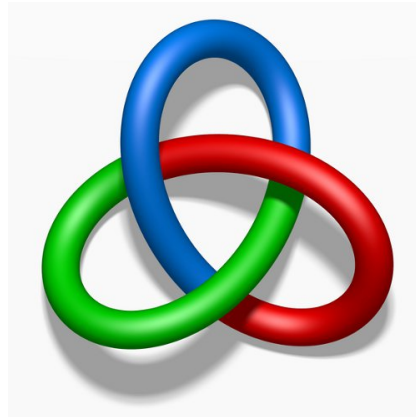


9. Scientific Computing



Applications of Scientific Computing

Science and engineering challenges.

- Fluid dynamics.
- Seismic surveys.
- Plasma dynamics.
- Ocean circulation.
- Electronics design.
- Pharmaceutical design.
- Human genome project.
- Vehicle crash simulation.
- Global climate simulation.
- Nuclear weapons simulation.
- Molecular dynamics simulation.

Commercial applications.

- Web search.
- Financial modeling.
- Computer graphics.
- Digital audio and video.
- Architecture walk-throughs.
- Natural language processing.
- Medical diagnostics (MRI, CAT).

Common features.

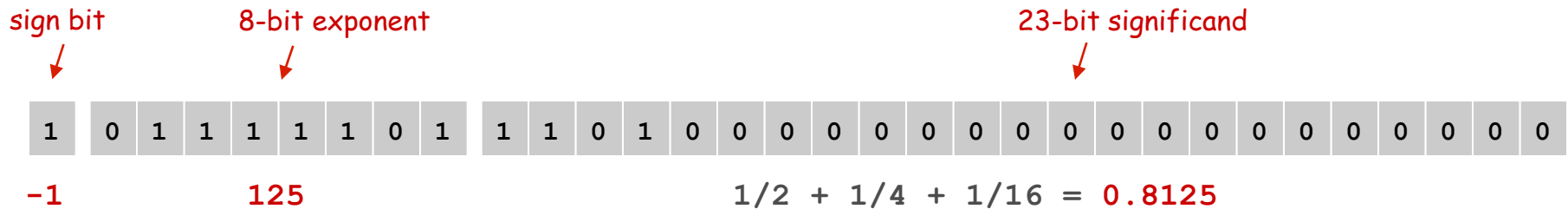
- Problems tend to be **continuous** instead of discrete.
- Algorithms must **scale** to handle huge problems.

Floating Point

IEEE 754 representation.

- Used by all modern computers.
- Scientific notation, but in binary.
- Single precision: `float` = 32 bits.
- Double precision: `double` = 64 bits.

Ex. Single precision representation of -0.453125 .



$$-1 \times 2^{\text{bias} - 127} \times 1.\text{phantom bit}8125 = -0.453125$$

Floating Point

Remark. Most real numbers are not representable, including π and $1/10$.

Roundoff error. When result of calculation is not representable.

Consequence. Non-intuitive behavior for uninitialized.

```
if (0.1 + 0.2 == 0.3) { /* false */ }  
if (0.1 + 0.3 == 0.4) { /* true  */ }
```

Financial computing. Calculate 9% sales tax on a 50¢ phone call.

Banker's rounding. Round to nearest integer, to even integer if tie.

```
double a1 = 1.14 * 75;      // 85.49999999999999  
double a2 = Math.round(a1); // 85 ← you lost 1¢  
  
double b1 = 1.09 * 50;      // 54.50000000000001  
double b2 = Math.round(b1); // 55 ← SEC violation (!)
```

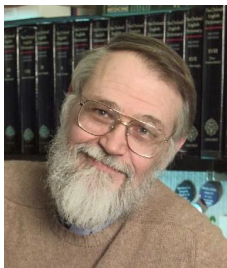
Floating Point

Remark. Most real numbers are not representable, including π and $1/10$.

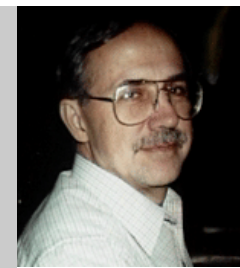
Roundoff error. When result of calculation is not representable.

