Matrix Multiplication

CPS343

Parallel and High Performance Computing

Spring 2020

Outline

1. Matrix operations
   - Importance
   - Dense and sparse matrices
   - Matrices and arrays
2. Matrix-vector multiplication
   - Row-sweep algorithm
   - Column-sweep algorithm
3. Matrix-matrix multiplication
   - "Standard" algorithm
   - *ijk*-forms

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Definition of a matrix

- A *matrix* is a rectangular two-dimensional array of numbers.
- We say a matrix is $m \times n$ if it has m rows and n columns.
- These values are sometimes called the *dimensions* of the matrix.
- Note that, in contrast to Cartesian coordinates, we specify the number of rows (the vertical dimension) and then the number of columns (the horizontal dimension).
- In most contexts, the rows and columns are numbered starting with 1.
- Several programming APIs, however, index rows and columns from 0.
- We use a_{ij} to refer to the entry in i^{th} row and j^{th} column of the matrix A.

Matrices are extremely important in HPC

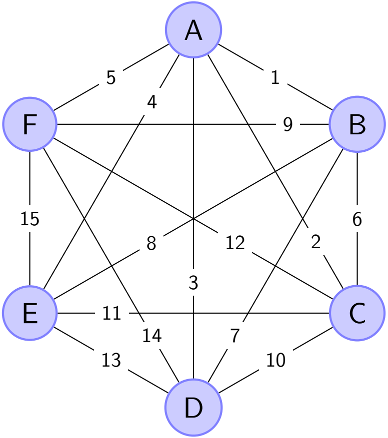
- While it's certainly not the case that high performance computing involves only computing with matrices, matrix operations are key to many important HPC applications.
- Many important applications can be "reduced" to operations on matrices, including (but not limited to)
  1. searching and sorting
  2. numerical simulation of physical processes
  3. optimization
- The list of the top 500 supercomputers in the world (found at `http://www.top500.org`) is determined by a benchmark program that performs matrix operations.
- Like most benchmark programs, this is just one measure, however, and does not predict the relative performance of a supercomputer on non-matrix problems, or even different matrix-based problems.

Outline

Dense matrices

- The $m \times n$ matrix A is *dense* if all or most of its entries are nonzero.
- Storing a dense matrix (sometimes called a *full* matrix) requires storing all mn elements of the matrix.
- Usually an array data structure is used to store a dense matrix.

Dense matrix example



Find a matrix to represent this complete graph if the ij entry contains the weight of the edge connecting node corresponding to row i with the node corresponding to column j. Use the value 0 if a connection is missing.

$$\begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 6 & 7 & 8 & 9 \\ 2 & 6 & 0 & 10 & 11 & 12 \\ 3 & 7 & 10 & 0 & 13 & 14 \\ 4 & 8 & 11 & 13 & 0 & 15 \\ 5 & 9 & 12 & 14 & 15 & 0 \end{bmatrix}$$

Dense matrix example

$$\begin{bmatrix} 0 & 1 & 2 & 3 & 4 & 5 \\ 1 & 0 & 6 & 7 & 8 & 9 \\ 2 & 6 & 0 & 10 & 11 & 12 \\ 3 & 7 & 10 & 0 & 13 & 14 \\ 4 & 8 & 11 & 13 & 0 & 15 \\ 5 & 9 & 12 & 14 & 15 & 0 \end{bmatrix}$$

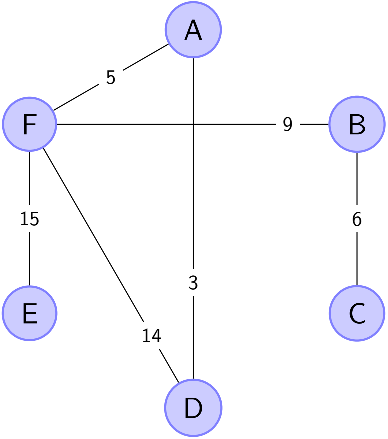
Note:

- This is considered a dense matrix even though it contains zeros.
- This matrix is *symmetric*, meaning that $a_{ij} = a_{ji}$.
- What would be a good way to store this matrix?

