

# Numerical Programming 1 (CSE)

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# 1 What can't be ignored

## 1.1 Floating point numbers (25.10.)

We use  $p$  digits  $d_1, \dots, d_p$  and an exponent  $e$  to write a floating point number with base  $b$  as

$$x = \pm b^e \left( \frac{d_1}{b} + \frac{d_2}{b^2} + \dots + \frac{d_p}{b^p} \right).$$

For  $b = 10$ , this means  $x = \pm 10^e \cdot 0.d_1d_2\dots d_p$ .

**Definition.**

$$\mathbb{F} = \mathbb{F}(b, p, [e_{\min}, e_{\max}]) = \{ \pm m \cdot b^{e-p} \mid b^{p-1} \leq m < b^p, e_{\min} \leq e \leq e_{\max} \}$$

function floating\_point

b=2; p=3; emi=-1; ema=3; F = 0;

for m = b^(p-1):b^p-1, F = [F, m\*b.^([emi:ema]-p)]; end

plot(F,zeros(length(F)), 'r\*')

**Range.** The range is  $x_{\min} = b^{e_{\min}-1} \leq |x| \leq b^{e_{\max}}(1 - b^{-p}) = x_{\max}$ .

**Gaps.** The spacing grows by a factor  $b$  at each power of  $b$ : Let  $\varepsilon = b^{1-p}$  be the machine precision, that is, the distance from 1 to the next larger  $x \in \mathbb{F}$ . The distance from  $x \in \mathbb{F}$  to the nearest  $y \in \mathbb{F}$ ,  $y \neq x$  is at least  $b^{-1}\varepsilon|x|$  and at most  $\varepsilon|x|$ .

function IEEE\_double

realmin, realmax, eps

Let  $\mathbb{F}_{\infty} = \mathbb{F}(b, p, ] - \infty, \infty[)$  and  $\text{fl} : \mathbb{R} \rightarrow \mathbb{F}_{\infty}$ ,  $x \mapsto$  nearest  $y \in \mathbb{F}_{\infty}$ . In case of a tie,  $\text{fl}(x)$  is the  $y$  with even  $d_p$  (round to even). Overflow, if  $|\text{fl}(x)| > x_{\max}$ , underflow, if  $0 < |\text{fl}(x)| < x_{\min}$ .

**Theorem.** For all  $|x| \in [x_{\min}, x_{\max}]$  there exists  $|\delta| \leq \frac{\varepsilon}{2}$  with  $\text{fl}(x) = x(1 + \delta)$ .

```
function wobbling
x=linspace(1,16,1e3);
plot(x,eps(single(x))./x);
```

**Wobbling.** The relative distance to the next larger  $x \in \mathbb{F}$  varies by  $b$ . Therefore,  $b = 2$  is favoured.

**Standard model.** Let  $\star$  be one of the arithmetic operations  $+, -, \cdot, /$  and  $\tilde{\star}$  its floating point analogue. For all  $x, y \in \mathbb{F}$  with  $|x \star y| \in [x_{\min}, x_{\max}]$ , there exists  $|\delta| \leq \frac{\varepsilon}{2}$  with  $x \tilde{\star} y = (x \star y)(1 + \delta)$ .

**Literature.** [TB, Lecture 13], [H, Chapter 2], [O]

## 1.2 Conditioning (27.10.)

We want to evaluate a function  $f$  in  $x$ . How sensitive is  $f(x)$  to slight perturbations of  $x$ ?

**Definition.** Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$  and  $x \in \mathbb{R}^n$ .

$$\kappa_f(x) = \lim_{\delta \rightarrow 0} \sup_{\|\Delta x\| < \delta} \frac{\|f(x + \Delta x) - f(x)\|}{\|f(x)\|} \cdot \frac{\|x\|}{\|\Delta x\|}.$$

For continuously differentiable  $f$ , we have  $f(x + \Delta x) - f(x) = f'(x)\Delta x + o(\Delta x)$  as  $\Delta x \rightarrow 0$  by Taylor's theorem. In this case,  $\kappa_f(x) = \|f'(x)\| \cdot \|x\| / \|f(x)\|$ .

**Matrix norms.** We will use three norms on  $\mathbb{R}^n$ :

$$\|x\|_1 = \sum_{j=1}^n |x_j|, \quad \|x\|_2 = \sqrt{\sum_{j=1}^n |x_j|^2}, \quad \|x\|_\infty = \max\{|x_j| : j = 1, \dots, n\}.$$

The corresponding matrix norms  $\|A\| = \max\{\|Ax\| \cdot \|x\|^{-1} : \|x\| \leq 1\}$  are

$$\begin{aligned} \|A\|_1 &= \max\{\|A(:, j)\|_1 : j = 1, \dots, n\} && \text{(maximum column sum)} \\ \|A\|_2 &= \sigma_{\max}(A) = \sqrt{\lambda_{\max}(A^*A)} && \text{(largest singular value)} \\ \|A\|_\infty &= \max\{\|A(i, :)\|_1 : i = 1, \dots, m\} && \text{(maximum row sum)} \end{aligned}$$

**Scalar multiplication.**  $f : \mathbb{R} \rightarrow \mathbb{R}$ ,  $x \mapsto \frac{x}{2}$ ,  $\kappa_f(x) = \frac{1}{2} \cdot \frac{|x|}{|x/2|} = 1$ .

**Square root.**  $f : [0, \infty) \rightarrow [0, \infty)$ ,  $x \mapsto \sqrt{x}$ ,  $\kappa_f(x) = \frac{|x^{-1/2}/2| \cdot |x|}{|x^{1/2}|} = \frac{1}{2}$ .

**Cancellation.**  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $x \mapsto x_1 - x_2$ ,  $f'(x) = (1, -1)$ ,  $\|f'(x)\|_\infty = 2$ ,  $\kappa_f(x) = 2\|x\|_\infty / |x_1 - x_2|$ .

**Literature.** [TB, Lecture 3 & 12]

### 1.3 Stability (3.11.)

Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$  and  $\tilde{f} : \mathbb{R}^n \rightarrow \mathbb{R}^m$  a corresponding algorithm. Analysing a computation's accuracy, we estimate

$$\begin{aligned} \frac{\|f(x) - \tilde{f}(x + \Delta x)\|}{\|f(x)\|} &\leq \frac{\|f(x) - f(x + \Delta x)\|}{\|f(x)\|} + \frac{\|f(x + \Delta x) - \tilde{f}(x + \Delta x)\|}{\|f(x)\|} \\ &\leq \kappa_f(x) \|\Delta x\| / \|x\| + ? \end{aligned}$$

**Definition.**

$$\sigma_{\tilde{f}}(x) = \limsup_{\delta \rightarrow 0} \sup_{\varepsilon < \delta} \frac{\|f(x) - \tilde{f}(x)\|}{\|f(x)\| \cdot (\kappa_f(x) + 1) \cdot \varepsilon}$$

**Discussion.** With machine precision  $\varepsilon$ , the input is  $x + \Delta x$  with  $\|\Delta x\| / \|x\| = O(\varepsilon)$ . Then,

$$\frac{\|f(x) - \tilde{f}(x + \Delta x)\|}{\|f(x)\|} \leq \kappa_f(x) \cdot O(\varepsilon) + \sigma_{\tilde{f}}(x) \cdot (\kappa_f(x) + 1) \cdot O(\varepsilon).$$

For well-conditioned problems forward stable algorithms achieve  $O(\varepsilon)$  accuracy.

**Definition.**

$$\rho_{\tilde{f}}(x) = \limsup_{\delta \rightarrow 0} \left\{ \frac{\|\Delta x\|}{\|x\| \cdot \varepsilon} : \tilde{f}(x) = f(x + \Delta x), \varepsilon < \delta \right\}$$

**Discussion.** For well-conditioned problems, a forward stable algorithm computes nearly the right answer to nearly the right question, whereas a backward stable algorithm computes the exact answer to nearly the right problem. More precisely,  $\sigma_{\tilde{f}}(x) \leq \rho_{\tilde{f}}(x)$ .

**Subtraction.**  $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ ,  $x \mapsto x_1 - x_2$ ,  $\tilde{f}(x) = \text{fl}(x_1) \tilde{-} \text{fl}(x_2)$   
backward stable.

