PracticeSession03

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Numerical Linear Algebra for Computational Science and Information Engineering

Floating-Point Arithmetic and Error Analysis

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[1]:
```
using LinearAlgebra, Random, Plots, Printf, Latexify, LaTeXStrings
```

Preamble: Cancellation error

The relative error of a scalar is indicative of the number of correct digits of its approximation. For example, consider $\pi = 3.1415926\ldots$, we have

$\widehat{\pi}$	$\lvert\widehat{\pi} - \pi\rvert/\lvert\pi\rvert$
3.1	1.323935×10^{-2}
3.141	1.886475×10^{-4}
3.141592	2.080440×10^{-7}
3.1415926	1.705816×10^{-8}

When we subtract two nearly equal numbers, their most significant digits cancel out, leading to a floating-point number that less accurately approximates the difference. This is **cancellation error**.

For example, consider the number π stored in 32 bits, i.e., 32, and its representation error:

[2]:
```
 32 = Float32(pi)
rel_error_ 32 = abs(Float64( 32) - pi) / abs(pi)
@printf "  = %.8f,  32 = %.8f, rel. error = %.2E"   32 rel_error_ 32
```

```
  = 3.14159265,  32 = 3.14159274, rel. error = 2.78E-08
```

We see that 32 has around 8 significant digits.

Then, we want to evaluate the difference between π and a nearly equal number, say $\Delta = \pi - 3.14$. We also are interested in the approximation $\Delta 32$ of this number, done by evaluating 32 - 3.14 in 32 bits, and we look at the relative error between Δ and $\Delta 32$:

[3]:
```
Δ32 = Float32(3.14) -  32
Δ = 3.14 - pi
rel_error_Δ = abs(Float64(Δ32) - Δ) / abs(Δ)
@printf "Δ = %.5E, Δ32 %.5E, rel_error_Δ = %.2E" Δ Δ32 rel_error_Δ
```

```
Δ = -1.59265E-03, Δ32 -1.59264E-03, rel_error_Δ = 1.10E-05
```

We see the number of significant digits of Δ32 dropped to 5, from previously 8 digits for 32.

However, the representation of Δ with 32 bits still has around 8 significant digits:

[4]:
```
rel_error_Δ32 = abs(Float64(Float32(Δ)) - Δ) / abs(Δ)
@printf "Δ = %.5E, Float32(Δ) %.5E, rel_error_Δ32 = %.2E" Δ Float64(Float32(Δ))␣
 ↪rel_error_Δ32
```

```
Δ = -1.59265E-03, Float32(Δ) -1.59265E-03, rel_error_Δ32 = 1.20E-08
```

So, the increase of relative error obtained when evaluating Δ32 using floating-point arithmetic with 32 bits is indeed due to cancellation.

Exercise #1: Catastrophic cancellation

Let us consider the integral $I_n = \int_0^1 x^n e^{-x} dx$, which we wish to evalue as a function of n.

Upon integrating by parts we get the recursive formula $I_n = n \cdot I_{n-1} - 1/e$ with a base case $I_0 = 1 - 1/e$.

The recursive formula is implemented as follows:

[2]:
```
function I(n)
  if n == 0
    return 1. - exp(-1)
  end
  return n * I(n-1) - exp(-1)
end;
```

Now, we wish to test `I(n)`. We know that $I_{100} \approx 3.678430281 \times 10^{-3}$. What does `I(100)` give us?

[3]:
```
I0   = 6.321205588e-1;
I10  = 3.646133462e-2;
I50  = 7.354706796e-3;
I100 = 3.678430281e-3;
I300 = 1.226251224e-3;

II100 = I(100)
println("I_100 = ", II100)
println("rel. error: ", abs(I100 - II100) / abs(I100))
```

```
I_100 = -3.1530126806564304e141
rel. error: 8.571625502711085e143
```

The value returned by `I(100)` is completely off from the expected result, showing a breakdown of the numerical method. Why is that?

