Matrices

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Matrices

- Major topic in mathematics
- Very important in numerical computation
- Illustrate some of the limitations of current technology
- Show where we should not use simplify assumptions such as all memory is random access

Definitions

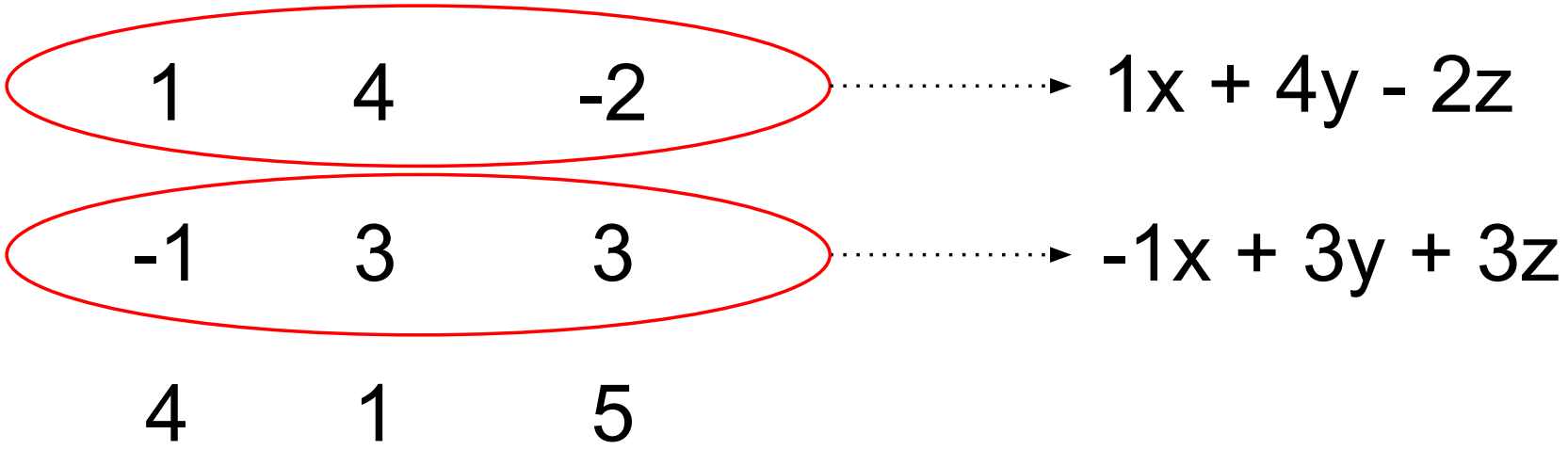
A matrix is a 2D table of numbers (rows, columns)

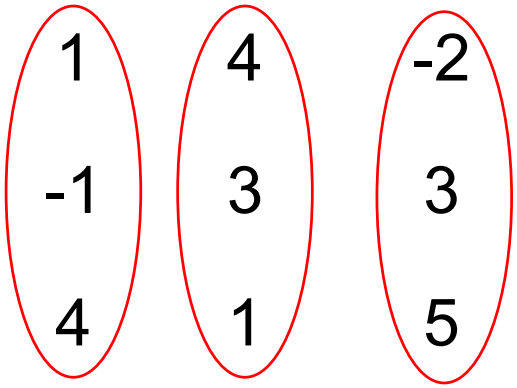
Matrices can be thought of in a number of ways

- A set of rows each representing the coefficients of a linear equation
- A set of columns each representing an n-dimensional vector

$$\begin{pmatrix} 1 & 4 & -2 \\ 2 & 9 & 2 \\ 3 & -2 & 1 \end{pmatrix}$$

Two ways of Looking at Matrices





Matrix Type

A square matrix is a matrix where the number of rows and columns are equal

The main diagonal is the locations in the matrix where row = column

The identity matrix has all zeros except for ones down the main diagonal

Example:

1	0	0	0
0	1	0	0
0	0	1	0
0	0	0	1

Identity Matrix

In an Algebra, there must exist an identity element such that

$$Ix = xI = x$$

For scalars this is the number 1. For matrices it is the identity matrix:

$$I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$ The same definition will apply, but in order to understand it we must define matrix multiplication

