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.
- Natural language processing.
- Architecture walk-throughs.
- Medical diagnostics (MRI, CAT).

Common features.

- Problems tend to be continuous instead of discrete.
- Algorithms often need to scale to handle huge problems.

Representing Real Numbers

Challenge: use fixed size words to represent, e.g.,

- `2.1`
- `0.0000000000000000000000000000000000345878778`
- `-1020455.000322`
- `365090807000000000000000000000000.0`

We appear to need:

- A sign bit
- An exponent, which might need to be negative
- A “significand” or “mantissa”

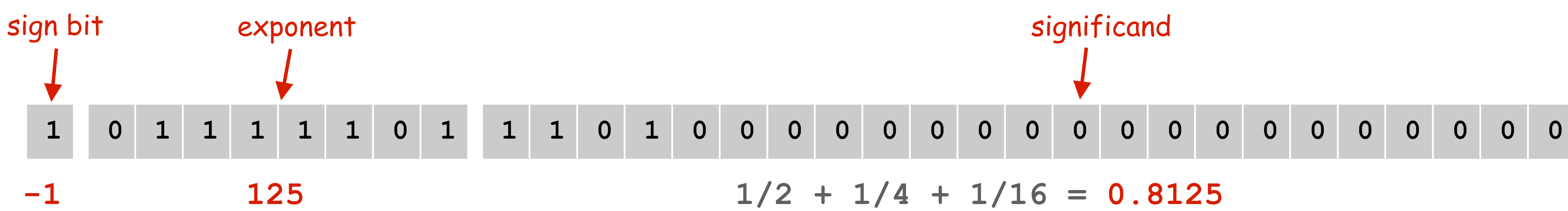
- AND a way to cram all this into 32 or 64 bits.

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`.



$$-1 \times 2^{125 - \overbrace{127}^{\text{bias}}} \times \overbrace{1}^{\text{hidden bit}}.8125 = -0.453125$$

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 uninitiated.

```
if (0.1 + 0.2 == 0.3) { // NO  }
if (0.1 + 0.3 == 0.4) { // YES }
```

Financial computing. Calculate 9% sales tax on a 50¢ phone call.
Banker's rounding. Round to nearest integer, to even integer if tie.

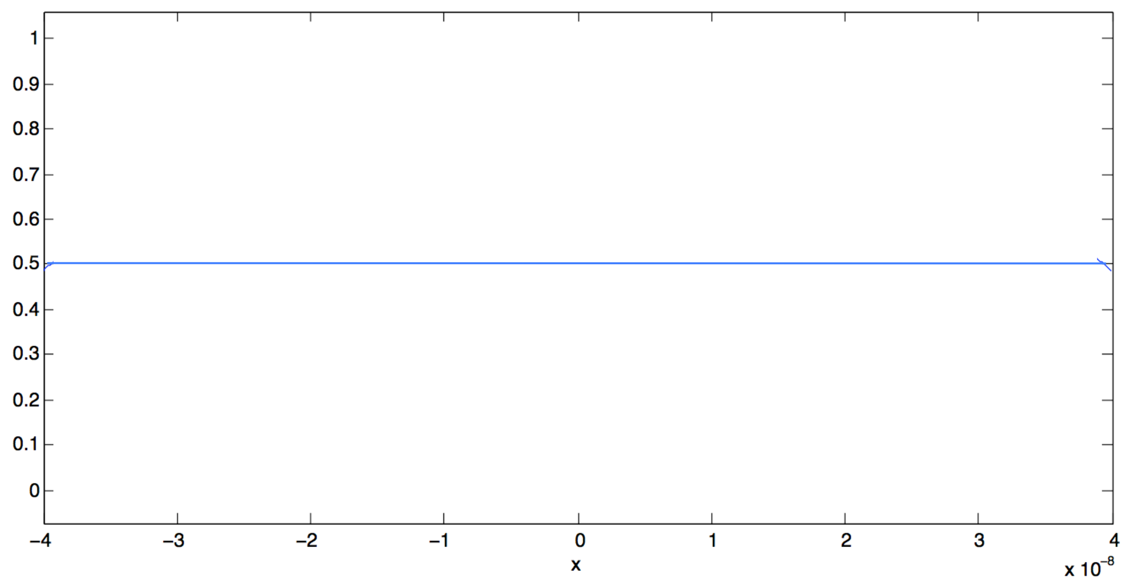
```
double a1 = 1.14 * 75;       // 85.49999999999999
double a2 = Math.round(a1); // 85              you lost 1¢

double b1 = 1.09 * 50;       // 54.50000000000001
double b2 = Math.round(b1); // 55              SEC violation (!)
```