To answer this question, let us first look at what comes into the recursive computation of I_{n+1} for different values of n, namely $n \cdot I_{n-1}$ and $1/e$:

[4]:
```
println("1 * I0 = ", I0, ", exp(-1) = ", exp(-1));
println("11 * I10 = ", 10 * I10, ", exp(-1) = ", exp(-1));
println("51 * I50 = ", 51 * I50, ", exp(-1) = ", exp(-1));
println("101 * I100 = ", 101 * I100, ", exp(-1) = ", exp(-1));
```

```
1 * I0 = 0.6321205588, exp(-1) = 0.36787944117144233
11 * I10 = 0.3646133462, exp(-1) = 0.36787944117144233
51 * I50 = 0.37509004659600004, exp(-1) = 0.36787944117144233
101 * I100 = 0.371521458381, exp(-1) = 0.36787944117144233
```

We see that the true value of $n \cdot I_{n-1}$ grows closer to $1/e$ as n increases. Then, `I(n)` attempts to evaluate I_n by subtracting these increasingly close numbers, which leads to **cancellation error**. In addition to this, I_n is then multiplied by $n+1$ in order to compute I_{n+1}. As n grows, this means the cancellation error may be maginified, accelerating the propagation of errors.

In order to circumvent this issue, we should try and reformulate the recursion so as to not have differences of nearly equal numbers multiplied by large numbers.

For that, note that the recursion can be recast into $I_{n-1} = 1/n \cdot (I_n + 1/e)$, which is used backwards, from a base case I_m with $m > n$. Let us for instance use I_{300} as a base case. The backward recursion is implemented as follows:

[5]:
```
function J(n)
  J = 1.226251224e-3
  i = 300
  while (i > n)
    J = (1. / i) * (J + exp(-1))
    i -= 1
  end
  return J
end;
```

Let us now test `J(n)` to compute I_{100}.

[6]:
```
J100 = J(100)
println("J_100 = ", J100)
println("rel. error: ", abs(I100 - J100) / abs(I100))
```

```
J_100 = 0.0036784302813674887
rel. error: 9.990364464392733e-11
```

The problem now is fixed.

This problem was suggested by Luc Giraud from Inria, Bordeaux.

Exercise #2: Ill-conditioned linear system

Let us consider the linear system $Ax = b$ given by

$$A = \begin{bmatrix} 1 & 1 \\ 1+\varepsilon & 1 \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} b_1 \\ b_1+\varepsilon \end{bmatrix} \quad \text{with} \quad \varepsilon > 0.$$

The unique exact solution of this system is given by

$$x = \begin{bmatrix} 1 \\ b_1 - 1 \end{bmatrix}.$$

The matrix A has eigenvalues $\lambda_{min} = 1 - \sqrt{1+\varepsilon}$ and $\lambda_{max} = 1 + \sqrt{1+\varepsilon}$, so that $\|A\|_2 = \lambda_{max} = 1 + \sqrt{1+\varepsilon}$ and, the condition number for solving a linear system with A is

$$\kappa(A) = \|A^{-1}\|_2 \|A\|_2 = \frac{|\lambda_{max}(A)|}{|\lambda_{min}(A)|} = \frac{1+\sqrt{1+\varepsilon}}{|1-\sqrt{1+\varepsilon}|} = \frac{(1+\sqrt{1+\varepsilon})^2}{\varepsilon} \qquad (A \text{ is normal}).$$

That is, solving for x is an ill-conditioned problem for sufficiently small values of ε. For example, we have

[7]:
```
function get_A( )
  return [1.    1.;
          1+   1.]
end;

get_b(b1,  ) = [b1;b1+ ];
get_ ( ) = (1 + sqrt(1+ ))^2/ ;
get_x(b,  ) = [1.; b[1]-1.];

for    (1e-3, 1e-4, 1e-5, 1e-6)
    = get_ ( );
  @printf "  = %.0E,   = %.1E\n"
end
```

```
 = 1E-03,   = 4.0E+03
 = 1E-04,   = 4.0E+04
 = 1E-05,   = 4.0E+05
 = 1E-06,   = 4.0E+06
```

Now, in practice some of the components of A and b may not be exactly stored. In particular, we may rather have

$$B = \begin{bmatrix} 1 & 1 \\ \mathrm{fl}(1+\varepsilon) & 1 \end{bmatrix} \quad \text{and} \quad c = \begin{bmatrix} \mathrm{fl}(b_1) \\ \mathrm{fl}(b_1+\varepsilon) \end{bmatrix} \quad \text{with} \quad \varepsilon > 0.$$

If that is so, assuming $\mathrm{fl}(1+\varepsilon) > 1$ so that B remains invertible, the true solution y of $By = c$ is

$$y = \frac{1}{\mathrm{fl}(1+\varepsilon) - 1} \begin{bmatrix} \mathrm{fl}(b_1+\varepsilon) - \mathrm{fl}(b_1) \\ \mathrm{fl}(1+\varepsilon)\cdot\mathrm{fl}(b_1) - \mathrm{fl}(b_1+\varepsilon) \end{bmatrix}.$$