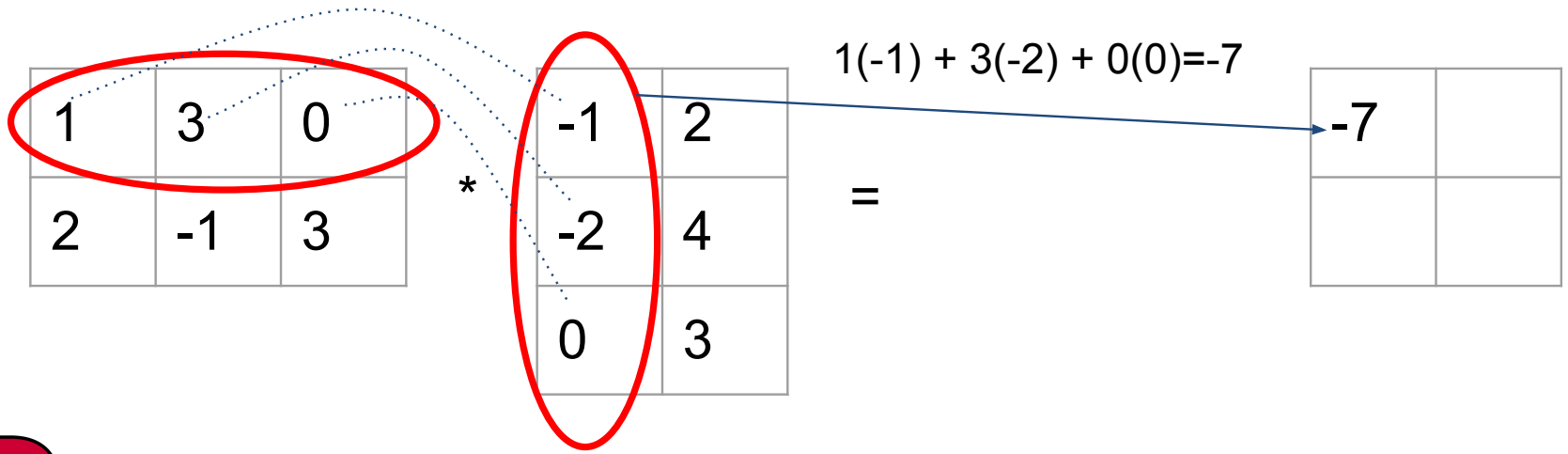
Matrix Multiplication

Matrix multiplication is defined on two matrices of size

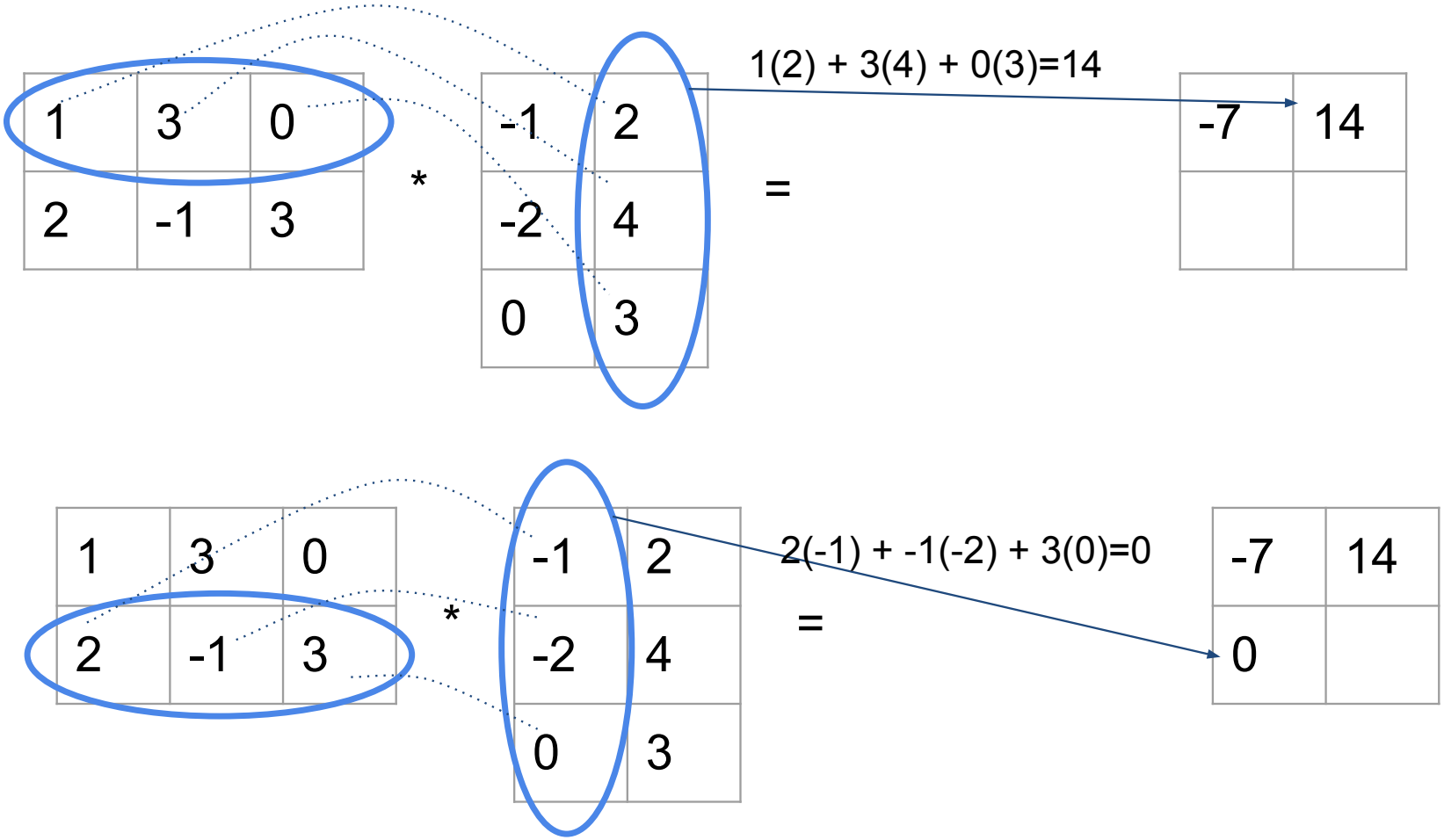
- m rows x n columns
- n rows x p columns