**Inner product.**  $f : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$ ,  $(x, y) \mapsto x^T \cdot y$ ,  $\tilde{f}(x, y) =$   
 $\widetilde{\sum}_j \text{fl}(x_j) \tilde{\cdot} \text{fl}(y_j)$  backward stable.

**Outer product.**  $f : \mathbb{R}^m \times \mathbb{R}^n \rightarrow \mathbb{R}^{m \times n}$ ,  $(x, y) \mapsto (x \otimes y)_{ij} =$   
 $x_i y_j$ ,  $\tilde{f}(x, y)_{ij} = \text{fl}(x_i) \tilde{\cdot} \text{fl}(y_j)$ , forward but not backward stable.

**Adding to one.**  $f : \mathbb{R} \rightarrow \mathbb{R}$ ,  $x \mapsto x + 1$ ,  $\tilde{f}(x) = \text{fl}(x) \tilde{+} 1$  is  
forward but not backward stable for small  $x$ .

**Literature.** [TB, Lecture 14 & 15]

## 1.4 Conditioning & Stability (8.11.)

```
function wilkinson_polynomial
a = poly(1:20); x = roots(a); plot(real(x),imag(x),'*'); hold on
for n=1:100, r = randn(size(a)); b = a.*(1 + 1e-10*r);
x = roots(b); plot(real(x),imag(x),'*'), end
```

Polynomial root finding is typically ill-conditioned.

**Multiple roots.** Consider  $p(x) = x^2 - 2x + 1 = (x - 1)^2$  and  $q(x) = x^2 - 2x + 0.9999 = (x - 0.99)(x - 1.01)$ . The roots of  $x^2 - 2x + a_0$  are  $2 \pm \sqrt{4 - 4a_0}$ . The condition number of  $f : [0, 1) \rightarrow \mathbb{R}, a_0 \mapsto \sqrt{1 - a_0}$  is

$$\kappa_f(a_0) = \frac{|f'(a_0)| \cdot |a_0|}{|f(a_0)|} = \frac{a_0}{2(1 - a_0)} \xrightarrow{a_0 \rightarrow 1} \infty.$$

**Simple roots.** Let  $a_i$  be the  $i$ th coefficient of  $p$  and  $x_j$  the  $j$ th root. Since  $p(x) = p'(x_j)(x - x_j) + O(|x - x_j|^2)$ ,

$$\kappa_{x_j}(a_i) = \lim_{\delta \rightarrow 0} \sup_{|\Delta a_i| < \delta} \frac{|x_j(a_i + \Delta a_i) - x_j(a_i)| \cdot |a_i|}{|x_j(a_i)| \cdot |\Delta a_i|} = \frac{|a_i x_j(a_i)^{i-1}|}{|p'(x_j)|}.$$

```
function wilkinson_condition
```

```
a = poly(1:20); kappa = a(6)*15^14/(factorial(14)*factorial(5))
```

**Eigenvalues.** Computing the eigenvalues of  $A \in \mathbb{R}^{n \times n}$  by root finding for the characteristic polynomial  $p(x) = \det(x\text{Id} - A)$  is not forward stable.

```
function eigenvalues
```

```
b = [1,1]; x = roots([1,-b(1)-b(2),b(1)*b(2)])
```

```
b(1) = 1+1e-14; y = roots([1,-b(1)-b(2),b(1)*b(2)])
```

**Product estimates.** Let  $f = h \circ g$ , that is  $f(x) = h(g(x)) = h(y)$ , and  $\tilde{f} = \tilde{h} \circ \tilde{g}$ . Then,

$$\begin{aligned}\sigma_{\tilde{f}}(x)\kappa_f(x) &\leq \kappa_h(y) \cdot (\sigma_{\tilde{h}}(\tilde{y}) + \sigma_{\tilde{g}}(x)\kappa_g(x)), \\ \rho_{\tilde{f}}(x) &\leq \rho_{\tilde{g}}(x) + \kappa_{g^{-1}}(y)\rho_{\tilde{h}}(\tilde{y}).\end{aligned}$$

**Rules of Thumb.** Algorithms built on well-conditioned problems solved by forward stable algorithms are forward stable. For backward stability, the intermediate steps should have a well-conditioned inverse mapping.

**Literature.** [TB, Lecture 12 & 15], [B]

## 2 Nonlinear equations

### 2.1 Newton's method (10.11.)

Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  be a bounded function with continuous derivatives. We compute zeros of  $f$ , that is,  $x_*$  with  $f(x_*) = 0$ .

**Conditioning.** We use the norm

$$\|\Delta f\|_\infty = \sup\{|\Delta f(x)| : x \in \mathbb{R}\}.$$

We assume that  $f + \Delta f$  has a zero  $\tilde{x}_*$  with  $\tilde{x}_* \rightarrow x_*$  as  $\|\Delta f\|_\infty \rightarrow 0$ . Since  $f(\tilde{x}_*) = -\Delta f(\tilde{x}_*)$  and  $f(\tilde{x}_*) = f'(x_*)(\tilde{x}_* - x_*) + O(|\tilde{x}_* - x_*|^2)$ , we obtain

$$\kappa_{x_*}(f) = \lim_{\delta \rightarrow 0} \sup_{\|\Delta f\|_\infty < \delta} \frac{|\tilde{x}_* - x_*| \cdot \|f\|_\infty}{\|\Delta f\|_\infty \cdot |x_*|} = \frac{\|f\|_\infty}{|f'(x_*)| \cdot |x_*|}.$$

Therefore, zeros with small first derivative are badly conditioned.

**Newton's method.** Starting from  $x_0$ , we construct a sequence  $x_1, x_2, \dots$  with  $\lim_{k \rightarrow \infty} x_k = x_*$ . Newton's method defines

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}.$$

This can be motivated geometrically as well as analytically via  $0 = f(x_*) = f(x_k) + f'(x_k)(x_* - x_k) + O(|x_* - x_k|^2)$ .

```
function newton_reciprocal
```

```
a = 0.5; x = 0.1; x = 2*x - a*x^2; x-1/a,
```

```
a = 0.5; x = 10; x = 2*x - a*x^2; x-1/a
```

```
a = 1e-10; x = a; x = 2*x - a*x^2; x-1/a
```

```
function newton_square_root
```

```
x = 2; x = (x + 2/x)/2, x-sqrt(2)
```

**Theorem.** If  $f'(x_*) \neq 0$  and  $x_0$  is sufficiently close to  $x_*$ , then  $\lim_{k \rightarrow \infty} x_k = x_*$  and

$$\lim_{k \rightarrow \infty} \frac{x_{k+1} - x_*}{(x_k - x_*)^2} = \frac{f''(x_*)}{2f'(x_*)}$$

**Remark.** The theorem says that Newton's method is quadratically convergent.

**Literature.** [S, Lectures 2 & 5]

## 2.2 Newton's method for systems (17.11.)

**Fixed point methods.** Let  $\varphi(x) = x - f(x)/f'(x)$ . Newton's method is  $x_{k+1} = \varphi(x_k)$  and computes a fixed point of  $\varphi$ , that is,  $x_*$  with

$$\varphi(x_*) = x_*.$$

We observe that  $\varphi'(x_*) = 0$ ,  $\varphi''(x_*) = f''(x_*)/f'(x_*)$ .

**Theorem.** Let  $|\varphi'(x_*)| < 1$ . If  $\varphi^{(p)}(x_*) \neq 0$ ,  $\varphi'(x_*) = \dots = \varphi^{(p-1)}(x_*) = 0$  and  $x_0$  is sufficiently close to a fixed point  $x_*$  of  $\varphi$ , then  $x_{k+1} = \varphi(x_k)$  converges to  $x_*$  and

$$\lim_{k \rightarrow \infty} \frac{x_{k+1} - x_*}{(x_k - x_*)^p} = \frac{1}{p!} \varphi^{(p)}(x_*).$$

**Systems.** For zeros of  $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ , Newton's method is

$$x_{k+1} = x_k - f'(x_k)^{-1} f(x_k),$$

where  $f'(x_k) \in \mathbb{R}^{n \times n}$  is the Jacobian of  $f$  at  $x_k$ . This requires two steps: solve the linear system  $f'(x_k)y_k = f(x_k)$ , update  $x_{k+1} = x_k - y_k$ .