In case of non-zero representation errors, y is only an approximation of x, i.e., the true solution of the non-perturbed system $Ax = b$. We saw in class that the minimally normed perturbations δA and δb such that $(A + \delta A)y = b + \delta b$ are given by

$$\delta A = \frac{\|A\|_2}{\|y\|_2 \cdot (\|A\|_2 \cdot \|y\|_2 + \|b\|_2)}\, ry^T \ \text{ and } \ \delta b = -\frac{\|b\|_2}{\|A\|_2 \cdot \|y\|_2 + \|b\|_2}\, r$$

where $r = b - Ay$, and so that

$$\eta_{A,b}(y) = \frac{\|r\|_2}{\|A\|_2 \cdot \|y\|_2 + \|b\|_2} = \frac{\|\delta A\|_2}{\|A\|_2} = \frac{\|\delta b\|_2}{\|b\|_2}.$$

In this particular case, since $B - A$ and $c - a$ are very small, we actually have

$$\eta_{A,b}(y) \approx \frac{\|B - A\|_2}{\|A\|_2} = \frac{\|c - b\|_2}{\|b\|_2}.$$

Now, what we wish to show is that, **even though the backward error $\eta_{A,b}(y)$ may be small, the relative forward error $\|x - y\|_2 / \|x\|_2$ may actually be large, because of the ill-conditioned nature of the problem reflected by the values of $\kappa(A)$.**

[8]:
```
function get_y(b, )
    arithmetic = :fl64 # fl32
    if (arithmetic == :fl32)
      a21_32 = Float32(1+ )
      b1_32  = Float32(b[1])
      b2_32  = Float32(b[1]+ )
      return [Float64((b2_32-b1_32)/(a21_32-1));
              Float64((a21_32*b1_32-b2_32)/(a21_32-1))]
    else
      a21_64 = Float64(Float32(1+ ))
      b1_64  = Float64(Float32(b[1]))
      b2_64  = Float64(Float32(b[1]+ ))
      return [(b2_64-b1_64)/(a21_64-1);
              (a21_64*b1_64-b2_64)/(a21_64-1)]
    end
end

function get_ (y,  , b, r)
  A_2norm = 1+sqrt(1+ )
  b_2norm = sqrt(b'b)
  r_2norm = sqrt(r'r)
  y_2norm = sqrt(y'y)
  d = A_2norm * y_2norm + b_2norm
  return r_2norm / d
end;

function get_ A(y,  , b, r)
  A_2norm = 1+sqrt(1+ )
  b_2norm = sqrt(b'b)
```

```
  y_2norm = sqrt(y'y)
  c = A_2norm / y_2norm / (A_2norm * y_2norm + b_2norm)
  return c * r * y'
end;

function get_ b(y,  , b, r)
  A_2norm = 1+sqrt(1+ )
  b_2norm = sqrt(b'b)
  y_2norm = sqrt(y'y)
  c = - b_2norm / (A_2norm * y_2norm + b_2norm)
  return c * r
end;

function check(y,  , A, b, r)
   A = get_ A(y,  , b, r)
   b = get_ b(y,  , b, r)
  z = (A +  A) \ (b +  b)
  println(norm(y - z))
end

b1 = 22.

for    (1e-3, 1e-4, 1e-5, 1e-6)
  A = get_A( );
  b = get_b(b1,  );
    = get_ ( );
  x = get_x(b,  );
  y = get_y(b,  );
  r = b - A * y;
  forward_error = sqrt((x-y)'*(x-y))/sqrt(x'x);
  backward_error = get_ (y,  , b, r);
  # check(y,  , A, b, r);
  @printf "  = %.0E,   = %.1E, backward_error = %.4E, forward_error = %.4E\n"
  ↪backward_error forward_error
end
```

```
 = 1E-03,   = 4.0E+03, backward_error = 8.1454E-09, forward_error = 4.0093E-05
 = 1E-04,   = 4.0E+04, backward_error = 1.1401E-08, forward_error = 5.6123E-04
 = 1E-05,   = 4.0E+05, backward_error = 6.5008E-09, forward_error = 3.2032E-03
 = 1E-06,   = 4.0E+06, backward_error = 1.4023E-08, forward_error = 6.7267E-02
```

We can see that, as the condition number $\kappa(A)$ of the problem increases, the backward error $\eta_{A,b}(y)$, which characterizes the approximation y of x, becomes less and less indicative of the relative forward error. Indeed, we do have

$$\frac{\|x-y\|_2}{\|x\|_2} \lesssim \kappa(A) \times \eta_{A,b}(y).$$

Exercise #3: Ill-conditioned eigenvalue problem

We saw during the lecture that the condition number was a problem-dependent quantity. In order to showcase this, we take a look at a specific type of matrix which is well-conditioned for linear solves, but has ill-conditioned eigenvalues.