Notice that the columns(A) = rows(B)

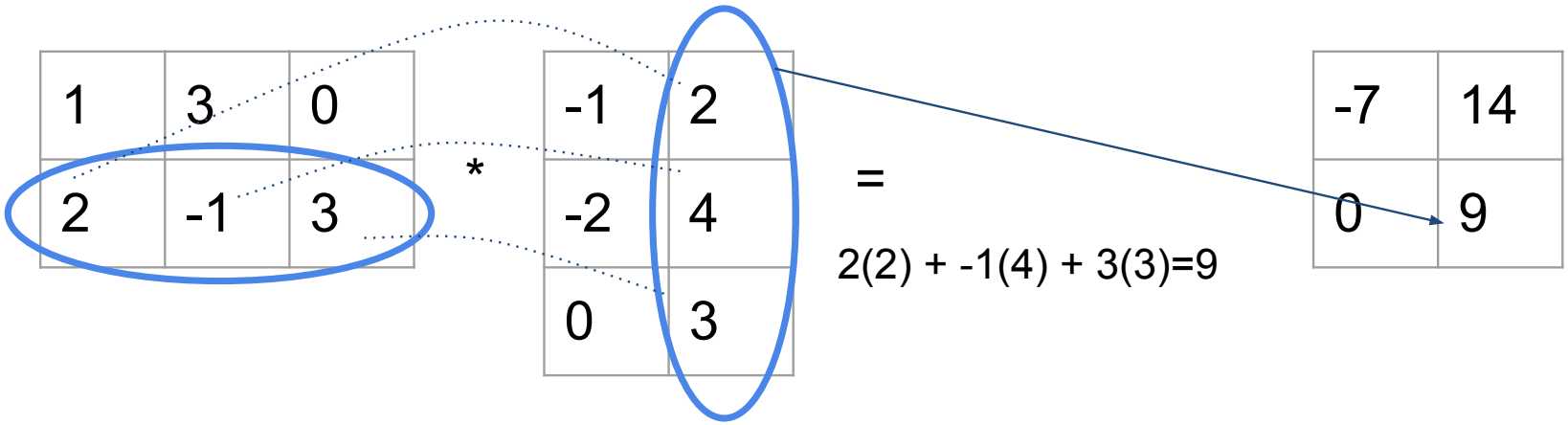
Each element of the answer C_{jk} is the dot product of a row(A) column(B)



Matrix Multiplication, contd



Matrix Multiplication, done!



