## Recap lecture MATH3230A

## Outline

- Numerical integration
- Polynomial interpolation
- Linear systems of equations
- Nonlinear equations/systems
- Floating point arithmetic


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## Numerical integration

General quadrature rule for approximating the integral of $f:[a, b] \rightarrow \mathbb{R}$ with $n+1$ points $x_{0}, \ldots, x_{n} \in[a, b]$

$$
\int_{a}^{b} f(x) \mathrm{dx} \approx \alpha_{0} f\left(x_{0}\right)+\cdots+\alpha_{n} f\left(x_{n}\right)
$$

such that it is exact for polynomials of certain degrees.

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$$

such that it is exact for polynomials of certain degrees.
Newton-Cotes rules:

- Equally-spaced points $a=x_{0}<x_{1}<\cdots<x_{n}=b, x_{i}=a+i h$ with $h=\frac{b-a}{n}$.
- Exact for polynomials of degree $\leq n$.

Gaussian (Gauss-Legendre) rules:

- Points are roots of certain (Legendre) polynomials (not equally-spaced).
- Exact for polynomials of degree $\leq 2 n+1$.


## Newton-Cotes

2-point Newton-Cotes (aka Trapezoidal rule) $x_{0}=a, x_{1}=b$ :

$$
\int_{a}^{b} f(x) \mathrm{dx} \approx \frac{b-a}{2}(f(a)+f(b)) .
$$

Composite Trapezoidal rule with $h=x_{i+1}-x_{i}=\frac{b-a}{n}$
$\int_{x_{i}}^{x_{i+1}} f(x) \mathrm{dx} \approx \frac{h}{2}\left(f\left(x_{i}\right)+f\left(x_{i+1}\right)\right), \quad \int_{a}^{b} f(x) \mathrm{dx} \approx \sum_{i=0}^{n-1} \frac{h}{2}\left(f\left(x_{i}\right)+f\left(x_{i+1}\right)\right)$

## Newton-Cotes

3-point Newton-Cotes (aka Simpson's rule) $x_{0}=a, x_{1}=\frac{1}{2}(a+b)$, $x_{2}=b$ :

$$
\int_{a}^{b} f(x) \mathrm{dx} \approx \frac{b-a}{6}(f(a)+4 f((a+b) / 2)+f(b)) .
$$

Composite Simpson's rule

$$
\int_{a}^{b} f(x) \mathrm{dx} \approx \sum_{i=0}^{n-1} \frac{h}{6}\left(f\left(x_{i}\right)+4 f\left(\left(x_{i}+x_{i+1}\right) / 2\right)+f\left(x_{i+1}\right)\right)
$$

## Newton-Cotes

General procedure:

- Set $x_{i}=a+i h, h=\frac{b-a}{n}$ as the equally-spaced partition of $[a, b]$.
- Since Newton-Cotes must be exact for all polynomials of degree $\leq n$, compute for $0 \leq k \leq n$

$$
I_{k}:=\int_{a}^{b} x^{k} \mathrm{dx}=\sum_{i=0}^{n} \alpha_{i} x_{i}^{k} .
$$

- Deduce $\alpha_{i}$ by solving a linear system

$$
\left(\begin{array}{cccc}
1 & 1 & \cdots & 1 \\
x_{0} & x_{1} & \cdots & x_{n} \\
\vdots & \vdots & \ddots & \vdots \\
x_{1}^{n} & x_{2}^{n} & \cdots & x_{n}^{n}
\end{array}\right)\left(\begin{array}{c}
\alpha_{0} \\
\alpha_{1} \\
\vdots \\
\alpha_{n}
\end{array}\right)=\left(\begin{array}{c}
I_{0} \\
I_{1} \\
\vdots \\
I_{n}
\end{array}\right)
$$

- Alternatively

$$
\alpha_{i}=\int_{a}^{b} l_{i}(x) \mathrm{dx}=\int_{a}^{b} \prod_{j=0, j \neq i}^{n} \frac{x-x_{j}}{x_{i}-x_{j}} \mathrm{dx} .
$$

## Gaussian/Gauss-Legendre

Procedure for $f:[-1,1] \rightarrow \mathbb{R}$ :
■ Set $x_{0}, \ldots, x_{n}$ as the roots of the $(n+1)^{\text {th }}$ Legendre polynomial $P_{n+1}(x)$.