**Termination.** For  $x_k$  sufficiently close to  $x_*$ ,

$$\frac{1}{4\kappa} \cdot \frac{\|x_k - x_*\|}{\|x_k - x_0\|} \leq \frac{\|f(x_k)\|}{\|f(x_0)\|} \leq 4\kappa \cdot \frac{\|x_k - x_*\|}{\|x_k - x_0\|},$$

where  $\kappa = \|f'(x_*)\| \cdot \|f'(x_*)^{-1}\|$  is the condition number of the Jacobian  $f'(x_*)$ . One might terminate, if

$$\|f(x_k)\| \leq \tau_{\text{rel}} \|f(x_0)\| + \tau_{\text{abs}}.$$

Alternatively, one might terminate, if  $\|y_k\| \leq \tau_{\text{rel}} \|x_k - x_0\|$ , since  $\|x_k - x_*\| = \|y_k\| + O(\|x_k - x_*\|^2)$ .

```

function newton_system
x = linspace(-2,2); [X1,X2] = meshgrid(x);
Y = sin(pi/2*X1) + X2.^3; contour(X1,X2,Y), colorbar
hold on, t = linspace(0,2*pi); plot(cos(t),sin(t),'-r')
x = [1;1]; plot(x(1),x(2),'*r')
x = x - [2*x(1), 2*x(2); pi/2*cos(pi/2*x(1)), 3*x(2)^2]\...
[x(1)^2 + x(2)^2-1; sin(pi/2*x(1)) + x(2)^3];

```

**Literature.** [S, Lecture 3], [K, Chapter 5]

### 3 Interpolation

#### 3.1 Polynomial interpolation (22.11.)

Let  $x_0, \dots, x_n$  be distinct points in  $[-1, 1]$  and  $y_0, \dots, y_n \in \mathbb{R}$ . Polynomial interpolation provides *the* polynomial  $p$  of degree  $\leq n$  such that  $p(x_j) = y_j$  for all  $j = 0, \dots, n$ .

**Lagrange polynomials.** Let  $\ell_j(x)$  be the polynomial of degree  $\leq n$  such that  $\ell_j(x_k) = \delta_{kj}$ . Then,

$$p(x) = \sum_{j=0}^n y_j \ell_j(x).$$

```
x = linspace(-1,1,7); y = [0 0 0 0 0 1 0]; p = polyfit(x,y,6);  
xx = linspace(-1,1); yy = polyval(p,xx); plot(xx,yy,x,y,'*')
```

**Conditioning.** Let the nodes  $x_0, \dots, x_n$  be given and  $P_n(y)$  be the interpolating polynomial for  $y = (y_0, \dots, y_n)$ . The absolute condition number is

$$\kappa_P(y) = \lim_{\delta \rightarrow 0} \sup_{\|\Delta y\|_\infty < \delta} \frac{\|P_n(y + \Delta y) - P_n(y)\|_\infty}{\|\Delta y\|_\infty} = \sup_{x \in [-1,1]} \sum_{j=0}^n |\ell_j(x)| =: \Lambda_n,$$

the Lebesgue constant of the nodes. Always,  $\Lambda_n \geq \frac{2}{\pi} \log(n + 1) + 0.5$ .

```
n = [10:10:1000]; c = 2/pi*log(n+1)+1; e = 2.^(n-2)./n.^2;  
subplot(2,1,1), plot(n,c,'b'), subplot(2,1,2), semilogy(n,e,'r')
```

**First barycentric interpolation formula.**  $\ell_j(x) = \frac{\prod_{k \neq j} (x - x_k)}{\prod_{k \neq j} (x_j - x_k)} = \ell(x) \frac{w_j}{x - x_j}$  with  $\ell(x) = \prod_{k=0}^n (x - x_k)$  the node polynomial. This gives

$$p(x) = \ell(x) \sum_{j=0}^n \frac{y_j w_j}{x - x_j}.$$

The formula is backward stable and requires  $O(n)$  flops for pre-computed weights.

**Interpolation error.** If  $y_j = f(x_j)$ , then  $f(x) - p(x) = \ell(x)f^{(n+1)}(\xi)/(n+1)!$  for some  $\xi \in [-1, 1]$ .

```
n = 8; x = cos(pi/n*[0:n]); % x = linspace(-1,1,n+1);
y = 1./(1+25*x.^2);
for j=1:n+1, w(j) = prod(1./(x(j) - x([1:j-1, j+1:end]))); end
xx = linspace(-1,1); yy = 1./(1+25*xx.^2); l = 1; s = 0;
for j=1:n+1, l = l.*(xx-x(j)); s = s + y(j)*w(j)./(xx-x(j)); end
p = l.*s; plot(xx,yy,xx,p,x,y,'*')
```

**Literature.** [T, Chapter 5 & 15]

### 3.2 Trigonometric interpolation (24.11)

Let  $x_0, \dots, x_{n-1}$  be distinct points in  $[0, 2\pi]$  and  $y_0, \dots, y_{n-1} \in \mathbb{C}$ . Trigonometric interpolation provides *the* trigonometric polynomial

$$p(x) = \sum_{j=0}^{n-1} c_j e^{ijx}$$

such that  $p(x_j) = y_j$  for all  $j = 0, \dots, n-1$ . From now on,  $x_j = 2\pi j/n$ .

**Conditioning.** As for algebraic interpolation, the absolute condition number is the Lebesgue constant  $\Lambda_n$ , and one can prove  $\Lambda_n \leq \frac{2}{\pi} \log(n) + \frac{5}{3}$ .

**Fast Fourier Transform.** We observe  $e^{ijx_k} = e^{2\pi ijk/n} = \omega_n^{jk}$ , write  $y_k = \sum_{j=0}^{n-1} c_j \omega_n^{jk}$  and compute  $c_l = \frac{1}{n} \sum_{k=0}^{n-1} \omega_n^{-lk} y_k$ . Let  $n = 2^m$ . Since  $\omega_{2n}^2 = \omega_n$ ,

$$c_l = \frac{1}{n} \sum_{k=0}^{n/2-1} \omega_{n/2}^{-lk} y_{2k} + \frac{1}{n} \omega_n^{-l} \sum_{k=0}^{n/2-1} \omega_{n/2}^{-lk} y_{2k+1} = \dots$$

This is the basic observation for the FFT, the computation of  $c = (c_0, \dots, c_{n-1})$  in  $O(n \log(n))$  flops, which can be done with a backward stable algorithm.

```
n = 32; y = zeros(1,n); y(1) = 1; p = fft(y);
subplot(1,2,1), plot([0:n-1],real(p), 'b-*'),
subplot(1,2,2), plot([0:n-1],imag(p), 'r-*')
```

**Fourier Series.** Let  $f : [-\pi, \pi] \rightarrow \mathbb{C}$  be  $2\pi$ -periodic, continuously differentiable. Then,  $f(x) = \sum_{j=-\infty}^{\infty} \widehat{f}_j e^{ijx}$ , where

$$\widehat{f}_j = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ijx} dx$$

is the  $j$ th Fourier coefficient. We write the trigonometric interpolant for  $x_j = 2\pi j/n$ ,  $y_j = f(x_j)$  as  $p(x) = \sum_{j=-n/2}^{n/2-1} c_j e^{ijx}$  and observe

$$c_j = \frac{1}{n} \sum_{k=-n/2}^{n/2-1} y_k \omega_n^{-jk} = \frac{1}{2\pi} \cdot \frac{2\pi}{n} \sum_{k=-n/2}^{n/2-1} f(x_k) e^{-ijx_k} \approx \hat{f}_j.$$

**Aliasing.** The interpolation property yields  $c_j = \sum_{k=-\infty}^{\infty} \hat{f}_{j+kn}$ .

```
n = 8; x = 2*pi/n*[0:n-1]; y = sin(x) + 3*sin(5*x);
xx = linspace(0,2*pi,100); yy = sin(xx) + 3*sin(5*xx);
z = interpft(y,100); plot(xx,yy,'b-',xx,z,'r-',x,y,'ro')
n = 16; x = 2*pi/n*[0:n-1]; y = sin(x) + 3*sin(5*x);
z = interpft(y,100); hold on, plot(xx,z,'g-')
```