Inverse

The inverse of a matrix A^{-1} is a matrix such that
$AA^{-1} = A^{-1}A = I$
With scalars, only the number 0 has no inverse.
Many matrices are singular matrix and have no inverse

Example: $\begin{matrix} 1 & -2 \\ -3 & 6 \end{matrix}$

Matrix Multiplication Pseudocode

```
for i ← 0 to m−1
  for j ← 0 to p−1
    dot ← 0                          // dot product of A_i * B_j \\
    for k ← 0 to n−1
      dot ← dot + A_ik B_kj
    end
    C_ij ← dot
  end
```

Matrix Multiplication is not Commutative

With scalars $AB = BA$

Example: $2 * 3 = 3 * 2$

With matrices, not only is AB $\neq$ BA, they are not even the same dimension

Example (let's use octave to see this)

$$A = \begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$$

$$A = 1 \quad 2 \quad 3$$

$$B = \begin{bmatrix} 1; 2; 3; \end{bmatrix}$$

$$B = \begin{matrix} 1 \\ 2 \\ 3 \end{matrix}$$

$$A * B = 14$$

$$B * A = \begin{matrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 6 & 9 \end{matrix}$$

Complexity of Matrix Multiplication

$(m \times n) * (n \times p) \rightarrow (m \times p)$

Each element of the answer is the dot product of n elements $\rightarrow O(mnp)$

If $m = n = p$ then $O(n^3)$

Everything interesting in matrices is $O(n^3)$

In fact, just to read every element of a matrix of size $n \times n$ is $O(n^2)$

Faster Matrix Multiplication

It turns out that while the brute force matrix multiplication is $O(n^3)$ there is a cleverer way to beat that

It is not that useful in practice, but it points to a general pattern

Brute force algorithm $O(n^2)$ (sorting) $\rightarrow$ O(n log n) (quicksort, heapsort, mergesort)

Many things that seem to be $O(n^2)$ can be done faster

- Multiplication of two n-digit numbers
- Fourier Transform

Strassen: Faster Multiplication

In 1969 Volker Strassen derived an algorithm equivalent to matrix multiplication, but faster

Consider a matrix in which both dimensions are a power of 2

- Each matrix can be broken up into quarters
- The relationship between the quarters is as shown

$$C_{11} = A_{11}B_{11} + A_{12}B_{21}$$
$$C_{12} = A_{11}B_{12} + A_{12}B_{22}$$

Notice, there are 8 multiplications

Each is $(\frac{1}{2})(\frac{1}{2})(\frac{1}{2}) = \frac{1}{8}$ the size

Complexity is the same as the original problem

Strassen, continued

The genius of Strassen's solution was in figuring out how to combine terms and do less computation

$$M_1 = (A_{11} + A_{22})(B_{11} + B_{22})$$
$$M_2 = (A_{21} + A_{22})B_{11}$$
$$M_3 = A_{11}(B_{12} - B_{22})$$

7 multiplications $= (\frac{7}{8}n)^3$

18 additions $= 18n^2$

$O(2^{\log 7}) = O(n^{2.8074})$

$$M_4 = A_{22}(B_{21} - B_{11})$$
$$M_5 = (A_{11} + A_{12})B_{22}$$
$$M_6 = (A_{21} - A_{11})(B_{11} + B_{12})$$
$$M_7 = (A_{12} - A_{22})(B_{21} + B_{22})$$

$$C_{11} = M_1 + M_4 - M_5 + M_7$$
$$C_{12} = M_3 + M_5$$
$$C_{21} = M_2 + M_4$$
$$C_{22} = M_1 - M_2 + M_3 + M_6$$

Practical Applications

Strassen is important theoretically

- It means it is possible to multiply matrices in less than $O(n^3)$
- Strassen is $O(n^{2.807})$
- Others have followed: Coppersmith-Winograd $O(n^{2.36})$
- None are very practical for most cases
    - Require copying and reordering that are slow (faster with very large matrices)
    - Numerical results become less stable (see later chapter on numerical methods)

In practice faster methods are not used, but the idea that $O(n^3)$ algorithms can be faster is important