Catastrophic Cancellation

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

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

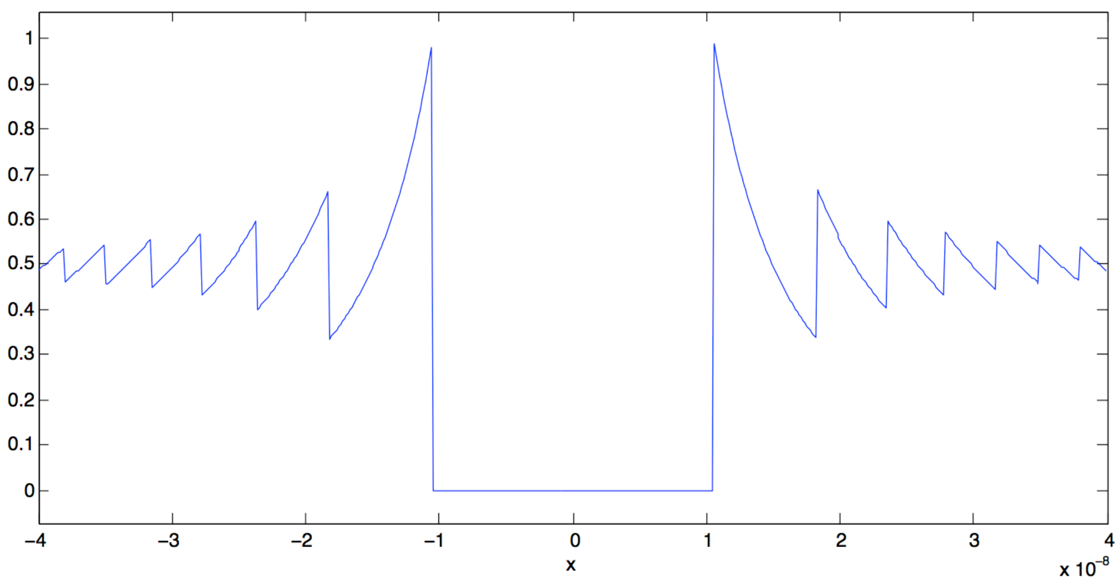


Exact answer

Catastrophic Cancellation

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

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



IEEE 754 double precision answer

Catastrophic Cancellation

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

Ex. Evaluate `fl(x)` for `x = 1.1e-8`.

- `Math.cos(x) = 0.99999999999999988897769753748434595763683319091796875.`

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

- `(1.0 - Math.cos(x)) = 1.1102e-16`

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

- `(1.0 - 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.

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.

Gaussian Elimination

Linear System of Equations

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

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

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

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.

$$x_0 C_3H_8 + x_1 O_2 \Rightarrow x_2 CO_2 + x_3 H_2O$$

Stoichiometric constraints.

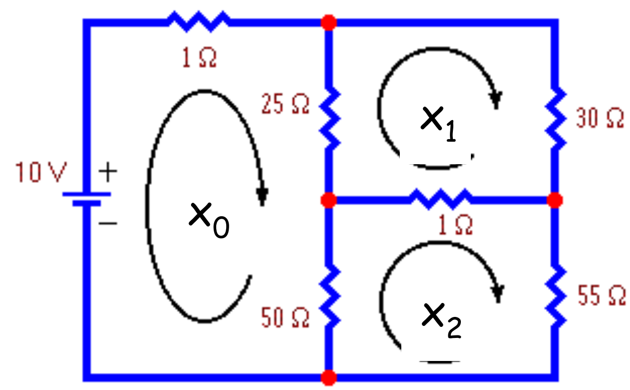
$$\left.\begin{array}{ll} \text{Carbon:} & 3x_0 = x_2. \\ \text{Hydrogen:} & 8x_0 = 2x_3. \\ \text{Oxygen:} & 2x_1 = 2x_2 + x_3. \end{array}\right\} \text{conservation of mass}$$

- Normalize: $x_0 = 1$.

$$C_3H_8 + 5O_2 \Rightarrow 3CO_2 + 4H_2O$$

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

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 $i > j$.