Consequence. Non-intuitive behavior for uninitialized.

```
if (0.1 + 0.2 == 0.3) { /* false */ }  
if (0.1 + 0.3 == 0.4) { /* true  */ }
```



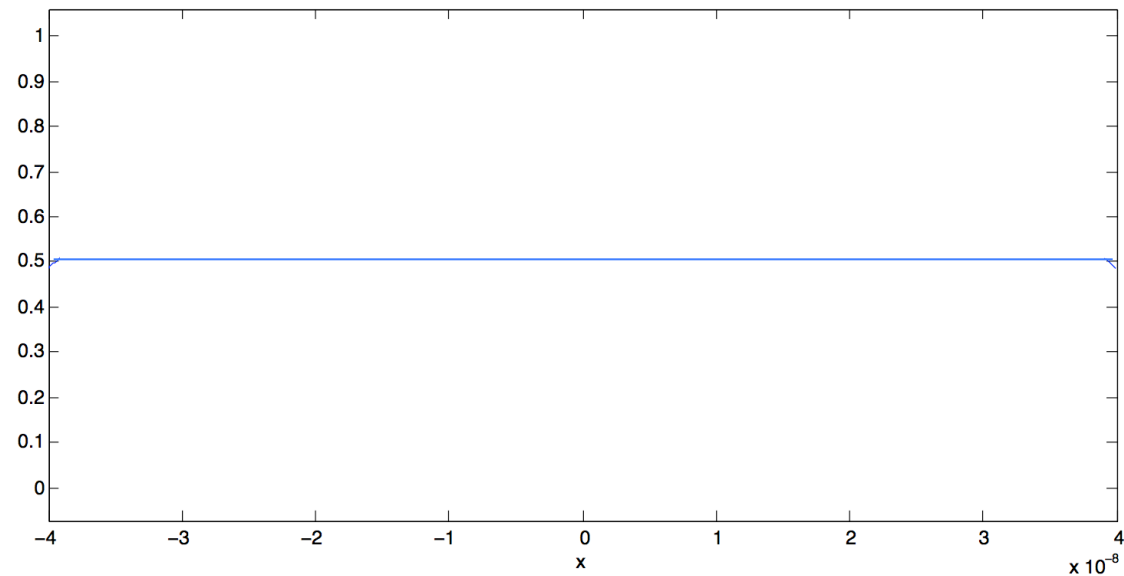
“ Floating point numbers are like piles of sand; every time you move them around, you lose a little sand and pick up a little dirt. ” — Brian Kernighan and P. J. Plauger



Catastrophic Cancellation

A simple function. $f(x) = \frac{1 - \cos x}{x^2}$

Goal. Plot $f(x)$ for $-4 \cdot 10^{-8} \leq x \leq 4 \cdot 10^{-8}$.

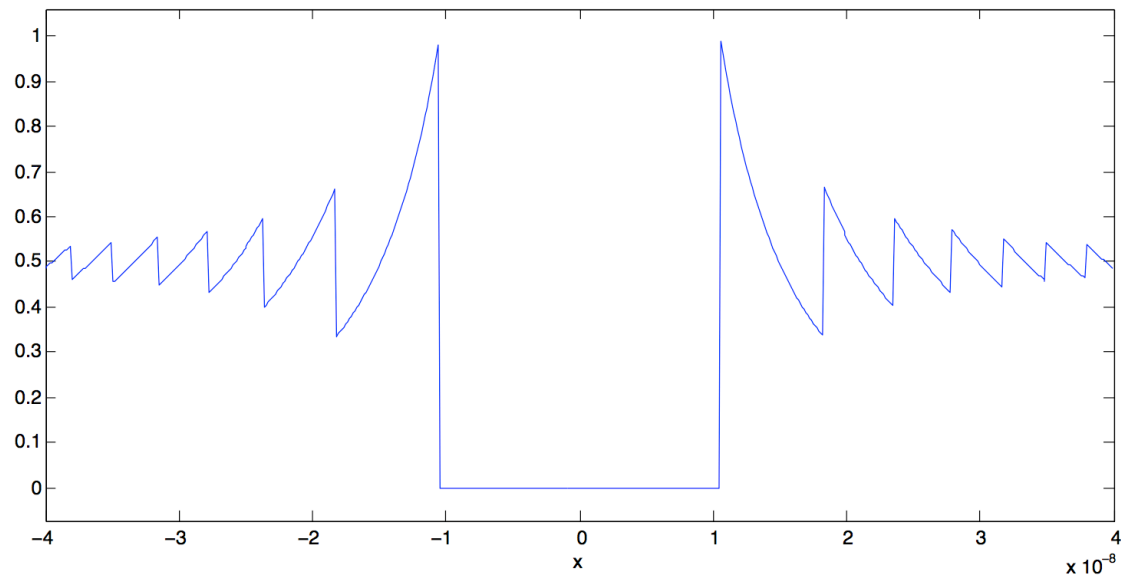


Exact answer

Catastrophic Cancellation

A simple function. $f(x) = \frac{1 - \cos x}{x^2}$

Goal. Plot $f(x)$ for $-4 \cdot 10^{-8} \leq x \leq 4 \cdot 10^{-8}$.