Matrix Addition

Matrix addition requires two matrices with the same number of rows and columns

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & -1 & 1 \end{pmatrix} + \begin{pmatrix} 3 & 0 & -1 \\ 1 & -2 & -3 \end{pmatrix} = \begin{pmatrix} 4 & 2 & 2 \\ 3 & -3 & -2 \end{pmatrix}$$

It results in a matrix where each element is the sum of the corresponding element in the other two

Solving Systems of Linear Equations

In high school, you learned to solve systems of linear equations

$$\begin{aligned} x + 2y + z &= 4 \\ 3x + 2y - z &= 15 \\ -x + y + 2z &= 5 \end{aligned}$$

1	2	1	4
3	2	-1	15
-1	1	2	5

You might have been taught to do this either by

- substitution (figure out what z is and replace it)
- add/subtract equations from each other (row reduction)

Row reduction works better as the problems scale up. Neither solution is numerically stable without help

How did they do it in high school? They cheated

The methods taught in high school for solving systems of linear equations do not work in general

- So how did they make it work? They cheated
- The analogy is to shoot a hole in a wall, then paint the bullseye around it
- Perfect shot! You are an expert marksman

1. Pick a set of answers at random: x=3, y = 4, z = 2
2. Pick a random set of coefficients (must be linearly independent, more later)
   $x + 2y + z =$
   $3x + 2y - z =$
   $-x + y + 2z =$

How did they do it in high school (contd)

Compute the answers. You now know that there is a perfect solution to this problem

$$\begin{aligned} x + 2y + z = &\quad 3 + 2(4) + 2 &&= 13 \\ 3x + 2y - z = &\quad 3(3) + 2(4) - 2 &&= 15 \\ -x + y + 2z = &\quad -3 + 4 + 2(2) &&= 5 \end{aligned}$$

Error Conditions with Systems of Linear Equations

For Solving a set of linear equations

- No row may be zero (undetermined)
- **There must be as many rows as columns (n equations, n unknowns)**
- Each row must be linearly independent from the others
- Each column must contain some information

Not enough equations

$$3x + 2y + z = 5$$
$$4x - y + 3z = 7$$

Error Conditions with Systems of Linear Equations

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Too many equations (overdetermined)

$$3x + 2y + z = 5$$
$$4x - y + 3z = 7$$
$$2x + 3y - 4z = 11$$
$$x - 4y + 2z = 5$$

Error Conditions with Systems of Linear Equations, case 2

For Solving a set of linear equations

- No row may be zero (undetermined)
- There must be as many rows as columns (n equations, n unknowns)
- **Each row must be linearly independent from the others**
- Each column must contain some information

Equations are not linearly independent

$$4x + 2y + z = 5$$
$$2x + y + 1/2z = 6$$
$$x - 3y + 4z = 19$$

Error Conditions with Systems of Linear Equations, case 2

For Solving a set of linear equations

- No row may be zero (undetermined)
- There must be as many rows as columns (n equations, n unknowns)
- Each row must be linearly independent from the others
- **Each column must contain some information**

One variable is not used at all

$$4x + 0y + z = 5$$
$$2x + 0y + 1/2z = 6$$
$$x - 0y + 4z = 19$$

Solving a System of Linear Equations with Row Reduction

Row Reduction, called Gauss-Jordan (yes, that Gauss!)

Augment the matrix with one extra column (the answers)

Reduce to a upper-triangular form by multiplying each row by a constant

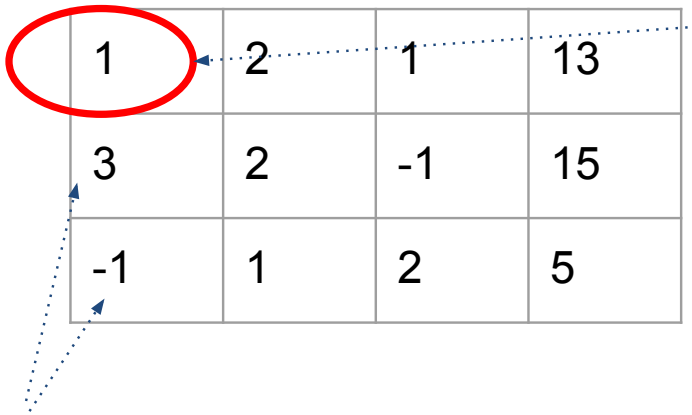
Add to the other row to zero out specific values