We consider the Grcar matrix (see https://math.nist.gov/MatrixMarket/data/NEP/mvmgrc/mvmgrc.html) which is upper Hessenberg, and thus, non-normal.

[9]:
```
function get_A(n)
  A = zeros(n, n);
  A[diagind(A, -1)] .= -1.;
  for i in 0:3
    A[diagind(A, i)] .= 1.;
  end
  return A
end

println("For n=10, the Grcar matrix looks like this:")
latex_string = L"A = " * latexify(get_A(10));
display("text/latex", latex_string);
```

```
For n=10, the Grcar matrix looks like this:
```

$A =$

$$\begin{bmatrix} 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & -1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & -1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & -1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.0 & 1.0 \end{bmatrix} \tag{1}$$

This matrix has a small condition number (A) with respect to linear solves. In particular, for n=100, we have:

[10]:
```
n = 100;
A = get_A(n);
 = cond(A)
```

[10]: `3.5911104629805917`

The small value of $\kappa = \|A^{-1}\|_2 \|A\|_2$ means that the solution x of the linear system $Ax = b$ is not highly sensitive to perturbations. That is, the true solution y of $(A + \delta A)y = b + \delta b$ remains close to x, as long as $\|\delta A\|_2$ and $\|\delta b\|_2$ are small. We can put this to the test as follows:

[11]:
```
Random.seed!(123467);
b = 1 .+ rand(n);
A_2norm = norm(A);
b_2norm = norm(b);

x = A \ b

 A0 = rand(n, n);  A0 ./= norm( A0);
 b0 = rand(n);  b0 ./= norm( b0);

for    (1e-5, 1e-4, 1e-3, 1e-2)
   A =   * A0
   b =   * b0
  y = (A +  A) \ (b +  b)
  rel_error = norm(y - x) / norm(x)
  @printf "|| A||_2/||A||_2 = %.2E, || b||_2/||b||_2 = %2.E, ||y - x||_2/||x||_2 = %.2E\n" norm( A)/A_2norm norm( b)/b_2norm rel_error
end
```

```
|| A||_2/||A||_2 = 4.50E-07, || b||_2/||b||_2 = 6E-07, ||y - x||_2/||x||_2 =
2.28E-06
|| A||_2/||A||_2 = 4.50E-06, || b||_2/||b||_2 = 6E-06, ||y - x||_2/||x||_2 =
2.28E-05
|| A||_2/||A||_2 = 4.50E-05, || b||_2/||b||_2 = 6E-05, ||y - x||_2/||x||_2 =
2.28E-04
|| A||_2/||A||_2 = 4.50E-04, || b||_2/||b||_2 = 6E-04, ||y - x||_2/||x||_2 =
2.28E-03
```

where we see that the forward error $\|y-x\|_2/\|x\|_2$ is properly measured by the relative perturbations $\|\delta A\|_2/\|A\|_2$ and $\|\delta b\|_2/\|b\|_2$ multiplied by the moderatly small condition number $\kappa(A)$.

Now, let us look into the eigenvalues of A.

We remember the condition number $\kappa(A, \lambda)$ of an eigenvalue λ with normalized right- and left-eigenvectors u and v, respectively, i.e., such that

$$Au = \lambda u, \quad A^H v = \bar{\lambda} v, \quad \|u\|_2 = \|v\|_2 = 1$$

is given by

$$\kappa(A, \lambda) = \frac{1}{|v^H u|}$$

so that $\kappa(A, \lambda)$ becomes increasingly large as the right- and left-eigenvectors u and v are close to be orthogonal.