- Compute

$$
\alpha_{i}=\int_{a}^{b} l_{i}(x) \mathrm{dx}=\int_{a}^{b} \prod_{j=0, j \neq i}^{n} \frac{x-x_{j}}{x_{i}-x_{j}} \mathrm{dx} .
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## Gaussian/Gauss-Legendre

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- Compute

$$
\alpha_{i}=\int_{a}^{b} I_{i}(x) \mathrm{dx}=\int_{a}^{b} \prod_{j=0, j \neq i}^{n} \frac{x-x_{j}}{x_{i}-x_{j}} \mathrm{dx}
$$

Procedure for $f:[a, b] \rightarrow \mathbb{R}$ :

- Use linear transformation

$$
L(x)=\frac{b+a}{2}+\frac{b-a}{2} x .
$$

- Transform the integrals:

$$
\int_{a}^{b} f(y) d y=\int_{-1}^{1} f(L(x)) \frac{b-a}{2} \mathrm{dx}=: \int_{-1}^{1} g(x) \mathrm{dx} \approx \sum_{i=0}^{n} \alpha_{i} g\left(x_{i}\right)
$$

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## Interpolating data

General problem: given a data set of a function $f: \mathbb{R} \rightarrow \mathbb{R}$ :

| $x$ | $x_{0}$ | $x_{1}$ | $\cdots$ | $x_{n}$ |
| :---: | :---: | :---: | :---: | :---: |
| $f(x)$ | $f_{0}$ | $f_{1}$ | $\cdots$ | $f_{n}$ |

find a polynomial $p(x)$ of degree $\leq n$ such that

$$
p\left(x_{i}\right)=f_{i} .
$$

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find a polynomial $p(x)$ of degree $\leq n$ such that

$$
p\left(x_{i}\right)=f_{i} .
$$

Method 1: Vandermonde interpolation - Solve the matrix-vector problem

$$
\left(\begin{array}{ccccc}
1 & x_{0} & x_{0}^{2} & \cdots & x_{0}^{n} \\
1 & x_{1} & x_{1}^{2} & \cdots & x_{1}^{n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & x_{n} & x_{n}^{2} & \cdots & x_{n}^{n}
\end{array}\right)\left(\begin{array}{c}
\alpha_{0} \\
\alpha_{1} \\
\vdots \\
\alpha_{n}
\end{array}\right)=\left(\begin{array}{c}
f_{0} \\
f_{1} \\
\vdots \\
f_{n}
\end{array}\right)
$$

and set

$$
V(x)=\alpha_{0}+\alpha_{1} x+\cdots+\alpha_{n} x^{n} .
$$

## Interpolating data

General problem: given a data set of a function $f: \mathbb{R} \rightarrow \mathbb{R}$ :

| $x$ | $x_{0}$ | $x_{1}$ | $\cdots$ | $x_{n}$ |
| :---: | :---: | :---: | :---: | :---: |
| $f(x)$ | $f_{0}$ | $f_{1}$ | $\cdots$ | $f_{n}$ |

find a polynomial $p(x)$ of degree $\leq n$ such that

$$
p\left(x_{i}\right)=f_{i} .
$$

Method 2: Lagrange interpolation - Define

$$
I_{i}(x)=\prod_{j=0, j \neq i}^{n} \frac{x-x_{j}}{x_{i}-x_{j}}
$$

and set

$$
L(x)=f_{0} l_{0}(x)+f_{1} I_{1}(x)+\cdots+f_{n} I_{n}(x) .
$$

## Interpolating data

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| :---: | :---: | :---: | :---: | :---: |
| $f(x)$ | $f_{0}$ | $f_{1}$ | $\cdots$ | $f_{n}$ |

find a polynomial $p(x)$ of degree $\leq n$ such that

$$
p\left(x_{i}\right)=f_{i} .
$$

Method 3: Newton interpolation - Compute the divided difference table and obtain

$$
c_{k}=f\left[x_{0}, \ldots, x_{k}\right] \text { for } 0 \leq k \leq n,
$$

and set

$$
N(x)=c_{0}+c_{1}\left(x-x_{0}\right)+c_{2}\left(x-x_{0}\right)\left(x-x_{1}\right)+\cdots+c_{n} \prod_{j=0}^{n-1}\left(x-x_{j}\right)
$$