**Literature.** [M, Chapter 8]

### 3.3 Spline interpolation (29.11.)

**Linear splines.** Let  $x_0, \dots, x_n \in [a, b]$  with  $a = x_0 < \dots < x_n = b$  and  $y_0, \dots, y_n \in \mathbb{R}$ . The continuous function  $s : [a, b] \rightarrow \mathbb{R}$ , which is linear on each interval  $[x_j, x_{j+1}]$  and satisfies  $s(x_j) = y_j$  for all  $j = 0, \dots, n$ , is *the* interpolating linear spline:

$$s(x) = y_j + \frac{y_{j+1} - y_j}{x_{j+1} - x_j}(x - x_j), \quad x \in [x_j, x_{j+1}].$$

**Approximation error.** Let  $f : [a, b] \rightarrow \mathbb{R}$  be twice continuously differentiable and  $y_j = f(x_j)$  for all  $j$ . Then,  $f(x) - s(x) = \frac{1}{2}f''(\xi)(x - x_j)(x - x_{j+1})$  for  $x \in [x_j, x_{j+1}]$ . If  $h_j = x_{j+1} - x_j$  and  $h = \max\{h_0, \dots, h_{n-1}\}$ , then

$$\|f - s\|_\infty \leq \frac{h^2}{8} \|f''\|_\infty.$$

```
x = linspace(-2,8,6); y = x.^2 + 10./(sin(x)+1.2);
xx = linspace(-2,8); yy = xx.^2 + 10./(sin(xx)+1.2);
z = interp1(x,y,xx); plot(xx,yy,'b-',xx,z,'r-',x,y,'ro')
```

**Cubic splines.** Twice continuously differentiable functions  $s : [a, b] \rightarrow \mathbb{R}$ , which are cubic polynomials on each interval  $[x_j, x_{j+1}]$  and satisfy  $s(x_j) = y_j$  for all  $j = 0, \dots, n$ , are interpolating cubic splines:

$$s(x) = a_j + b_j(x - x_j) + \frac{s_j}{6h_j}(x_{j+1} - x)^3 + \frac{s_{j+1}}{6h_j}(x - x_j)^3$$

with  $a_j = y_j - \frac{1}{6}s_j h_j^2$ ,  $b_j = d_j - \frac{1}{6}(s_{j+1} - s_j)h_j$ ,  $d_j = (y_{j+1} - y_j)/h_j$ . The second derivatives  $s_j = s''(x_j)$  satisfy

$$\frac{h_j}{6}s_j + \frac{h_j + h_{j+1}}{3}s_{j+1} + \frac{h_{j+1}}{6}s_{j+2} = d_{j+1} - d_j, \quad j = 1, \dots, n-2.$$

**End conditions.**  $s'(a) = f'(a)$ ,  $s'(b) = f'(b)$  yields *the* complete spline. The not-a-knot condition is

$$s|_{[x_0,x_1]} = s|_{[x_1,x_2]}, \quad s|_{[x_{n-2},x_{n-1}]} = s|_{[x_{n-1},x_n]}.$$

The resulting tridiagonal linear systems are well-conditioned and can always be solved in a backward stable way in  $O(n)$  flops.

**Approximation error.** If  $f$  is four times continuously differentiable, then both cubic splines satisfy

$$\|f^{(r)} - s^{(r)}\|_\infty \leq C_r h^{4-r} \|f^{(4)}\|_\infty, \quad r = 0, 1, 2.$$

`z = interp1(x,y,xx,'spline'); hold on, plot(xx,z,'g-')`

**Literature.** [S2, Chapter 10 & 11]

## 4 Quadrature

### 4.1 Basics (1.12.)

Let  $f : [a, b] \rightarrow \mathbb{R}$  be continuous. Let  $x_0, \dots, x_n \in [a, b]$  and  $w_0, \dots, w_n \in \mathbb{R}$ . We approximate

$$I(f) = \int_a^b f(x)dx \approx \sum_{j=0}^n w_j f(x_j) = Q(f).$$

**Conditioning.** If  $\|w\|_1 = |w_0| + \dots + |w_n|$ , then

$$\kappa_I(f) = \frac{(b-a)\|f\|_\infty}{|I(f)|}, \quad \kappa_Q(f) = \frac{\|w\|_1\|f\|_\infty}{|Q(f)|}.$$

Hence, integration and quadrature of oscillatory functions are ill-conditioned.

**Stability.** If  $Q(1) = I(1)$ , then

$$\kappa_Q(f) \geq \kappa_I(f) + (b-a)\|f\|_\infty \cdot r(I(f), Q(f)) \quad (*)$$

with  $|r(I(f), Q(f))| \leq |I(f) - Q(f)|$ . (\*) is an equality iff  $w_0, \dots, w_n \geq 0$ . Therefore, positive weights are preferred.

**Simple interpolatory rules.** Let  $p_1, p_2, p_3$  be the interpolating polynomials for the nodes  $\{\frac{a+b}{2}\}$ ,  $\{a, b\}$ , and  $\{a, \frac{a+b}{2}, b\}$ , respectively. Then,

$$\begin{aligned} M_{[a,b]}(f) &= I(p_1) = (b-a)f\left(\frac{a+b}{2}\right), \\ T_{[a,b]}(f) &= I(p_2) = \frac{b-a}{2}(f(a) + f(b)), \\ S_{[a,b]}(f) &= I(p_3) = \frac{b-a}{6}(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)). \end{aligned}$$

$M$  and  $T$  are exact for linear integrands,  $S$  for cubic ones.

**Composite rules.** Let  $n$  be even and  $x_j = a + jh$ ,  $j = 0, \dots, n$  with  $h = (b - a)/n$  and  $f_j = f(x_j)$ . The composite rules are

$$M_n(f) = \sum_{j=0}^{n/2-1} M_{[x_{2j}, x_{2(j+1)}]}(f) = \sum_{j=0}^{n/2-1} 2hf_{2j+1},$$

$$T_n(f) = \sum_{j=1}^n T_{[x_{j-1}, x_j]}(f) = \frac{h}{2}(f_0 + f_n) + \sum_{j=1}^{n-1} hf_j,$$

$$S_n(f) = \sum_{j=0}^{n/2-1} S_{[x_{2j}, x_{2(j+1)}]}(f) = \frac{h}{3}(f_0 + \sum_{j=0}^{n/2-1} 4f_{2j+1} + \sum_{j=1}^{n/2-1} 2f_{2j} + f_n)$$

$M_n$  and  $T_n$  are both  $O(h^2)$ ,  $S_n$  is  $O(h^4)$  accurate.

```
n = 10; x = linspace(-1,1,n); y = exp(-x.^2/2)/sqrt(2*pi);
T = trapz(x,y), I = quad('exp(-x.^2/2)/sqrt(2*pi)',-1,1)
```

**Literature.** [S, Chapter 21]

## 4.2 Gauß quadrature (6.12.)

Let  $w : [a, b] \rightarrow [0, \infty[$ . We compute

$$I_w(f) = \int_a^b f(x)w(x)dx \approx Q(f) = \sum_{j=0}^n w_j f(x_j)$$

for  $f : [a, b] \rightarrow \mathbb{R}$  continuous. Let  $\mathbb{P}_n$  the space of polynomials of degree  $\leq n$ .

**Weights.**  $\forall p \in \mathbb{P}_n : Q(p) = I_w(p)$  if and only if  $\forall j = 0, \dots, n : w_j = I_w(\ell_j)$ . Moreover,  $\forall p \in \mathbb{P}_{2n} : Q(p) = I_w(p)$  implies  $\forall j = 0, \dots, n : w_j \geq 0$ .