IEEE 754 double precision answer

Catastrophic Cancellation

```
public static double fl(double x) {  
    return (1.0 - Math.cos(x)) / (x*x);  
}
```

Ex. Evaluate $f_1(x)$ for $x = 1.1e-8$.

▪ $\text{Math.cos}(x) = 0.9999999999999999888897769753748434595763683319091796875.$

← nearest floating point value agrees with exact answer to 16 decimal places.

▪ $(1.0 - \text{Math.cos}(x)) = 1.1102e-16$

← inaccurate estimate of exact answer ($6.05 \cdot 10^{-17}$)

▪ $(1.0 - \text{Math.cos}(x)) / (x*x) = 0.9175$

← 80% larger than exact answer (about 0.5)

Catastrophic cancellation. Devastating loss of precision when small numbers are computed from large numbers, which themselves are subject to roundoff error.

Numerical Catastrophes

Ariane 5 rocket. [June 4, 1996]

- 10 year, \$7 billion ESA project exploded after launch.
- 64-bit float converted to 16 bit signed int.
- Unanticipated overflow.



Copyright, Arianespace

Vancouver stock exchange. [November, 1983]

- Index undervalued by 44%.
- Recalculated index after each trade by adding **change** in price.
- 22 months of accumulated truncation error.

Patriot missile accident. [February 25, 1991]


- Failed to track scud; hit Army barracks, killed 28.
- Inaccuracy in measuring time in 1/20 of a second since using 24 bit binary floating point.



War Story


Bugs. Java Virtual Machine and compiler struggle with 2^{-1022} .

Double.MIN_NORMAL



```
public class RuntimeHang {  
    public static void main(String[] args) {  
        double d = Double.parseDouble("2.2250738585072012e-308");  
        System.out.println(d);  
    }  
}
```

should be converted to 2^{-1022}



```
public class CompileHang {  
    public static void main(String[] args) {  
        double d = 2.2250738585072012e-308;  
        System.out.println(d);  
    }  
}
```

Bugs identified and fixed. February, 2011.

<http://www.exploringbinary.com/java-hangs-when-converting-2-2250738585072012e-308>

Gaussian Elimination

$$Ax = b$$

Linear System of Equations

Linear system of equations. N linear equations in N unknowns.

$$\begin{array}{rclcl} 0x_0 & + & 1x_1 & + & 1x_2 & = & 4 \\ 2x_0 & + & 4x_1 & - & 2x_2 & = & 2 \\ 0x_0 & + & 3x_1 & + & 15x_2 & = & 36 \end{array}$$

$$A = \begin{bmatrix} 0 & 1 & 1 \\ 2 & 4 & -2 \\ 0 & 3 & 15 \end{bmatrix}, \quad b = \begin{bmatrix} 4 \\ 2 \\ 36 \end{bmatrix}$$

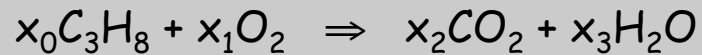
matrix notation: find x such that $Ax = b$

Fundamental problems in science and engineering.

- Chemical equilibrium.
- Linear and nonlinear optimization.
- Kirchoff's current and voltage laws.
- Hooke's law for finite element methods.
- Leontief's model of economic equilibrium.
- Numerical solutions to differential equations.
- ...

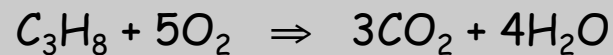
Chemical Equilibrium

Ex. Combustion of propane.



Stoichiometric constraints.