## Properties

- Any two polynomials $p(x)$ and $q(x)$ of deg $\leq n$ agreeing on $n+1$ points must coincide.
- The Lagrange interpolation $L(x)$ and the Newton interpolation $N(x)$ are the same polynomial.
- The divided difference is symmetric with respect to perturbations in the argument:

$$
f\left[x_{0}, \ldots, x_{k}\right]=f\left[z_{0}, \cdots, z_{k}\right]
$$

for any perturbation $\left(z_{0}, \cdots, z_{k}\right)$ of $\left(x_{0}, \ldots, x_{k}\right)$.

- The ordering in the divided difference table does not matter.
- The error of interpolating $f(x)$ with polynomial $p(x)$ of degree $\leq n$ with $n+1$ distinct points is

$$
f(x)-p(x)=\frac{f^{(n+1)}\left(\xi_{x}\right)}{(n+1)!}\left(x-x_{0}\right) \cdots\left(x-x_{n}\right) .
$$

## Chebyshev polynomials

Aim: to find the best points $x_{0}<x_{1}<\cdots<x_{n}$ in [a,b] such that the interpolation error

$$
f(x)-p(x)=\frac{f^{(n+1)}\left(\xi_{x}\right)}{(n+1)!}\left(x-x_{0}\right) \cdots\left(x-x_{n}\right)
$$

is minimized.

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$$

is minimized.
For a monic polynomial $g:[-1,1] \rightarrow \mathbb{R}$ of degree $n+1$, it holds that

$$
\max _{x \in[-1,1]}|g(x)| \geq 2^{-n}
$$

and so for $f:[-1,1] \rightarrow \mathbb{R}$, the best error estimate is

$$
|f(x)-p(x)| \leq \frac{\max _{x \in[-1,1]}\left|f^{(n+1)}(x)\right|}{2^{n}(n+1)!}
$$

if we choose $x_{0}, \ldots, x_{n}$ as roots of the Chebyshev polynomial $T_{n+1}(x)$.

## Chebyshev polynomials

The Chebyshev polynomials are defined recursively:

$$
T_{0}(x)=1, \quad T_{1}(x)=x, \quad T_{n+1}(x)=2 x T_{n}(x)-T_{n-1}(x)
$$

Properties include:

- $T_{n}(x)=\cos \left(n \cos ^{-1}(x)\right)$ for $x \in[-1,1]$.
- $\left|T_{n}(x)\right| \leq 1$ for $x \in[-1,1]$.
- $T_{n}\left(\cos \frac{j \pi}{n}\right)=(-1)^{j}$ for $0 \leq j \leq n$.
- $T_{n}\left(\cos \frac{2 j-1}{2 n} \pi\right)=0$ for $0 \leq j \leq n$.
- The monic polynomial $\hat{T}_{n+1}(x)=2^{-n} T_{n+1}(x)$ satisfies

$$
\max _{x \in[-1,1]}\left|\widehat{T}_{n+1}(x)\right|=2^{-n} .
$$

## Hermite's interpolation

General problem: given a data set of a function $f: \mathbb{R} \rightarrow \mathbb{R}$ and its derivative:

| $x$ | $x_{0}$ | $x_{1}$ | $\cdots$ | $x_{n}$ |
| :---: | :---: | :---: | :---: | :---: |
| $f(x)$ | $f_{0}$ | $f_{1}$ | $\cdots$ | $f_{n}$ |
| $f^{\prime}(x)$ | $f_{0}^{\prime}$ | $f_{1}^{\prime}$ | $\cdots$ | $f_{n}^{\prime}$ |

find a polynomial $p(x)$ of degree $\leq 2 n+1$ such that

$$
p\left(x_{i}\right)=f_{i}, \quad p^{\prime}\left(x_{i}\right)=f_{i}^{\prime} .
$$