**Idea of Gauß quadrature.** Let  $Q$  be exact on  $\mathbb{P}_n$ . We determine nodes such that  $Q$  is exact on  $\mathbb{P}_{2n+1}$ . Let  $p \in \mathbb{P}_{2n+1}$  and  $p_{n+1} \in \mathbb{P}_{n+1}$ . We write  $p = qp_{n+1} + r$  with  $q, r \in \mathbb{P}_n$ . Then,  $I_w(p) = I_w(qp_{n+1}) + Q(r)$  and we obtain  $I_w(p) = Q(p)$ , if

$$\forall q \in \mathbb{P}_n : I_w(qp_{n+1}) = 0 = Q(qp_{n+1}).$$

This works, if  $x_0, \dots, x_n$  are the roots of  $p_{n+1}$  and  $p_{n+1}$  is orthogonal on  $\mathbb{P}_n$ .

**Orthogonal polynomials.**  $(p_n)_{n \geq 0}$  is a family of orthogonal polynomials, if  $p_n \in \mathbb{P}_n$ ,  $p_n \neq 0$  for all  $n$  and

$$\forall n \neq m : I_w(p_n p_m) = 0.$$

Each family satisfies a 3-term recurrence

$$a_n p_{n+1}(x) = (b_n + c_n x) p_n(x) - d_n p_{n-1}(x)$$

with  $(b_n)_{n \geq 0}$ ,  $(c_n)_{n \geq 0}$ ,  $(d_n)_{n \geq 0}$  sequences of real numbers.

	$[a, b]$	$w$	$a_n$	$b_n$	$c_n$	$d_n$
Legendre $P_n$	$[-1, 1]$	1	$n + 1$	0	$2n + 1$	$n$
Hermite $H_n$	$]-\infty, +\infty[$	$e^{-x^2}$	1	0	2	$2n$
Laguerre $L_n$	$[0, \infty[$	$e^{-x}$	$n + 1$	$2n + 1$	-1	$n$

**Eigenvalue problems.** The 3-tem recurrence allows to characterize the nodes as the eigenvalues of a symmetric tridiagonal eigenvalue problem, while the weights can be obtained from the eigenvectors.

```
function gauss_legendre
n = 6; beta = .5./sqrt(1-(2*(1:n)).^(-2));
T = diag(beta,1) + diag(beta,-1); [V,D] = eig(T);
x = diag(D); w = 2*V(1,:).^2; I = w*cos(x);
error = I - 2*sin(1)
```

**Literature.** [S, Chapter 23]

### 4.3 Monte Carlo quadrature (13.12.)

Let  $\Omega \subset \mathbb{R}^d$  and  $w : \Omega \rightarrow [0, \infty[$  such that  $\int_{\Omega} w(x)dx = 1$ . Then,

$$I_w(f) = \int_{\Omega} f(x)w(x)dx = \mathbb{E}_w(f).$$

Here,  $I_w(f)$ ,  $I_w(f^2)$  exist and are finite.

**Strong law of large numbers.** Let  $(X_n)_{n>0}$  be independent identically distributed random variables distributed according to  $w$ . Then,

$$\mathbb{P}\left(\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{j=1}^n f(X_j) - \mathbb{E}_w(f)\right) = 1.$$

function plain\_mc

```
n = 10; x = rand(n,1); plot(x,zeros(n,1),'ro'), I = sum(x)/n
```

**Expectation & variance.** Let  $Q_n(f) = \frac{1}{n} \sum_{j=1}^n f(X_j)$ . Then,  $\mathbb{E}(Q_n(f)) = \mathbb{E}_w(f)$  and  $\mathbb{V}(Q_n(f)) = \mathbb{V}_w(f)/n$ . Therefore,

$$\sqrt{\mathbb{E}([Q_n(f) - \mathbb{E}_w(f)]^2)} = \frac{\sigma_w(f)}{\sqrt{n}}.$$

**Statistics.** Let  $q_1, \dots, q_m$  be independent runs of  $Q_n(f)$ . Then,

$$\bar{q} = \frac{1}{m} \sum_{j=1}^m q_j, \quad \bar{v} = \frac{1}{m-1} \sum_{j=1}^m (q_j - \bar{q})^2$$

are unbiased estimators of  $\mathbb{E}_w(f)$  and  $\mathbb{V}_w(f)$ , respectively. That is,  $\mathbb{E}(\bar{q}) = \mathbb{E}(Q_n(f))$  and  $\mathbb{E}(\bar{v}) = \mathbb{V}(Q_n(f))$ .

```

function integrate_mc
n = 1e+4; for j=1:10, q(j) = sum(rand(n,1))/n; end,
error = abs(mean(q)-0.5), error_est = sqrt(var(q)),
error_L2 = 1/2/sqrt(n)

function normal_distr
n = 1e+4; for j=1:10, x = 1+randn(n,1)*2; q(j) = sum(x)/n; end,
error = abs(mean(q)-1),
n = 100; m = 2; q = zeros(2,m);
for j=1:m, x = repmat([1,2],n,1)+randn(n,2)*chol([1,0.5;0.5,2]);
plot(x(:,1),x(:,2),'ro'); q(:,j) = sum(x,1)/n; end,
error = norm(mean(q,2)'-[1,2])

```

**Literature.** [DR, Chapter 5.9]

## 5 Linear systems

### 5.1 Basics (15.12.)

Let  $A \in \mathbb{R}^{n \times n}$  be invertible,  $b \in \mathbb{R}^n$ . We compute  $x \in \mathbb{R}^n$  with  $Ax = b$ .

**Conditioning.** Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ ,  $b \mapsto A^{-1}b$ . Then,

$$\kappa_f(b) = \lim_{\delta \rightarrow 0} \sup_{\|\Delta b\| < \delta} \frac{\|A^{-1}(b + \Delta b) - A^{-1}b\| \cdot \|b\|}{\|A^{-1}b\| \cdot \|\Delta b\|} = \frac{\|A^{-1}\| \cdot \|b\|}{\|A^{-1}b\|}$$

and  $\kappa_f(Ab) = \|A^{-1}\| \cdot \|Ab\|/\|b\| \leq \|A^{-1}\| \cdot \|A\| =: \kappa(A)$  for all  $b \in \mathbb{R}^n$ .

```
A = [0.2161, 0.1441; 1.2969 0.8648]; b = [0.144; 0.8642];  
x = A\b; b = b + 1e-8*rand(2,1); dev = A\b - x, kappa = cond(A)
```

**Preconditioning.** An invertible  $B \in \mathbb{R}^{n \times n}$  with  $\kappa(BA) \ll \kappa(A)$  is called a preconditioner for  $A$ .

**Literature.** [S, Lecture 16]

## 5.2 Gaussian elimination (20.12.)

**Triangular systems.** Let  $L, U \in \mathbb{R}^{n \times n}$  be a lower and upper triangular matrix,  $l_{ij} = 0$  for  $i < j$  and  $u_{ij} = 0$  for  $i > j$ , respectively. Let  $L, U$  be invertible, that is  $l_{ii} \neq 0$  and  $u_{ii} \neq 0$  for all  $i$ . We write  $Lx = b$  as

$$\begin{pmatrix} \lambda & 0 \\ l & L_* \end{pmatrix} \begin{pmatrix} x_1 \\ x_* \end{pmatrix} = \begin{pmatrix} \lambda y \\ x_1 l + L_* x_* \end{pmatrix} = \begin{pmatrix} \beta \\ b_* \end{pmatrix}$$

with  $L_* \in \mathbb{R}^{(n-1) \times (n-1)}$  upper triangular,  $l, x_*, b_* \in \mathbb{R}^{n-1}$ ,  $\lambda \neq 0$ ,  $x_1, \beta \in \mathbb{R}$ .

function forward\_sub

```
n = 100; L = tril(rand(n))+eye(n); spy(L);
```

```
b = rand(n,1); xx = L\b;
```

```
for i=1:n, x(i)=b(i)/L(i,i); b(i+1:n)=b(i+1:n)-x(i)*L(i+1:n,i);
```

```
end, error = norm(x-xx)
```

**Substitution.** Forward (back) substitution is a backward stable algorithm for solving lower (upper) triangular systems using  $\sum_{i=1}^n (2(n-i) + 1) = n^2$  flops.