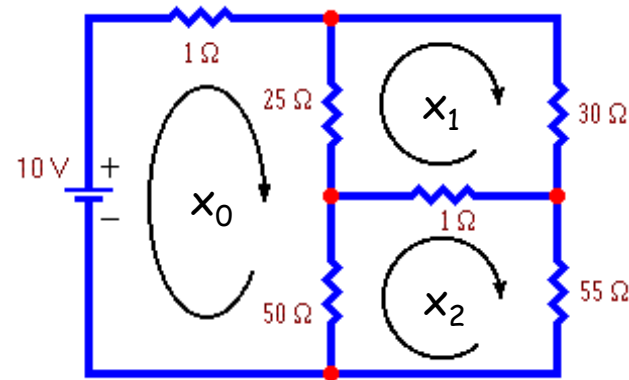
- Carbon: $3x_0 = x_2.$
 - Hydrogen: $8x_0 = 2x_3.$
 - Oxygen: $2x_1 = 2x_2 + x_3.$
 - Normalize: $x_0 = 1.$
- } conservation of mass



Remark. Stoichiometric coefficients tend to be small integers; among first hints suggesting the atomic nature of matter.

Kirchoff's Current Law

Ex. Find current flowing in each branch of a circuit.



Kirchoff's current law.

- $10 = 1x_0 + 25(x_0 - x_1) + 50(x_0 - x_2).$
 - $0 = 25(x_1 - x_0) + 30x_1 + 1(x_1 - x_2).$
 - $0 = 50(x_2 - x_0) + 1(x_2 - x_1) + 55x_2.$
- } conservation of electrical charge

Solution. $x_0 = 0.2449$, $x_1 = 0.1114$, $x_2 = 0.1166.$

Upper Triangular System of Equations

Upper triangular system. $a_{ij} = 0$ for $i > j$.

$$\begin{array}{rclcl} 2x_0 & + & 4x_1 & - & 2x_2 & = & 2 \\ 0x_0 & + & 1x_1 & + & 1x_2 & = & 4 \\ 0x_0 & + & 0x_1 & + & 12x_2 & = & 24 \end{array}$$

Back substitution. Solve by examining equations in reverse order.

- Equation 2: $x_2 = 24/12 = 2$.
- Equation 1: $x_1 = 4 - x_2 = 2$.
- Equation 0: $x_0 = (2 - 4x_1 + 2x_2) / 2 = -1$.

```
for (int i = N-1; i >= 0; i--) {
    double sum = 0.0;
    for (int j = i+1; j < N; j++)
        sum += A[i][j] * x[j];
    x[i] = (b[i] - sum) / A[i][i];
}
```

$$x_i = \frac{1}{a_{ii}} \left[b_i - \sum_{j=i+1}^{N-1} a_{ij} x_j \right]$$

Gaussian Elimination

Gaussian elimination.

- Among oldest and most widely used solutions.
- Repeatedly apply **row operations** to make system upper triangular.
- Solve upper triangular system by back substitution.

Elementary row operations.

- Exchange row p and row q.
- Add a multiple α of row p to row q.



Key invariant. Row operations preserve solutions.

Gaussian Elimination: Row Operations

Elementary row operations.

$$\begin{array}{rclcrcl} 0x_0 & + & 1x_1 & + & 1x_2 & = & 4 \\ 2x_0 & + & 4x_1 & - & 2x_2 & = & 2 \\ 0x_0 & + & 3x_1 & + & 15x_2 & = & 36 \end{array}$$

↓ (interchange row 0 and 1)

$$\begin{array}{rclcrcl} 2x_0 & + & 4x_1 & - & 2x_2 & = & 2 \\ 0x_0 & + & 1x_1 & + & 1x_2 & = & 4 \\ 0x_0 & + & 3x_1 & + & 15x_2 & = & 36 \end{array}$$

↓ (subtract 3x row 1 from row 2)

$$\begin{array}{rclcrcl} 2x_0 & + & 4x_1 & - & 2x_2 & = & 2 \\ 0x_0 & + & 1x_1 & + & 1x_2 & = & 4 \\ 0x_0 & + & 0x_1 & + & 12x_2 & = & 24 \end{array}$$

Gaussian Elimination: Forward Elimination

Forward elimination. Apply row operations to make upper triangular.

Pivot. Zero out entries below pivot a_{pp} .

$$a_{ij} = a_{ij} - \frac{a_{ip}}{a_{pp}} a_{pj}$$
$$b_i = b_i - \frac{a_{ip}}{a_{pp}} b_p$$

The diagram illustrates the forward elimination step. On the left, a matrix is shown with a pivot element at row p , column p , highlighted with a blue circle. The matrix is represented as a grid of elements, with the pivot element at the intersection of row p and column p . An arrow points to the right, where the matrix is shown after the elimination step. The pivot element remains, but the entries below it in the p -th column are now zero, highlighted with a blue vertical bar.

```
for (int p = 0; p < N; p++) {  
    for (int i = p + 1; i < N; i++) {  
        double alpha = A[i][p] / A[p][p];  
        b[i] -= alpha * b[p];  
        for (int j = p; j < N; j++)  
            A[i][j] -= alpha * A[p][j];  
    }  
}
```

Gaussian Elimination: Forward Elimination

Forward elimination. Apply row operations to make upper triangular.