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

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];
}
```

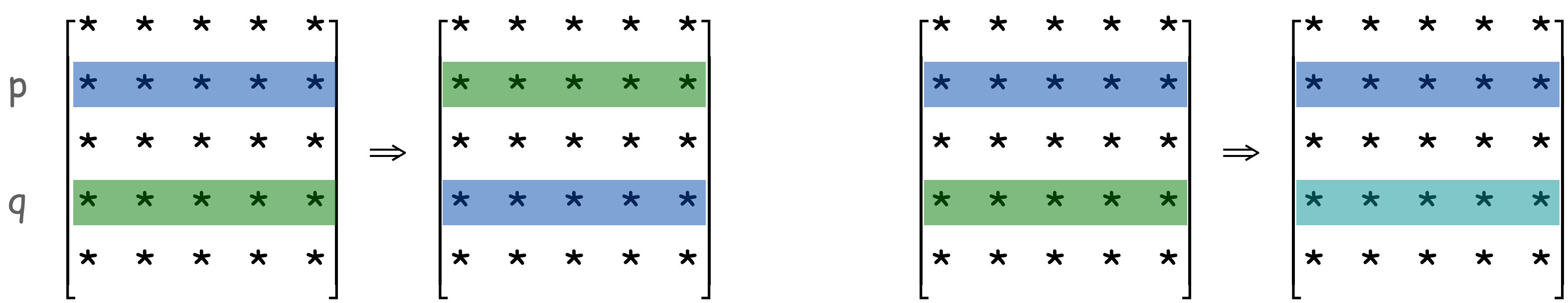
$$x_i = \frac{1}{a_{ii}} \left[b_i - \sum_{j=i+1}^{N-1} a_{ij}\, x_j \right]$$

Gaussian elimination.

- 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.

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

$\Downarrow$ (interchange row 0 and 1)

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

$\Downarrow$ (subtract 3x row 1 from row 2)

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

Gaussian Elimination: Forward Elimination

Forward elimination. Apply row operations to make upper triangular.

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

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

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

$$\begin{array}{cc} & \begin{array}{cccccc} & & p & & & \end{array} \\ \begin{array}{c} \\ \\ p \\ \\ \\ \\ \end{array} & \begin{bmatrix} * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & * & * & * & * \end{bmatrix} \end{array} \Rightarrow \begin{bmatrix} * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & * & * & * \end{bmatrix}$$

```
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

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

Gaussian Elimination Example

$$
\begin{array}{ccccccccc}
1\,x_0 & + & 0\,x_1 & + & 1\,x_2 & + & 4\,x_3 & = & 1 \\
0\,x_0 & + & -1\,x_1 & + & -1\,x_2 & + & -1\,x_3 & = & 0 \\
0\,x_0 & + & 1\,x_1 & + & 2\,x_2 & + & 2\,x_3 & = & 5 \\
0\,x_0 & + & 1\,x_1 & + & 0\,x_2 & + & 5\,x_3 & = & 3
\end{array}
$$

Gaussian Elimination Example

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

Gaussian Elimination Example

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

Gaussian Elimination Example

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

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

Gaussian Elimination: Partial Pivoting

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

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

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

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

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;
```

$$\begin{array}{cc} & \begin{matrix} & & p & & & \end{matrix} \\ \begin{matrix} \\ \\ p \\ \\ \text{max} \\ \\ \end{matrix} & \begin{bmatrix} * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 3 & * & * & * \\ 0 & 0 & 9 & * & * & * \\ 0 & 0 & 2 & * & * & * \end{bmatrix} \end{array}$$

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];
      }
   }
   // 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;
}
```