Back-propagate to solve the variables

$$\begin{bmatrix} 1 & 2 & 1 \\ 3 & 2 & -1 \\ -1 & 1 & 2 \end{bmatrix} * \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 13 \\ 15 \\ 5 \end{bmatrix}$$

Row Reduction, part 2

- Augment the matrix with one extra column (the answers)
- For the first column, use the top element to zero out the others



$$s = 1$$

$$s * r + 3 = 0 \quad \leftarrow -3$$

$$s * r + (-1) = 0r \leftarrow 1$$

Row Reduction, part 3

Multiply the first row by -3 and add it to the second row: n+1 = O(n)

1	2	1	13
3	2	-1	15
-1	1	2	5

1	2	1	13
0	-4	-4	-24
-1	1	2	5

Row Reduction, part 3

Multiply the first row by 1 and add it to the third row

1	2	1	13
3	2	-1	15
-1	1	2	5

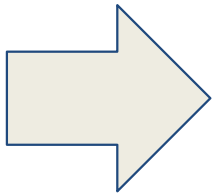
1	2	1	4
0	-4	-4	-24
0	3	3	9

Complexity: $n * (n-1) = \theta(n^2)$

Row Reduction, part 4

Repeat for the second column

1	2	1	13
0	-4	-4	-24
0	3	3	9



1	2	1	13
0	-4	-4	-24
0	**0**	0	11.25

Complexity: $n * (n-1) = \Theta(n^2)$

r=-3/-4=.75
-4*.75 + 3 → 0
3*.75+9 → 11 1/4

Oops!

Complexity

For this small example, that's all the row reduction, but in general

$$n(n-1) + (n-1)(n-2) + ... + (2)(1) = O(n^3)$$

The system is not yet solved. It must be back-propagated

Ill-Conditioned Systems

A system that has all zeros on one row, or two rows that are linearly dependent cannot be solved

The Unpleasant Reality: Matrices are Hard

It is extremely easy to get an ill conditioned matrix just by row reduction

This happens when a pivot value is too small Example:

$$\begin{pmatrix} .001 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 5 & -1 \end{pmatrix} \rightarrow \begin{pmatrix} .001 & 2 & 3 \\ 0 & -1997 & -2998 \\ 2 & 5 & -1 \end{pmatrix}$$

$row2 = row2 - 1000 * row1$ The resulting matrix is ill conditioned

Making Matrices More Stable: Partial Pivoting

In order to maximize the stability, use the biggest number
Swap rows until the biggest number is on top

Example: $\begin{pmatrix} .001 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 5 & -1 \end{pmatrix} \rightarrow \begin{pmatrix} 2 & 5 & -1 \\ 1 & 3 & 2 \\ .001 & 2 & 3 \end{pmatrix}$

Now, instead of multiplying by -1000, the coefficients are -0.5 and -0.0005

$$\begin{pmatrix} 2 & 5 & -1 \\ 0 & 0.5 & 2.5 \\ 0 & 1.9995 & 3.0005 \end{pmatrix}$$

Making Matrices More Stable: Full Pivoting

For even greater stability, at a cost in bookkeeping
Find the largest value in the matrix
Swap rows *and columns* to get the value with the largest absolute value to top-left

Example: $\begin{pmatrix} .001 & 2 & 3 \\ 1 & 3 & 2 \\ 2 & 5 & -1 \end{pmatrix} \rightarrow \begin{pmatrix} 5 & 2 & -1 \\ 3 & 1 & 2 \\ 2 & .001 & 3 \end{pmatrix}$

However, now you must track which columns have been transposed
This can be done by augmenting the matrix with a new first row of length n Each element stores the position of the variable in that column

Complexity of Partial and Full Pivoting

1. Reducing a row $O(n)$
2. Reducing n rows $O(n^2)$. This zeros one column
3. Reducing n columns $O(n^3)$
4. Finding largest value in a column $O(n)$
5. Doing that for n columns (Partial Pivoting) $O(n^2)$