Pivot. Zero out entries below pivot a_{pp} .

$$\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \Rightarrow \begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \\ 0 & * & * & * & * \end{bmatrix} \Rightarrow \begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & * & * & * \end{bmatrix} \Rightarrow \begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & * & * \end{bmatrix} \Rightarrow \begin{bmatrix} * & * & * & * & * \\ 0 & * & * & * & * \\ 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * \\ 0 & 0 & 0 & 0 & * \end{bmatrix}$$

```
for (int p = 0; p < N; p++) {
    for (int i = p + 1; i < N; i++) {
        double alpha = A[i][p] / A[p][p];
        b[i] -= alpha * b[p];
        for (int j = p; j < N; j++)
            A[i][j] -= alpha * A[p][j];
    }
}
```

Gaussian Elimination Example

$$\begin{array}{rcccccc} 1 x_0 & + & 0 x_1 & + & 1 x_2 & + & 4 x_3 & = & 1 \\ 2 x_0 & + & -1 x_1 & + & 1 x_2 & + & 7 x_3 & = & 2 \\ -2 x_0 & + & 1 x_1 & + & 0 x_2 & + & -6 x_3 & = & 3 \\ 1 x_0 & + & 1 x_1 & + & 1 x_2 & + & 9 x_3 & = & 4 \end{array}$$

Gaussian Elimination Example

$1 x_0$	+	$0 x_1$	+	$1 x_2$	+	$4 x_3$	=	1
$0 x_0$	+	$-1 x_1$	+	$-1 x_2$	+	$-1 x_3$	=	0
$0 x_0$	+	$1 x_1$	+	$2 x_2$	+	$2 x_3$	=	5
$0 x_0$	+	$1 x_1$	+	$0 x_2$	+	$5 x_3$	=	3

Gaussian Elimination Example

$1 x_0$	+	$0 x_1$	+	$1 x_2$	+	$4 x_3$	=	1
$0 x_0$	+	$-1 x_1$	+	$-1 x_2$	+	$-1 x_3$	=	0
$0 x_0$	+	$0 x_1$	+	$1 x_2$	+	$1 x_3$	=	5
$0 x_0$	+	$0 x_1$	+	$-1 x_2$	+	$4 x_3$	=	3

Gaussian Elimination Example

$$1 x_0 + 0 x_1 + 1 x_2 + 4 x_3 = 1$$

$$0 x_0 + -1 x_1 + -1 x_2 + -1 x_3 = 0$$

$$0 x_0 + 0 x_1 + 1 x_2 + 1 x_3 = 5$$

$$0 x_0 + 0 x_1 + 0 x_2 + 5 x_3 = 8$$

Gaussian Elimination Example

$$\begin{array}{rccccrcr} 1x_0 & + & 0x_1 & + & 1x_2 & + & 4x_3 & = & 1 \\ 0x_0 & + & -1x_1 & + & -1x_2 & + & -1x_3 & = & 0 \\ 0x_0 & + & 0x_1 & + & 1x_2 & + & 1x_3 & = & 5 \\ 0x_0 & + & 0x_1 & + & 0x_2 & + & 5x_3 & = & 8 \end{array}$$

$$\begin{array}{l} x_3 = 8/5 \\ x_2 = 5 - x_3 = 17/5 \\ x_1 = 0 - x_2 - x_3 = -25/5 \\ x_0 = 1 - x_2 - 4x_3 = -44/5 \end{array}$$

Gaussian Elimination: Partial Pivoting

Remark. Previous code fails spectacularly if pivot $a_{pp} = 0$.

$$\begin{array}{rclclcl} 1 x_0 & + & 1 x_1 & + & 0 x_3 & = & 1 \\ 2 x_0 & + & 2 x_1 & + & -2 x_3 & = & -2 \\ 0 x_0 & + & 3 x_1 & + & 15 x_3 & = & 33 \end{array}$$

$$\begin{array}{rclclcl} 1 x_0 & + & 1 x_1 & + & 0 x_3 & = & 1 \\ 0 x_0 & + & 0 x_1 & + & -2 x_3 & = & -4 \\ 0 x_0 & + & 3 x_1 & + & 15 x_3 & = & 33 \end{array}$$