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

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

Stability and Conditioning

Numerically Unstable Algorithms

Stability. Algorithm `fl(x)` for computing f(x) is numerically stable if `fl(x)` ≈ f(x+ε) 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 fl(double x) {
   return (1.0 - Math.cos(x)) / (x * x);
}
```

- `fl(1.1e-8) = 0.9175.`

true answer ≈ 1/2.

$$f(x) = \frac{2 \sin^2(x/2)}{x^2}$$

a numerically stable formula

Numerically Unstable Algorithms

Stability. Algorithm `fl(x)` for computing f(x) is **numerically stable** if `fl(x)` $\approx$ f(x+ε) 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.

$a = 10^{-17}$

$$\begin{aligned} a\,x_0 &+ 1\,x_1 &= 1 \\ 1\,x_0 &+ 2\,x_1 &= 3 \end{aligned}$$

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. 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.

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 solutions.
Lesson 2. Some problems are unsuitable to floating point solutions.

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.

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

Edward Lorenz

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 + Δt according to tangent line.
- Increment time to t + Δt.
- Repeat.

$$
\begin{aligned}
x_{t+\Delta t} &= x_t + \Delta t \, \tfrac{dx}{dt}(x_t, y_t, z_t) \\
y_{t+\Delta t} &= y_t + \Delta t \, \tfrac{dy}{dt}(x_t, y_t, z_t) \\
z_{t+\Delta t} &= z_t + \Delta t \, \tfrac{dz}{dt}(x_t, y_t, z_t)
\end{aligned}
$$

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 Lorenz {
   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 Lorenz
```

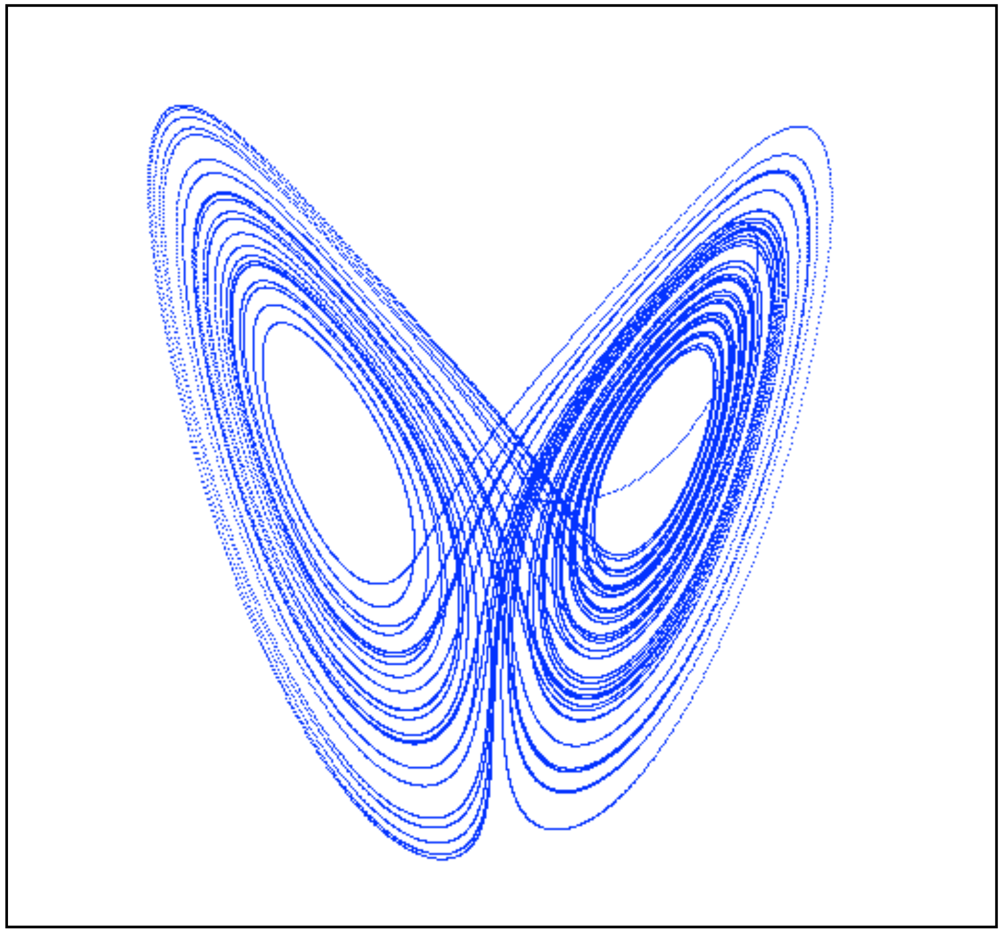
(25, 50)

(-25, 0)

The Lorenz Attractor

```
% java Lorenz
```

(25, 50)



(-25, 0)

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 1972 talk by Edward Lorenz