-Sm)/h;

D1c = (Sp-Sm)/(2*h);

D2  = (Sp-2*I+Sm)/h^2;
```

The important observation is that no separate construction of the diagonals is required. The operators are generated automatically from

$$I, \qquad S_+, \qquad S_-.$$

6.11 Visualization of Sparsity

Finite-difference matrices are sparse.

MATLAB provides the command `spy` to visualize their structure.

```
figure

subplot(2,2,1)
spy(D1p)
title('Forward difference')

subplot(2,2,2)
spy(D1c)
title('Central difference')

subplot(2,2,3)
spy(D2)
title('Second derivative')
```

The resulting figures show:

- bidiagonal structure for $D_{1,+}$;
- tridiagonal structure for $D_{1,c}$;
- tridiagonal structure for D_2.

6.12 Applying the Operators to a Function

Consider

$$u(x) = \sin(2\pi x).$$

Its exact derivative is

$$u'(x) = 2\pi \cos(2\pi x),$$

and its second derivative is

$$u''(x) = -4\pi^2 \sin(2\pi x).$$

The MATLAB implementation is:

```
n = 100;

x = linspace(0,1,n)';

h = x(2)-x(1);

u = sin(2*pi*x);

up_exact = 2*pi*cos(2*pi*x);

upp_exact = -4*pi^2*sin(2*pi*x);
```

```
12
13
14  [Sp,Sm] = shift_matrices(n);
15
16  I = eye(n);
17
18  D1c = (Sp-Sm)/(2*h);
19
20  D2 = (Sp-2*I+Sm)/h^2;
21
22
23  up_num = D1c*u;
24
25  upp_num = D2*u;
26
27
28  figure
29
30  plot(x,up_exact,'k','LineWidth',2)
31  hold on
32  plot(x,up_num,'r--')
33
34  legend('exact','finite difference')
35
36  title('First derivative')
37
38
39  figure
40
41  plot(x,upp_exact,'k','LineWidth',2)
42  hold on
43  plot(x,upp_num,'b--')
44
45  legend('exact','finite difference')
46
47  title('Second derivative')
```

6.13 Eigenvalues of Difference Matrices

The eigenvalues give information about stability and spectral properties.

For example:

```
1
2  lambda1 = eig(D1c);
3
4  lambda2 = eig(D2);
5
6
7  figure
8
9  plot(real(lambda1),imag(lambda1),'o')
10
11 xlabel('Real part')
12 ylabel('Imaginary part')
13
14 title('Spectrum of D1c')
15
16
```

```
figure

plot(lambda2,'o')

title('Eigenvalues of D2')
```

Because

$$D_{1,c}^T = -D_{1,c},$$

the eigenvalues of the central difference matrix are purely imaginary.
Because

$$D_2^T = D_2,$$

the eigenvalues of D_2 are real.

6.14 Comparison of Different Stencils

The following example compares the three first derivative approximations.

```

n = 200;

x = linspace(0,1,n)';

h=x(2)-x(1);

u = exp(x);

exact = exp(x);


[Sp,Sm]=shift_matrices(n);

I=eye(n);


D1p=(Sp-I)/h;

D1m=(I-Sm)/h;

D1c=(Sp-Sm)/(2*h);


figure

plot(x,D1p*u,'r')
hold on

plot(x,D1m*u,'b')
plot(x,D1c*u,'k')

plot(x,exact,'g--','LineWidth',2)