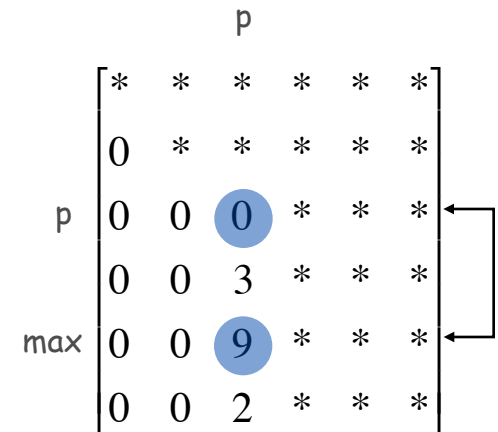
$$\begin{array}{rclclcl} 1 x_0 & + & 1 x_1 & + & 0 x_3 & = & 1 \\ 0 x_0 & + & 0 x_1 & + & -2 x_3 & = & -4 \\ 0 x_0 & + & \text{Nan } x_1 & + & \text{Inf } x_3 & = & \text{Inf} \end{array}$$

Gaussian Elimination: Partial Pivoting

Partial pivoting. Swap row p with the row that has **largest** entry in column p among rows i below the diagonal.

```
// find pivot row
int max = p;
for (int i = p + 1; i < N; i++)
    if (Math.abs(A[i][p]) > Math.abs(A[max][p]))
        max = i;

// swap rows p and max
double[] T = A[p]; A[p] = A[max]; A[max] = T;
double t = b[p]; b[p] = b[max]; b[max] = t;
```



Q. What if pivot $a_{pp} = 0$ while partial pivoting?

A. System has no solutions or infinitely many solutions.

Gaussian Elimination with Partial Pivoting

```
public static double[] lsolve(double[][] A, double[] b) {
    int N = b.length;

    // Gaussian elimination
    for (int p = 0; p < N; p++) {
        // partial pivot
        int max = p;
        for (int i = p+1; i < N; i++)
            if (Math.abs(A[i][p]) > Math.abs(A[max][p]))
                max = i;
        double[] T = A[p]; A[p] = A[max]; A[max] = T;
        double t = b[p]; b[p] = b[max]; b[max] = t;

        // zero out entries of A and b using pivot A[p][p]
        for (int i = p+1; i < N; i++) {
            double alpha = A[i][p] / A[p][p];
            b[i] -= alpha * b[p];
            for (int j = p; j < N; j++)
                A[i][j] -= alpha * A[p][j];
        }
    }
}
```

~ $N^3/3$ additions,
~ $N^3/3$ multiplications

```
// back substitution
double[] x = new double[N];
for (int i = N-1; i >= 0; i--) {
    double sum = 0.0;
    for (int j = i+1; j < N; j++)
        sum += A[i][j] * x[j];
    x[i] = (b[i] - sum) / A[i][i];
}
return x;
```

~ $N^2/2$ additions,
~ $N^2/2$ multiplications

```
}
```

Stability and Conditioning

Numerically-Unstable Algorithms

Stability. Algorithm $f1(x)$ for computing $f(x)$ is **numerically stable** if $f1(x) \approx f(x + \epsilon)$ for **some** small perturbation ϵ .

Nearly the right answer to nearly the right problem.

Ex 1. Numerically unstable way to compute $f(x) = \frac{1 - \cos x}{x^2}$

```
public static double f1(double x) {  
    return (1.0 - Math.cos(x)) / (x * x);  
}
```

▪ `f1(1.1e-8) = 0.9175.`

 true answer $\approx 1/2$.

Note. Numerically stable formula: $f(x) = \frac{2 \sin^2(x/2)}{x^2}$

Numerically-Unstable Algorithms

Stability. Algorithm $\mathbf{fl}(x)$ for computing $f(x)$ is **numerically stable** if $\mathbf{fl}(x) \approx f(x + \varepsilon)$ for **some** small perturbation ε .

Nearly the right answer to nearly the right problem.

Ex 2. Gaussian elimination (w/o partial pivoting) can fail spectacularly.