Sparse matrices

- A matrix is *sparse* if most of its entries are zero.
- Here "most" is not usually just a simple majority, rather we expect the number of zeros to far exceed the number of nonzeros.
- It is often most efficient to store only the nonzero entries of a sparse matrix, but this requires that location information also be stored.
- Arrays and lists are most commonly used to store sparse matrices.

Sparse matrix example



Find a matrix to represent this graph if the ij entry contains the weight of the edge connecting node corresponding to row i with the node corresponding to column j. As before, use the value 0 if a connection is missing.

$$\begin{bmatrix} 0 & 0 & 0 & 3 & 0 & 5 \\ 0 & 0 & 6 & 0 & 0 & 9 \\ 0 & 6 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 14 \\ 0 & 0 & 0 & 0 & 0 & 15 \\ 5 & 9 & 0 & 14 & 15 & 0 \end{bmatrix}$$

Sparse matrix example

Sometimes its helpful to leave out the zeros to better see the structure of the matrix

$$\begin{bmatrix} 0 & 0 & 0 & 3 & 0 & 5 \\ 0 & 0 & 6 & 0 & 0 & 9 \\ 0 & 6 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 0 & 14 \\ 0 & 0 & 0 & 0 & 0 & 15 \\ 5 & 9 & 0 & 14 & 15 & 0 \end{bmatrix} = \begin{bmatrix} & & & 3 & & 5 \\ & & 6 & & & 9 \\ & 6 & & & & \\ 3 & & & & & 14 \\ & & & & & 15 \\ 5 & 9 & & 14 & 15 & \end{bmatrix}$$

- This matrix is also symmetric.
- How could it be stored efficiently?

Banded matrices

- An important type of sparse matrices are *banded matrices*.
- Nonzeros are along diagonals close to main diagonal.
- Example:

$$\begin{bmatrix} 3 & 1 & 6 & 0 & 0 & 0 & 0 \\ 4 & 8 & 5 & 0 & 0 & 0 & 0 \\ 1 & 2 & 1 & 1 & 3 & 0 & 0 \\ 0 & 1 & 0 & 4 & 2 & 6 & 0 \\ 0 & 0 & 6 & 9 & 5 & 2 & 5 \\ 0 & 0 & 0 & 7 & 1 & 8 & 7 \\ 0 & 0 & 0 & 0 & 4 & 4 & 9 \end{bmatrix} = \begin{bmatrix} 3 & 1 & 6 & & & & \\ 4 & 8 & 5 & 0 & & & \\ 1 & 2 & 1 & 1 & 3 & & \\ & 1 & 0 & 4 & 2 & 6 & \\ & & 6 & 9 & 5 & 2 & 5 \\ & & & 7 & 1 & 8 & 7 \\ & & & & 4 & 4 & 9 \end{bmatrix}$$

- The *bandwidth* of this matrix is 5.

Outline

Using a two-dimensional arrays

It is natural to use a 2D array to store a dense or banded matrix. Unfortunately, there are a couple of significant issues that complicate this seemingly simple approach.

1. Row-major vs. column-major storage pattern is language dependent.
2. It is not possible to dynamically allocate two-dimensional arrays in C and C++; at least not without pointer storage and manipulation overhead.

Row-major storage

Both C and C++ (and Java and Python and ...) use what is often called a *row-major* storage pattern for 2D arrays.

- In C and C++, the last index in a multidimensional array indexes contiguous memory locations. Thus `a[i][j]` and `a[i][j+1]` are adjacent in memory.
- Example:

0	1	2	3	4
5	6	7	8	9

0	1	2	3	4	5	6	7	8	9

- The *stride* between adjacent elements in the same row is 1. The stride between adjacent elements in the same column is the row length (5 in this example).

Column-major storage

In contrast to this, Fortran stores 2D arrays in *column-major* form.