**LU decomposition.** Consider an invertible  $A \in \mathbb{R}^{n \times n}$  admitting a decomposition  $A = LU$  with  $L$  lower unit triangular and  $U$  upper triangular such that

$$\begin{pmatrix} \alpha & a^T \\ b & A_* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ l & L_* \end{pmatrix} \begin{pmatrix} \mu & u^T \\ 0 & U_* \end{pmatrix} = \begin{pmatrix} \mu & u^T \\ \mu l & lu^T + L_* U_* \end{pmatrix}$$

with  $A_*, L_*, U_* \in \mathbb{R}^{(n-1) \times (n-1)}$ ,  $a, b, l, u \in \mathbb{R}^{n-1}$ ,  $\alpha, \mu \neq 0$ .

function LU\_fac

```

n=100; A=rand(n); LL=tril(A,-1)+eye(n); UU=triu(A)+eye(n);
A=LL*UU; cond(A), L=eye(n); U=zeros(n,n);
for i=1:n, U(i,i:n)=A(i,i:n); L(i+1:n,i)=A(i+1:n,i)/A(i,i);
A(i+1:n,i+1:n)=A(i+1:n,i+1:n)-L(i+1:n,i)*U(i,i+1:n); end,
norm(L*U-LL*UU)

```

**Operation count.**  $\sum_{i=1}^n (2(n-i)^2 + (n-i)) \approx \int_0^n 2x^2 dx = \frac{2}{3}n^3$  flops. Solving  $Ax = b$  via  $Ly = b$ ,  $Ux = y$  is dominated by the cost for the  $LU$  decomposition.

**Pivoting.** The maximal entry in magnitude of each column vector  $a_{i:n,i}$  does not vanish. We permute rows to divide by this maximal entry. This also yields  $|l_{i,j}| \leq 1$  for all  $i, j$ , which is important for stability.

```

function pivoting
[y,ii]=max(abs(A(i:n,i))); ii=ii+i-1;
A([ii,i],i:n)=A([i,ii],i:n); L([ii,i],1:i-1)=L([i,ii],1:i-1);

```

**Literature.** [TB, Lecture 20 & 21]

### 5.3 Iterative methods (22.12.)

**Jacobi & Gauß-Seidel iteration.** We write the  $i$ th row of the linear system  $Ax = b$  as  $x_i = (b_i - \sum_{j \neq i} a_{ij}x_j)/a_{ii}$ . We construct a sequence  $(x^k)_{k>0}$  in  $\mathbb{R}^n$  by the Jacobi iteration

$$x_i^{k+1} = (b_i - \sum_{j \neq i} a_{ij}x_j^k)/a_{ii}$$

and hope for  $\lim_{k \rightarrow \infty} x^k = A^{-1}b$ . The Gauß-Seidel iteration is defined by

$$x_i^{k+1} = (b_i - \sum_{j < i} a_{ij}x_j^{k+1} - \sum_{j > i} a_{ij}x_j^k)/a_{ii}.$$

**Matrix form.** Let  $A = D - L - U = \text{diag}(A) + \text{tril}(A, -1) + \text{triu}(A, 1)$ . We write the Jacobi iteration as

$$x^{k+1} = D^{-1}b + D^{-1}(L + U)x^k.$$

The Gauß-Seidel iteration takes the form

$$x^{k+1} = D^{-1}(b + Lx^{k+1} + Ux^k) = (D - L)^{-1}b + (D - L)^{-1}Ux^k.$$

```
n = 100; A = rand(n); for i=1:n, A(i,i)= sum(abs(A(i,:))); end,
b = rand(n,1); D = diag(diag(A)); L = -tril(A,-1); U = -triu(A,1);
m = 10; x = rand(n,1); y = x;
for k=1:m, k; x=D\b + D\ (L+U)*x; y=(D-L)\b + (D-L)\U*y;
norm(x-A\b), norm(y-A\b), pause, end
```

**Splitting.** Let  $A = M - N$  with  $M$  invertible. We write  $Ax = (M - N)x = b$  as  $x = M^{-1}b + M^{-1}Nx$  and derive a stationary iteration

$$x^{k+1} = M^{-1}b + M^{-1}Nx^k.$$

The Jacobi and Gauß-Seidel iteration are stationary with  $A = D - (L + U)$  and  $A = (D - L) - U$ , respectively.

**Convergence.** We write  $x^{k+1} - x = M^{-1}N(x^k - x) = (M^{-1}N)^{k+1}(x^0 - x)$ . Sufficient conditions for convergence are

$$\lim_{k \rightarrow \infty} (M^{-1}N)^k = 0, \quad \|M^{-1}N\| < 1.$$

$\text{norm}(D \setminus (L+U))$ ,  $\text{norm}((D-L) \setminus U)$

**Literature.** [S2, Lecture 25]

## 6 Least-squares-problems

### 6.1 Normal equations (10.1.)

Let  $A \in \mathbb{R}^{m \times n}$ ,  $b \in \mathbb{R}^m$  with  $m \geq n$ . We seek a solution to the overdetermined linear system  $Ax = b$  in the following sense:  $x \in \mathbb{R}^n$  shall minimize

$$\|Ax - b\|_2 = \sqrt{\sum_{j=1}^m ((Ax)_j - b_j)^2}.$$

We solve a least squares problem.

**Polynomial data fit.** Fitting a polynomial of degree  $n-1$  to  $m$  data points  $(x_1, y_1), \dots, (x_m, y_m)$  with  $m \geq n$  can be formulated as a linear system  $Ac = y$  with  $A \in \mathbb{R}^{m \times n}$  a Vandermonde matrix,

$$A = \begin{pmatrix} x_1^{n-1} & x_1^{n-2} & \dots & 1 \\ x_2^{n-1} & x_2^{n-2} & \dots & 1 \\ \vdots & \vdots & \dots & \vdots \\ x_m^{n-1} & x_m^{n-2} & \dots & 1 \end{pmatrix}.$$

function polyfit

```
n = 11; x = linspace(-1,1,n); y = rand(n,1);
```

```
A = vander(x); cond(A), c = A\y;
```

```
xx = linspace(-1,1); plot(xx,polyval(c,xx),x,y,'o')
```

```
A = A(:,3:n); d = A\y; hold on, plot(xx,polyval(d,xx),'g')
```

**Normal equations.**  $x \in \mathbb{R}^n$  minimizes the residual norm  $\|r\|_2 = \|b - Ax\|_2$  if and only if  $r \perp \text{range}(A)$  if and only if  $A^T r = 0$  if and only if  $x$  satisfies the normal equations

$$A^T Ax = A^T b.$$

The solution  $x$  is unique if and only if  $\text{rank}(A) = n$ .

```
function laeuchli
d = 1e-7; A = [1,1; d,0; 0,d]; cond(A), b = [2;d;d]; xx = [1;1];
x = A'*A\(A'*b); y = A\b; norm(x-xx), norm(y-xx), cond(A'*A)
```

**Cholesky decomposition.**  $A^T A \in \mathbb{R}^{n \times n}$  is symmetric. If  $\text{rank}(A) = n$ , then  $A^T A$  is positive definite, that is,  $x^T (A^T A)x > 0$  for all  $x \neq 0$ . Therefore,

$$A^T A = LL^T$$

for a uniquely determined lower triangular matrix  $L$  with positive diagonal entries.  $L$  can be computed backward stably in approximately  $\frac{1}{3}n^3$  flops.

**Literature.** [TB, Lecture 11]

## 6.2 QR decomposition (12.1.)

**Orthogonal matrices.** A matrix  $Q \in \mathbb{R}^{n \times n}$  is orthogonal, if

$$Q^T = Q^{-1}.$$

From  $Q^T Q = \text{Id}$  we deduce  $q_i^T q_j = \delta_{ij}$  for the column vectors  $q_1, \dots, q_n$ . Moreover,  $(Qx)^T Qy = x^T y$  and  $\|Qx\|_2 = \|x\|_2$  for all  $x, y \in \mathbb{R}^n$ . Consequently  $\|Q\|_2 = 1$  and  $\kappa(Q) = 1$ .

**QR decomposition.** Any  $A \in \mathbb{R}^{m \times n}$  with  $m \geq n$  admits a QR decomposition

$$A = QR$$

with  $Q \in \mathbb{R}^{m \times m}$  an orthogonal matrix and  $R \in \mathbb{R}^{m \times n}$  upper triangular. If  $\text{rank}(A) = n$ , then  $R$  can be chosen with positive diagonal entries.