$a = 10^{-17}$

$$\begin{array}{rcl} a x_0 + 1 x_1 & = & 1 \\ 1 x_0 + 2 x_1 & = & 3 \end{array}$$

Algorithm	x_0	x_1
no pivoting	0.0	1.0
partial pivoting	1.0	1.0
exact	$\frac{1}{1-2a} \approx 1$	$\frac{1-3a}{1-2a} \approx 1$

Theorem. Partial pivoting improves numerical stability.

Ill-Conditioned Problems

Conditioning. Problem is **well-conditioned** if $f(x) \approx f(x + \varepsilon)$ for **all** small perturbation ε .

Solution varies gradually as problem varies.

Ex 1. arccos() and tan() functions.

- $\arccos(.99999991) \approx 0.000425$ $\tan(1.57078) \approx 6.12490 \times 10^5$
- $\arccos(.99999992) \approx 0.000400$ $\tan(1.57079) \approx 1.58058 \times 10^4$

Consequence. The following formula for computing the great circle distance between (x_1, y_1) and (x_2, y_2) is inaccurate for nearby points.

$$d = 60 \arccos(\sin x_1 \sin x_2 + \cos x_1 \cos x_2 \cos(y_1 - y_2))$$

 very close to 1 when two points are close

Ill-Conditioned Problems

Conditioning. Problem is **well-conditioned** if $f(x) \approx f(x + \varepsilon)$ for **all** small perturbation ε .

Solution varies gradually as problem varies.

Ex 2. Hilbert matrix.

- Tiny perturbation to H_n makes it singular.
- Cannot solve $H_{12} x = b$ using floating point.

$$H_4 = \begin{bmatrix} \frac{1}{1} & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} \\ \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \frac{1}{7} \end{bmatrix}$$

Hilbert matrix

Matrix condition number. [Turing, 1948] Widely-used concept for detecting ill-conditioned linear systems.

Numerically Solving an Initial Value ODE

Lorenz attractor.

- Idealized atmospheric model to describe turbulent flow.
- Convective rolls: warm fluid at bottom, rises to top, cools off, and falls down.

$$\begin{aligned}\frac{dx}{dt} &= -10(x+y) \\ \frac{dy}{dt} &= -xz + 28x - y \\ \frac{dz}{dt} &= xy - \frac{8}{3}z\end{aligned}$$

x = fluid flow velocity

y = ∇ temperature between ascending and descending currents

z = distortion of vertical temperature profile from linearity

Solution. No closed form solution for $x(t)$, $y(t)$, $z(t)$.

Approach. Numerically solve ODE.

Euler's Method

Euler's method. [to numerically solve initial value ODE]

- Choose Δt sufficiently small.
- Approximate function at time t by tangent line at t .
- Estimate value of function at time $t + \Delta t$ according to tangent line.
- Increment time to $t + \Delta t$.
- Repeat.

$$x_{t+\Delta t} = x_t + \Delta t \frac{dx}{dt}(x_t, y_t, z_t)$$

$$y_{t+\Delta t} = y_t + \Delta t \frac{dy}{dt}(x_t, y_t, z_t)$$

$$z_{t+\Delta t} = z_t + \Delta t \frac{dz}{dt}(x_t, y_t, z_t)$$

Advanced methods. Use less computation to achieve desired accuracy.

- 4th order Runge-Kutta: evaluate slope four times per step.
- Variable time step: automatically adjust timescale Δt .
- See COS 323.

Lorenz Attractor: Java Implementation

```
public class Butterfly {  
  
    public static double dx(double x, double y, double z)  
    { return -10*(x - y); }  
  
    public static double dy(double x, double y, double z)  
    { return -x*z + 28*x - y; }  
  
    public static double dz(double x, double y, double z)  
    { return x*y - 8*z/3; }  
  
}
```