legend('forward','backward',...
       'central','exact')

```

```
39 title('Comparison of first derivative formulas')
```

6.15 Final Remark

The MATLAB experiments confirm the theoretical structure developed in these notes:

$$\boxed{S_+, S_- \longrightarrow D_{1,+}, D_{1,-}, D_{1,c}, D_2 \longrightarrow \text{numerical differential operators.}}$$

The shift matrix viewpoint provides both a conceptual framework and a practical implementation strategy for finite-difference methods.

7 Appendix B: Periodic Shift Matrices and Fourier Analysis

The shift matrices introduced in the previous sections were defined with zero boundary values. This corresponds to a non-periodic grid.

For many problems in numerical analysis and partial differential equations, periodic boundary conditions are more appropriate.

In that case, the shift matrices are modified into cyclic shift matrices.

7.1 Periodic Shift Matrices

Consider a periodic grid with

$$u(x + L) = u(x).$$

The forward shift now moves the last grid point back to the first one.

The periodic forward shift matrix is

$$S_+^{per} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

The backward shift is

$$S_-^{per} = (S_+^{per})^T.$$

For a vector

$$u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix},$$

we now obtain

$$S_+^{per} u = \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ u_n \\ u_1 \end{pmatrix}.$$

The shift is therefore a true translation on the discrete periodic domain.

7.2 Periodic Difference Matrices

The same formulas as before can be used:

$$\boxed{D_{1,c}^{per} = \frac{1}{2h}(S_+^{per} - S_-^{per})}$$

and

$$\boxed{D_2^{per} = \frac{1}{h^2}(S_+^{per} - 2I + S_-^{per}).}$$

However, the resulting matrices are now circulant.
For example,

$$D_2^{per} = \frac{1}{h^2}\begin{pmatrix} -2 & 1 & 0 & \cdots & 1 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \ddots & 0 \\ \vdots & & \ddots & \ddots & 1 \\ 1 & 0 & 0 & 1 & -2 \end{pmatrix}.$$

The first and last grid points are now connected.

7.3 Circulant Structure

A periodic finite-difference matrix is a circulant matrix.
A circulant matrix has the form

$$C = \begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_{n-1} \\ c_{n-1} & c_0 & c_1 & \cdots & c_{n-2} \\ \vdots & & \ddots & & \vdots \\ c_1 & c_2 & \cdots & c_{n-1} & c_0 \end{pmatrix}.$$

Every row is obtained by a cyclic shift of the previous row.
This structure has a very important consequence:

$$\boxed{\text{Circulant matrices are diagonalized by Fourier modes.}}$$

7.4 Discrete Fourier Eigenvectors

Define the discrete Fourier vectors

$$v^{(k)} = \begin{pmatrix} 1 \\ e^{i\theta_k} \\ e^{2i\theta_k} \\ \vdots \\ e^{(n-1)i\theta_k} \end{pmatrix},$$

where

$$\theta_k = \frac{2\pi k}{n}.$$

For the periodic shift matrix,

$$S_+^{per} v^{(k)} = e^{i\theta_k} v^{(k)}.$$

Therefore,

$$\boxed{\lambda_k(S_+^{per}) = e^{i\theta_k}.}$$

The Fourier vectors are eigenvectors of the shift operator.

7.5 Eigenvalues of Difference Operators

Since the finite-difference matrices are constructed from the shifts, their eigenvalues follow immediately.

For the central difference matrix,

$$D_{1,c}^{per} = \frac{1}{2h}(S_+^{per} - S_-^{per}),$$

we obtain

$$\lambda_k(D_{1,c}^{per}) = \frac{1}{2h}\left(e^{i\theta_k} - e^{-i\theta_k}\right).$$

Using

$$e^{i\theta} - e^{-i\theta} = 2i\sin(\theta),$$

we find

$$\boxed{\lambda_k(D_{1,c}^{per}) = \frac{i}{h}\sin(\theta_k).}$$

Hence the eigenvalues are purely imaginary.

For the second derivative,

$$D_2^{per} = \frac{1}{h^2}(S_+^{per} - 2I + S_-^{per}),$$

we obtain

$$\lambda_k(D_2^{per}) = \frac{1}{h^2}(e^{i\theta_k} - 2 + e^{-i\theta_k}).$$

Therefore,

$$\boxed{\lambda_k(D_2^{per}) = -\frac{4}{h^2}\sin^2\left(\frac{\theta_k}{2}\right).}$$

All eigenvalues are real and non-positive.

7.6 MATLAB Example: Periodic Laplacian

The following code constructs a periodic second derivative matrix.

```
1
2  n = 50;
3
4  h = 1/n;
5
6  Sp = zeros(n);
7
8  for i=1:n-1
9      Sp(i,i+1)=1;
10 end
```

```
11
12  Sp(n,1)=1;
13
14  Sm = Sp';
15
16
17  D2per = (Sp-2*eye(n)+Sm)/h^2;
18
19
20  figure
21  spy(D2per)
22
23  title('Periodic second derivative matrix')
```

The sparsity pattern now shows the connection between the first and last grid points.

7.7 Connection with PDEs

For periodic PDEs, such as

$$u_t = u_{xx},$$

the semi-discrete approximation becomes

$$\frac{dU}{dt} = D_2^{per} U.$$

Because the matrix is diagonalized by Fourier modes, the solution can be analyzed mode by mode.

This provides the foundation of Fourier analysis of numerical PDE schemes.

7.8 Summary

The periodic case extends the shift-matrix framework:

$$\boxed{\text{Shift matrices} \rightarrow \text{Circulant matrices} \rightarrow \text{Fourier diagonalization}}$$

The main conclusions are:

$$\boxed{S_+^{per} \text{ has Fourier eigenvectors,}}$$

$$\boxed{D_{1,c}^{per} \text{ has imaginary eigenvalues,}}$$

and

$$\boxed{D_2^{per} \text{ has real negative eigenvalues.}}$$

This connection between shifts, finite differences, and Fourier analysis is one of the fundamental ideas behind the spectral analysis of numerical methods for PDEs.