**Least squares problem.** We write

$$\|b - Ax\|_2^2 = \|(Q^T b)(1:n) - R(1:n,:)x\|_2^2 + \|(Q^T b)(n+1:m)\|_2^2$$

and obtain the least squares solution by solving the upper triangular system  $R(1:n,:)x = (Q^T b)(1:n)$ .

```
function least_squares
```

```
d = 1e-7; A = [1,1; d,0; 0,d]; b = [2;d;d]; xx = [1;1];  
[Q,R] = qr(A); b = (Q'*b); x = R(1:2,:)\b(1:2); norm(x-xx)
```

**Gram-Schmidt orthogonalization.** Let  $\text{rank}(A) = n$  and set  $a_j = A(:,j)$ . We seek orthonormal vectors  $q_1, \dots, q_n \in \mathbb{R}^m$  such that

$$\forall j = 1, \dots, n : \text{span}\{a_1, \dots, a_j\} = \text{span}\{q_1, \dots, q_j\}.$$

This means  $a_1 = r_{11}q_1$ ,  $a_2 = r_{12}q_1 + r_{22}q_2$ ,  $\dots$ ,  $a_n = r_{1n}q_1 + \dots + r_{nn}q_n$  or

$$A = \hat{Q}\hat{R}$$

with  $\hat{Q} \in \mathbb{R}^{m \times n}$  a matrix with orthonormal columns and  $\hat{R} \in \mathbb{R}^{n \times n}$  upper triangular. This is a reduced QR decomposition.

**Existence.** From  $q_2 = (a_2 - r_{12}q_1)/r_{22}$  we deduce  $r_{12} = q_1^T a_2$ , and from  $q_3 = (a_3 - r_{13}q_1 - r_{23}q_2)/r_{33}$  we obtain  $r_{13} = q_1^T a_3$ ,  $r_{23} = q_2^T a_3$ . Hence,

$$\forall i < j : r_{ij} = q_i^T a_j,$$

and the diagonal elements of  $R$  are used for normalization.

**Literature.** [TB, Lecture 2 & 7]

### 6.3 Householder triangularization (17.1.)

```
function gram_schmidt
m=25; n=15; p=linspace(0,1,m); A=vander(p); A=A(:,11:end);
% classical
for j=1:n, v=A(:,j);
for i=1:(j-1), R(i,j)=Q(:,i)'*A(:,j); v=v-R(i,j)*Q(:,i); end
R(j,j)=norm(v); Q(:,j)=v/R(j,j); end,
norm(Q*R-A)/norm(A), norm(Q'*Q-eye(n)), cond(A)
% modified
V = A; for i=1:n, R(i,i)=norm(V(:,i)); Q(:,i)=V(:,i)/R(i,i);
for j=i+1:n, R(i,j)=Q(:,i)'*V(:,j); V(:,j)=V(:,j)-R(i,j)*Q(:,i);
end, end, norm(Q*R-A)/norm(A), norm(Q'*Q-eye(n))
```

**Gram-Schmidt orthogonalization (classical).** The classical method orthogonalizes  $q_j$  with respect to  $a_1, \dots, a_{j-1}$ . It might produce a not-orthogonal  $Q$ -factor. Operation count: approximately  $\sum_{i=1}^n \sum_{j=i+1}^n 4m \approx 2mn^2$  flops.

**Gram-Schmidt orthogonalization (modified).** The modified method orthogonalizes  $q_{j+1}, \dots, q_n$  with respect to  $q_j$ . It is backward stable with the same operation count as the classical method.

**Householder reflectors.** Instead of orthogonalizing one triangularizes by orthogonal elimination. One uses  $n$  orthogonal matrices of the form

$$Q_k = \begin{pmatrix} \text{Id}_{k-1} & 0 \\ 0 & F \end{pmatrix} \in \mathbb{R}^{m \times m} \quad (k = 1, \dots, n)$$

with  $F$  an orthogonal matrix called Householder reflector: For any vector  $v \in \mathbb{R}^{m-(k-1)}$ , the matrix

$$F = \text{Id} - 2vv^T/\|v\|^2$$

satisfies  $F = F^T$  and  $FF^T = \text{Id}$ .

**Literature.** [TB, Lecture 10 & 16]

## 7 Eigenvalue problems

### 7.1 Basics (19.1.)

**Householder reflectors, continued.** Let  $x$  be the last  $m - (k - 1)$  rows of the  $k$ th column of the matrix  $Q_{k-1}Q_2Q_1A$  and  $v = \text{sign}(x_1)\|x\|e_1 + x$ . Then,  $2v^T x = \|v\|^2$  and the Householder reflector  $F = \text{Id} - 2vv^T/\|v\|^2$  satisfies  $Fx = -\text{sign}(x_1)\|x\|e_1$ , as desired.  $F$  reflects across the hyperplane orthogonal to  $v$ . Altogether,

$$Q_n Q_{n-1} \dots Q_1 A = Q^T A = R.$$

Householder triangularization is backward stable and requires approximately  $2n^2(m - n/3)$  flops.

```
R = triu(randn(50)); [Q,X] = qr(randn(50)); A = Q*R;
[QQ,RR] = qr(A); norm(Q-QQ), norm(R-RR)/norm(R),
norm(A-QQ*RR)/norm(A), norm(QQ'*QQ-eye(50))
```

**Eigenvalues.** Let  $A \in \mathbb{C}^{n \times n}$ .  $\lambda \in \mathbb{C}$  is called an eigenvalue of  $A$ , if there exists a vector  $x \in \mathbb{C}^n$ ,  $x \neq 0$  such that  $Ax = \lambda x$ .

**Characteristic polynomial.**  $\lambda$  is an eigenvalue of  $A$  if and only if it is a zero of the characteristic polynomial

$$p(\lambda) = \det(\lambda \text{Id} - A) = \lambda^n + \dots + (-1)^n \det(A).$$

There are  $n$  not necessarily distinct zeros  $\lambda_1, \dots, \lambda_n \in \mathbb{C}$  such that  $p(\lambda) = (\lambda - \lambda_1) \cdot \dots \cdot (\lambda - \lambda_n)$ . The number of times  $\lambda_j$  appears in the factorization of  $p$  is the algebraic multiplicity of  $\lambda_j$ .

**The adjoint matrix.** The adjoint matrix  $A^* \in \mathbb{C}^{n \times n}$  is defined as

$$(A^*)_{i,j} = \overline{A_{j,i}}.$$

$\lambda$  is an eigenvalue of  $A$  if and only if  $\bar{\lambda}$  is an eigenvalue of  $A^*$ . Let  $y \in \mathbb{C}^n$ ,  $y \neq 0$  satisfy  $A^*y = \bar{\lambda}y$ . Then,  $y^*A = \lambda y^*$ , and  $y^*$  is called a left eigenvector of  $A$  corresponding to  $\lambda$ .

**Double eigenvalues.** The matrix

$$A_\varepsilon = \begin{pmatrix} 1 & 1 \\ \varepsilon & 1 \end{pmatrix}$$

has the characteristic polynomial  $p(\lambda) = (1 - \lambda)^2 - \varepsilon$  and the eigenvalues  $1 \pm \sqrt{\varepsilon}$ . Hence, an  $\varepsilon$ -perturbation of  $A_0$  perturbs the eigenvalue by  $\sqrt{\varepsilon}$ .