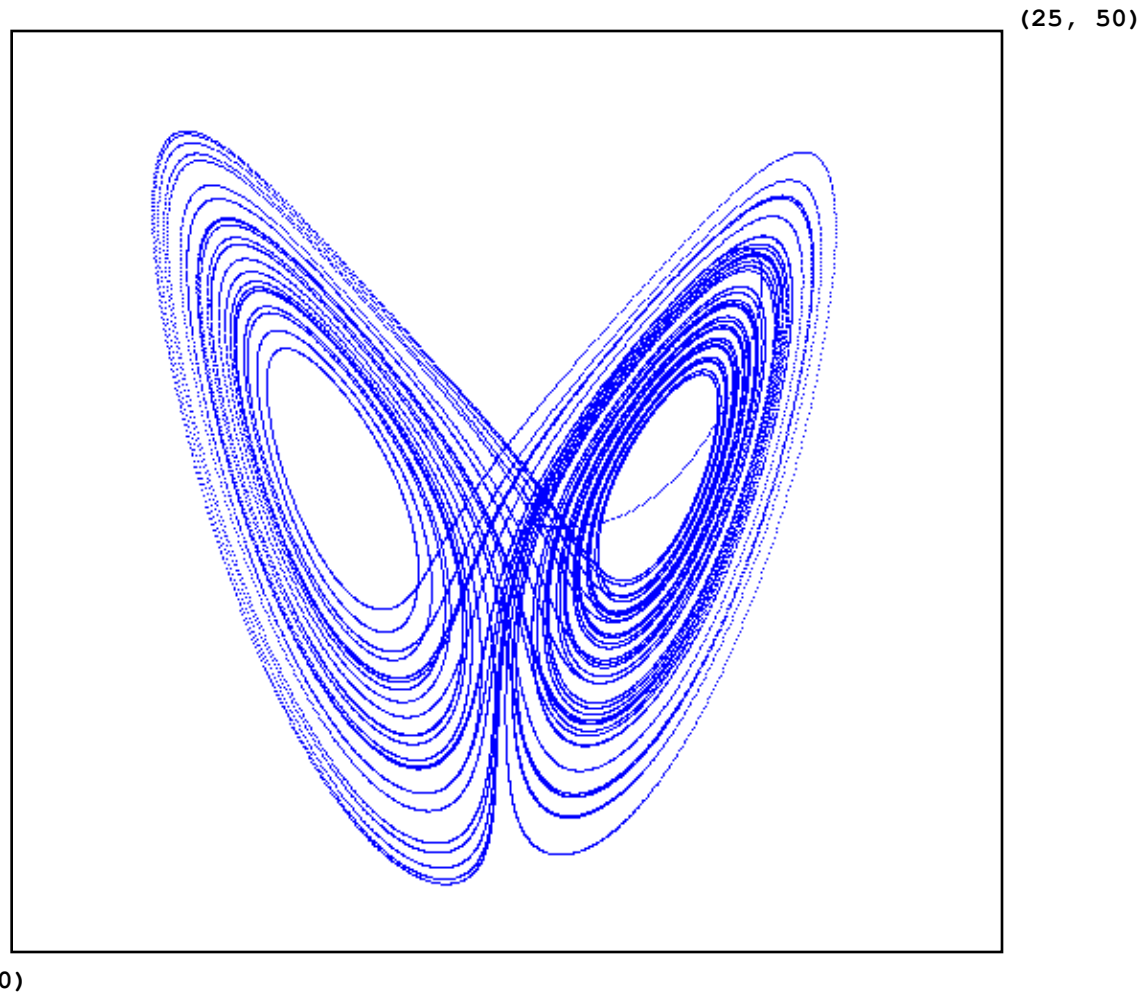
```
public static void main(String[] args) {  
    double x = 0.0, y = 20.0, z = 25.0;  
    double dt = 0.001;  
    StdDraw.setXscale(-25, 25);  
    StdDraw.setYscale( 0, 50);  
  
    while (true) {  
        double xnew = x + dt * dx(x, y, z);  
        double ynew = y + dt * dy(x, y, z);  
        double znew = z + dt * dz(x, y, z);  
        x = xnew; y = ynew; z = znew;  
        StdDraw.point(x, z);  
    }  
}
```

Euler's method

plot x vs. z

The Lorenz Attractor

```
% java Butterfly
```



Butterfly Effect

Experiment.

- Initialize $y = 20.01$ instead of $y = 20$.
- Plot original trajectory in blue, perturbed one in magenta.
- What happens?

Ill-conditioning.

- Sensitive dependence on initial conditions.
- Property of system, not of numerical solution approach.

Predictability: does the flap of a butterfly's wings in Brazil set off a tornado in Texas? — title of a 1972 talk by Edward Lorenz



Stability and Conditioning

Accuracy depends on both stability and conditioning.

- Danger: apply unstable algorithm to well-conditioned problem.
- Danger: apply stable algorithm to ill-conditioned problem.
- Safe: apply stable algorithm to well-conditioned problem.

Numerical analysis. Art and science of designing numerically stable algorithms for well-conditioned problems.

Lesson 1. Some **algorithms** are unsuitable for floating-point computation.

Lesson 2. Some **problems** are unsuitable to floating-point computation.