Gram-Schmidt Process

Gram Schmidt orthogonalization is an algorithm to make a matrix orthonormal

1. Each column vector becomes normal (unit length)
2. Each column vector is perpendicular to the others (orthogonal)

$$\begin{pmatrix} 5 & 2 & -1 \\ 3 & 1 & 2 \\ 2 & .001 & 3 \end{pmatrix}$$

Gram-Schmidt Complexity

1. To calculate the length of a vector is O(n)
2. To divide every element by that length is O(n)
3. To subtract the component of one vector in the direction of another is O(n)
4. $n + 2n + 3n + ..n^2 = O(n^3)$

Representation of Matrices

There are two ways

- Single block of contiguous memory
- Array of pointers

Row Major vs. Column Major Order

Indexing Equation for Row and Column Major Matrices

Impact of Sequential vs. Non-Sequential Memory Access

Normally in algorithms we don't worry about machine specifics

But in the case of matrices, memory order has a significant impact

Sparse Matrices

A sparse matrix is one where most of the elements are zero
An encoding scheme is needed to encode the non-zero elements
A general sparse matrix is not particularly common
Instead, we will deal with specific shapes

- Upper and Lower triangular matrices
- Diagonal matrices
- Tridiagonal matrices

Upper Triangular Matrices

In an upper-triangular matrix, all elements below the main diagonal are zero

This means:

- The first row has n elements
- The second row has n-1 elements
- The last row has 1 element

*	*	*	*	*
0	*	*	*	*
0	0	*	*	*
0	0	0	*	*
0	0	0	0	*

Lower Triangular Matrices

In a lower-triangular matrix, all elements above the main diagonal are zero

This means:

- The first row has 1 element
- The second row has 2 elements
- The last row has n elements

*	0	0	0	0
*	*	0	0	0
*	*	*	0	0
*	*	*	*	0
*	*	*	*	*

Diagonal Matrices

A Diagonal Matrix has non-zero elements only on the main diagonal

Because of this storage is only O(n)

Complexity of matrix multiplication is also O(n)

*	0	0	0	0
0	*	0	0	0
0	0	*	0	0
0	0	0	*	0
0	0	0	0	*

Applications of Diagonal Matrices

Calculating An for a matrix is quite expensive
$A * A$ is $O(n^3)$
Brute force would be $O(n^4)$

- We can do a lot better with number-theoretic algorithms, covered later
- The main problem is that multiplication is so expensive

However, if you could just decompose the matrix into three pieces:

$A = PDP^{-1}$ (this is called an EigenValue decomposition, $O(n^3)$)

where D is a diagonal matrix, then A^n can be computed as
$A = PD^nP^{-1}$ D^n is $O(n)$

Tridiagonal Matrices

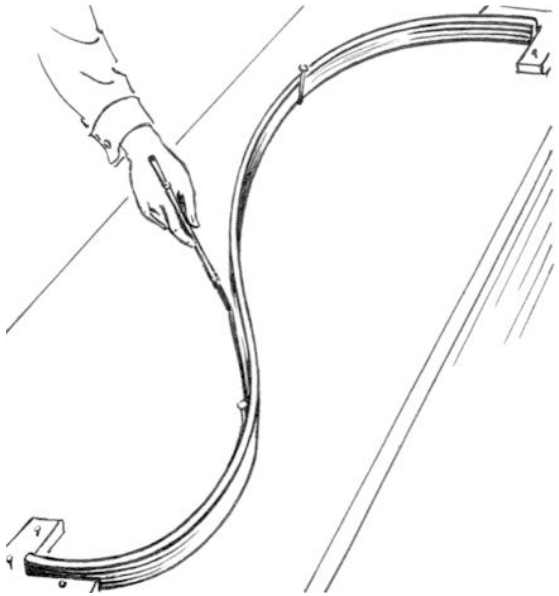
A Tridiagonal Matrix has non-zero elements on the main diagonal and one on each side

*	*	0	0	0
*	*	*	0	0
0	*	*	*	0
0	0	*	*	*
0	0	0	*	*

Applications of Tridiagonal Matrices: Numerical Splines

A spline was originally a thin strip of wood used to create smooth curves

- Used to create the shape for optimal boat hulls that have less drag (laminar flow)
- The thin wood means that the curvature is constant (2nd derivative is constant)



Applications of Tridiagonal Matrices: Numerical Splines, contd.

Once computers began to be used to design objects, question is how to simulate a spline?