**Literature.** [S2, Lecture 12]

## 7.2 Power iterations (24.1.)

**Dominant eigenvector.** Let  $A \in \mathbb{C}^{n \times n}$  have a basis of normalized eigenvectors,  $Ax_j = \lambda_j x_j$ ,  $j = 1, \dots, n$  with  $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ . Let  $v = \alpha_1 x_1 + \dots + \alpha_n x_n$  with  $\alpha_1 \neq 0$ . Then,

$$A^k v = \alpha_1 \lambda_1^k x_1 + |\lambda_1|^k \left( \alpha_2 \frac{\lambda_2^k}{|\lambda_1|^k} + \dots + \alpha_n \frac{\lambda_n^k}{|\lambda_1|^k} x_n \right),$$

and the distance of  $A^k v / \|A^k v\|$  to  $\text{span}(x_1)$  is  $O(|\lambda_2/\lambda_1|^k)$ .

```
A=[1 2;3 4]; [V,D]=eig(A);
plot([0,V(1,2),-V(1,2)],[0,V(2,2),-V(2,2)],'r-'),
axis([-1 1 -1 1]), hold on, v=[1;0]; plot(v(1),v(2),'o'),
for k=1:3, v=A*v/norm(A*v); plot(v(1),v(2),'o'), pause, end
```

**Rayleigh quotient.** Let  $A \in \mathbb{C}^{n \times n}$ . For  $x \in \mathbb{C}^n$  we define

$$r(x) = \frac{x^* A x}{x^* x}.$$

If  $(x, \lambda)$  is an eigenpair of  $A$ , then  $r(x) = \lambda$ . Let  $y \in \mathbb{C}^n$  with  $y^* y = 1$  and  $y^* x = 0$ . Then, for all  $h > 0$

$$r(x + hy) = \frac{\lambda + hx^* A y + h^2}{1 + h^2} = \lambda + O(h).$$

If  $A = A^*$ , then  $r(x + hy) = \lambda + O(h^2)$ .

```
A=[1 2;3 4]; l1=eig(A), v=[1;0];
for k=1:10, v=A*v/norm(A*v); l(k)=v'*A*v; end,
A=[1 2;2 3]; l1s=eig(A), v=[1;0];
for k=1:10, v=A*v/norm(A*v); ls(k)=v'*A*v; end,
semilogy([1:10],abs(l-11(2)), [1:10],abs(ls-11s(2)))
```

**Inverse iteration.** Let  $A \in \mathbb{C}^{n \times n}$  be invertible.  $(x, \lambda)$  is an eigenpair of  $A$  if and only if  $(x, 1/\lambda)$  is an eigenpair of  $A^{-1}$ . The inverse iteration approximates  $(x_n, \lambda_n)$  with convergence rate  $O(|\lambda_n/\lambda_{n-1}|^k)$ .

```
A=[1 2;3 4]; ll=eig(A); v=[1;0];  
for k=1:10, v=A\v; v=v/norm(v); l(k)=v'*A*v; end  
hold on, semilogy([1:10],abs(l-ll(1)), 'r')
```

**Literature.** [TB, Lecture 27]

### 7.3 QR algorithm (26.1)

**Shifted iterations.** Let  $A \in \mathbb{C}^{n \times n}$  be invertible and  $\mu \in \mathbb{C}$ .  $(x, \lambda)$  is an eigenpair of  $A$  if and only if  $(x, \lambda - \mu)$  is an eigenpair of  $A - \mu \text{Id}$ . The inverse iteration with shift  $\mu$  approximates the eigenvalue  $\lambda_j$  closest to  $\mu$  with convergence rate

$$O(|(\mu - \lambda_j)/(\mu - \lambda_{j'})|^k),$$

where  $\lambda_{j'}$  is the second closest eigenvalue to  $\mu$ .

```
A=ones(3,3)+diag([1,2,3]); ll=eig(A); mu=2.5; v=[1;0;0];
for k=1:10, v=(A-mu*eye(3))\v; v=v/norm(v); l(k)=v'*A*v; end
semilogy([1:10],abs(1-ll(2)))
```

**Similarity transformations.** Let  $X \in \mathbb{C}^{n \times n}$  be invertible. The matrix  $X^{-1}AX$  has the same eigenvalues as  $A$ . Let  $Q \in \mathbb{C}^{n \times n}$  be unitary. We decompose  $Q = (Q_\diamond, q_n)$  and obtain

$$Q^*AQ = \begin{pmatrix} Q_\diamond^*AQ_\diamond & Q_\diamond^*Aq_n \\ q_n^*AQ_\diamond & q_n^*Aq_n \end{pmatrix}.$$

If  $q_n^*A = \lambda q_n^*$ , then  $(Q^*AQ)(n, :) = \lambda e_n^*$ . By deflation, the process can be continued to obtain an upper triangular matrix whose diagonal elements are the eigenvalues of  $A$ . If  $A$  is hermitian, the resulting matrix is diagonal.

**QR iteration.** Let  $\kappa \in \mathbb{C}$  and

$$q_n^* = \frac{e_n^*(A - \kappa \text{Id})^{-1}}{\|e_n^*(A - \kappa \text{Id})^{-1}\|}.$$

If  $A - \kappa \text{Id} = QR$ , then  $q_n^* = r_{nn}e_n^*(A - \kappa \text{Id})^{-1}$ . That is, the  $n$ th column of  $Q$  is an approximate left eigenvector of  $A$ .

**Literature.** [S2, Lecture 15]

## 8 Exam preparation

### 8.1 Summary (31.1.)

**QR iteration.** If  $A - \kappa \text{Id} = QR$ , then

$$Q^*AQ = RQ + \kappa \text{Id}.$$

```
A=ones(3,3)+diag([1,2,3]);  
for k=1:10, [Q,R]=qr(A); A=R*Q, pause, end
```

**Rayleigh quotient shift.** Let  $A^{(k)}$  be the  $k$ th iterate. Then,

$$\kappa = e_n^* A^{(k)} e_n = a_{nn}$$

is viewed as an approximate eigenvalue.

```
A=ones(3,3)+diag([1,2,3]); l=[];  
while length(A(:))>1, kappa=A(end,end);  
[Q,R]=qr(A-kappa*eye(size(A))); A=R*Q+kappa*eye(size(A)), pause  
if norm(A(end,1:end-1))<1e-4, l=[1;A(end,end)];  
A=A(1:end-1,1:end-1); end, end, l=[1;A(end,end)]
```

**Summary.** What is ...?

**Newton's method.** We solve  $f(x_*) = 0$  by  $x_{k+1} = x_k - f'(x_k)^{-1} f(x_k)$ .

**Interpolation.** We construct  $p$  with  $p(x_j) = y_j$  for all  $j =$   
 $\dots, n$ .

**Algebraic.**  $p(x) = a_n x^n + \dots + a_0 = y_0 \ell_0(x) + \dots + y_n \ell_n(x)$ .

**Trigonometric.**  $p(x) = c_n e^{inx} + \dots + c_0$ . (FFT)

**Cubic spline.**  $p \in C^2[a, b]$  is cubic on all  $[x_{j-1}, x_j]$ .

**Quadrature.** We compute  $I(f) = \int_a^b f(x)dx$  by  $Q(f) = \sum_{j=0}^n w_j f(x_j)$ .

**Composite methods.**  $Q(f) = I(p)$  on each  $[x_{j-1}, x_j]$ .

**Gaussian rules.**  $I(p) = Q(p)$  for all  $p$  of degree  $\leq 2n + 1$ .

**Monte Carlo methods.** Pseudorandom nodes,  $w_j = 1/(n + 1)$  for all  $j$ .

**Linear systems.** We solve  $Ax = b$  for  $A \in \mathbb{C}^{n \times n}$  invertible.

**Gaussian elimination.** We triangularize  $A = LU$  by  $\frac{2}{3}n^3$  flops.

**Iterative methods.**  $A = M - N$ ,  $x_{k+1} = M^{-1}(b + Nx_k)$ .

**Least squares problems.** Minimize  $\|Ax - b\|_2$  for  $\text{rank}(A) = n \leq m$ .

**Normal equations.** We solve  $A^*Ax = A^*b$ . Cholesky:  $\frac{1}{3}n^3$  flops.

**QR factorization.**  $A = QR$ . Householder:  $2n^2(m - \frac{1}{3}n)$  flops.

**Eigenvalue problems.** We solve  $Ax = \lambda x$  for  $A \in \mathbb{C}^{n \times n}$ .

**Power iterations.**  $A^k x$  converges to a dominant eigenvector.

**QR iteration.**  $A_k - \kappa_k \text{Id} = QR$ ,  $A_{k+1} = RQ + \kappa_k \text{Id}$

8.2 Questions (2.2.)

8.3 Applications (7.2.)

8.4 Exam (9.2.)

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