For the case of the Grcar matrix, we can see that the condition number is very high, for all the eigenvalues. For example, we have

[12]:
```
Λ, U = eigen(A);
Θ, V = eigen(transpose(A));
 _ 1 = 1. / norm(U[:,1]'V[:,2]);
 _ n = 1. / norm(U[:,n]'V[:,n-1]);
```

```
@printf " _1 = %.2E,  _n = %.2E"  _1  _n
```

```
 _1 = 1.85E+14,  _n = 1.09E+06
```

Let us now showcase the ill-conditioning of these eigenvalues by applying small perturbation δA to A, and see what the effect is on the spectrum:

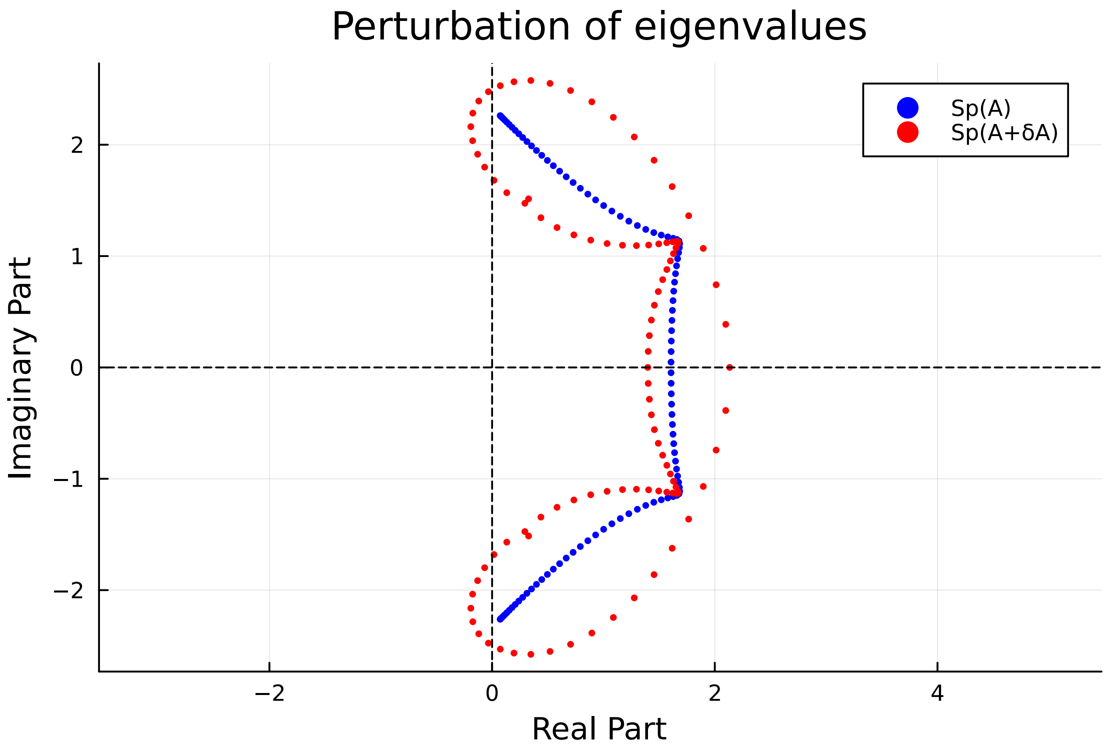
[13]:
```
 A = 1e-5 *  A0
Θ = eigvals(A +  A)
rel_error_1 = norm(Λ[1] - Θ[1]) / norm(Λ[1])
rel_error_n = norm(Λ[n] - Θ[n]) / norm(Λ[n])
@printf "|| A||_2/||A||_2 = %.2E, | 1 -  1|/| 1| = %.2E, | n -  n|/| n| = %.2E\n"
 ↪norm( A)/A_2norm  rel_error_1 rel_error_n
```

```
|| A||_2/||A||_2 = 4.50E-07, | 1 -  1|/| 1| = 1.25E-01, | n -  n|/| n| =
5.94E-01
```

We can see that despite the fact that the perturbation is small, the effect on the eigenvalues with smallest and largest magnitudes is very strong.

It is worth observing the effect of the entire spectrum:

[14]:
```
p = scatter(real.(Λ), imag.(Λ), xlabel="Real Part", ylabel="Imaginary Part",
 ↪title="Perturbation of eigenvalues",
            label="Sp(A)", marker=:circle, markersize=2, markerstrokewidth=0,
 ↪color=:blue, aspect_ratio=:equal)
scatter!(p, real.(Θ), imag.(Θ), label="Sp(A+ A)", marker=:circle, markersize=2,
 ↪markerstrokewidth=0, color=:red)
hline!([0], color=:black, linestyle=:dash, label="")
vline!([0], color=:black, linestyle=:dash, label="")
display(current())
```



Hence, we see that, despite being well-conditioned for linear solves, the Grcar matrix has ill-conditioned eigenvalues, which confirms that, indeed, **the condition number is a problem-dependent quantity**.