- The first index in a multidimensional array indexes contiguous memory locations. Thus `a(i,j)` and `a(i+1,j)` are adjacent in memory.
- Example:

0	1	2	3	4
5	6	7	8	9

0	5	1	6	2	7	3	8	4	9

- The stride between adjacent elements in the same row is the column length (2 in this example) while the stride between adjacent elements in the same column is 1.
- Notice that if C, Java, or Python is used to read a matrix stored in Fortran (or vice-versa), the *transpose* matrix will be read.

Significance of array ordering

There are two main reasons why HPC programmers need to be aware of this issue:

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1. Memory access patterns can have a dramatic impact on performance, especially on modern systems with a complicated memory hierarchy. These code segments access the same elements of an array, but the order of accesses is different.

Access by rows

```
for (i = 0; i < 2; i++)
  for (j = 0; j < 5; j++)
    a[i][j] = ...
```

Access by columns

```
for (j = 0; j < 5; j++)
  for (i = 0; i < 2; i++)
    a[i][j] = ...
```

Significance of array ordering

There are two main reasons why HPC programmers need to be aware of this issue:

1. Memory access patterns can have a dramatic impact on performance, especially on modern systems with a complicated memory hierarchy. These code segments access the same elements of an array, but the order of accesses is different.

   Access by rows

   ```
   for (i = 0; i < 2; i++)
     for (j = 0; j < 5; j++)
       a[i][j] = ...
   ```

   Access by columns

   ```
   for (j = 0; j < 5; j++)
     for (i = 0; i < 2; i++)
       a[i][j] = ...
   ```

2. Many important numerical libraries (e.g. LAPACK) are written in Fortran. To use them with row-major language the programmer must often work with a transposed matrix.

Outline

Row-sweep matrix-vector multiplication

Row-major matrix-vector product $\mathbf{y} = A\mathbf{x}$, where A is $M \times N$:

```
for (i = 0; i < M; i++)
{
    y[i] = 0.0;
    for (j = 0; j < N; j++)
    {
        y[i] += a[i][j] * x[j];
    }
}
```

- matrix elements accessed in row-major order
- repeated consecutive updates to `y[i]`...
- ...we can usually assume the compiler will optimize this
- also called *inner product form* since the i^{th} entry of $\mathbf{y}$ is the result of an inner product between the i^{th} row of A and the vector $\mathbf{x}$.

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Column-sweep matrix-vector multiplication

Column-major matrix-vector product $\mathbf{y} = A\mathbf{x}$, where A is $M \times N$:

```
for (i = 0; i < M; i++)
{
    y[i] = 0.0;
}

for (j = 0; j < N; j++)
{
    for (i = 0; i < M; i++)
    {
        y[i] += a[i][j] * x[j];
    }
}
```

- matrix elements accessed in column-major order
- repeated updates to `y[i]`, but every element in `y` array is updated before any element is updated again.
- also called *outer product form*.

Matrix-vector algorithm comparison

Which of these two algorithms will run faster? Why?

Row-Sweep Form

```
for (i = 0; i < M; i++)
{
  y[i] = 0.0;
  for (j = 0; j < N; j++)
  {
    y[i] += a[i][j] * x[j];
  }
}
```

Column-Sweep Form

```
for (i = 0; i < M; i++)
{
  y[i] = 0.0;
}

for (j = 0; j < N; j++)
{
  for (i = 0; i < M; i++)
  {
    y[i] += a[i][j] * x[j];
  }
}
```

Matrix-vector algorithm comparison

Answer: *it depends...*

- Both algorithms carry out the same operations, but do so in a different order.
- In particular, the memory access patterns are quite different.
- The row-sweep form will typically work better using a language like C or C++ which access 2D arrays in row-major form.
- Since Fortran accesses 2D arrays column-by-column, it is usually best to use the column-sweep form when working in that language.

Operation counts

- To compute the *computation rate* in FLOP/S, we need to know the number of FLOPs carried out and the elapsed time.
- Divisions are usually the most expensive of the four basic operations, followed by multiplication. Addition and subtraction are equivalent in terms of time and faster than multiplication or division.
- We usually count all four of these operations, but only when they involve floating point numbers. We typically ignore integer operations (e.g. array subscript calculations).
- In the case of a matrix-vector product, the innermost loop body contains a multiplication and an addition:

$$y_i = y_i + a_{ij}x_j$$

- The inner and outer loop are done M and N times respectively, so there are a total of $2MN$ FLOPs.

Outline

The textbook algorithm

Consider the problem of multiplying two matrices:

$$C = AB = \begin{bmatrix} 5 & 2 & 3 & 3 & 0 \\ 1 & 8 & 4 & 2 & 6 \\ 2 & 3 & 7 & 9 & 2 \end{bmatrix} \begin{bmatrix} 3 & 8 & 2 \\ 5 & 4 & 0 \\ 1 & 3 & 6 \\ 2 & 7 & 5 \\ 4 & 0 & 2 \end{bmatrix}$$

The standard "textbook" algorithm to form the product C of the $M \times P$ matrix A and the $P \times N$ matrix B is based on the inner product.

The c_{ij} entry in the product is the inner product (or *dot product*) of the i^{th} row of A and the j^{th} column of B.

The textbook algorithm

ijk-form Matrix-matrix product pseudocode:

```
for i = 1 to M
    for j = 1 to N
        c(i,j) = 0
        for k = 1 to P
            c(i,j) = c(i,j) + a(i,k) * b(k,j)
        end
    end
end
```

- known as the *ijk*-form of the product due to the loop ordering

The textbook algorithm

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```

- known as the *ijk*-form of the product due to the loop ordering
- What is the operation count. . . ?

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- What is the operation count. . . ?
- Number of FLOPs is $2MNP$.

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        end
    end
end
```

- known as the *ijk*-form of the product due to the loop ordering
- What is the operation count. . . ?
- Number of FLOPs is $2MNP$.
- For square matrices $M = N = P = n$ so number of FLOPs is $2n^3$.

The textbook algorithm

ijk-form Matrix-matrix product pseudocode:

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for i = 1 to M
    for j = 1 to N
        c(i,j) = 0
        for k = 1 to P
            c(i,j) = c(i,j) + a(i,k) * b(k,j)
        end
    end
end
```

- A is accessed row-by-row but B is accessed column-by-column.

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```

- A is accessed row-by-row but B is accessed column-by-column.
- The column index i for C varies faster than the row index j, but both of these are constant with respect to the inner loop. Compilers can easily optimize this.

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    end
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```

- A is accessed row-by-row but B is accessed column-by-column.
- The column index i for C varies faster than the row index j, but both of these are constant with respect to the inner loop. Compilers can easily optimize this.
- Regardless of the language we use (C or Fortran), we have an efficient access pattern for one matrix but not for the other.

The textbook algorithm

ijk-form Matrix-matrix product pseudocode:

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```

- A is accessed row-by-row but B is accessed column-by-column.
- The column index i for C varies faster than the row index j, but both of these are constant with respect to the inner loop. Compilers can easily optimize this.
- Regardless of the language we use (C or Fortran), we have an efficient access pattern for one matrix but not for the other.
- Can we improve things by rearranging the order of operations?

Outline

The *ijk* forms

From linear algebra we know that column i of the matrix-matrix product AB is defined as *"a linear combination of the columns of A using the values in the i^{th} column of B as weights."* The pseudocode for this is:

```
for j = 1 to N
    for i = 1 to M
        c(i,j) = 0.0
    end
    for k = 1 to P
        for i = 1 to M
            c(i,j) = c(i,j) + a(i,k) * b(k,j)
        end
    end
end
```

- the loop ordering changes but the innermost statement is unchanged
- the initialization of values in C is done one column at a time
- the operation count is still $2MNP$. This is the *jki* form.

The *ijk* forms

Other loop orderings are possible. . .

The *ijk* forms

Other loop orderings are possible...

How many ways can i, j, and k be arranged?

The *ijk* forms

Other loop orderings are possible. . .

How many ways can i, j, and k be arranged?

- Recall from discrete math that this is a *permutation* problem.
- "three ways to choose the first letter, two ways to choose the second, and one way to choose the third": $3 \times 2 \times 1 = 6$
- There are six possible loop orderings.
- We'll work with all six during our first hands-on exercise ☺.