## Hermite's interpolation

Method 1 - Lagrange form: Set

$$
u_{i}(x)=\left(1-2 l_{i}^{\prime}\left(x_{i}\right)\left(x-x_{i}\right)\right) l_{i}^{2}(x), \quad v_{i}(x)=\left(x-x_{i}\right) l_{i}^{2}(x)
$$

where

$$
\begin{aligned}
& u_{i}\left(x_{j}\right)=v_{i}^{\prime}\left(x_{j}\right)= \begin{cases}0 & \text { if } j \neq i, \\
1 & \text { if } j=i,\end{cases} \\
& u_{i}^{\prime}\left(x_{j}\right)=0, \quad v_{i}\left(x_{j}\right)=0 \text { for } 0 \leq j \leq n
\end{aligned}
$$

Then, define

$$
H_{2 n+1}(x)=\sum_{i=0}^{n} f_{i} u_{i}(x)+\sum_{i=0}^{n} f_{i}^{\prime} v_{i}(x) .
$$

## Hermite's interpolation

Method 2 - Newton form: Set

$$
z_{2 i}=z_{2 i+1}=x_{i} \text { for } i=0, \ldots n
$$

and

$$
f\left[z_{2 i}, z_{2 i+1}\right]=f_{i}^{\prime} \text { for } i=0, \ldots, n
$$

in the table of divided difference. Then, define

$$
H_{2 n+1}(x)=f\left[z_{0}\right]+\sum_{k=1}^{2 n+1} f\left[z_{0}, \ldots, z_{k}\right]\left(x-z_{0}\right) \cdots\left(x-z_{k-1}\right) .
$$

## Hermite's interpolation

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$$

Error estimate for $f \in C^{2 n+2}[a, b]$ and any $x \in[a, b]$ :

$$
f(x)-H_{2 n+1}(x)=\frac{f^{(2 n+2)}\left(\xi_{x}\right)}{(2 n+2)!}\left(x-x_{0}\right)^{2} \cdots\left(x-x_{n}\right)^{2}
$$

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## Vector and matrix norms

For $x \in \mathbb{R}^{n}$ and $p \geq 1$

$$
\|x\|_{p}= \begin{cases}\left(\sum_{i=1}^{n}\left|x_{i}\right|^{p}\right)^{1 / p} & \text { if } p<\infty, \\ \max _{1 \leq i \leq n}\left|x_{i}\right| & \text { if } p=\infty .\end{cases}
$$

For $A \in \mathbb{R}^{n \times n}$, the induced $p$-matrix norm is

$$
\|A\|_{p}=\max _{\|x\|_{p}=1}\|A x\|_{p}
$$

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$$

For $A \in \mathbb{R}^{n \times n}$, the induced $p$-matrix norm is

$$
\|A\|_{p}=\max _{\|\times\|_{p}=1}\|A x\|_{p}
$$

Properties:

- $\|A\|_{1}$ is the maximum column sum.
- $\|A\|_{\infty}$ is the maximum row sum.
- $\|A\|_{2}=\sqrt{\lambda_{\max }\left(A^{T} A\right)}$.
- $\|A B\|_{p} \leq\|A\|_{p}\|B\|_{p}$.
- $\|A x\|_{p} \leq\|A\|_{p}\|x\|_{p}$.


## Sensitivity of linear systems

Given invertible matrices $A$ and $\tilde{A}$ with vector $b$, and solutions $x$ and $\tilde{x}$ :

$$
A x=b, \quad \tilde{A} \tilde{x}=b,
$$

we seek an upper bound on the relative error $\frac{\|x-\tilde{x}\|}{\|x\|}$.

## Sensitivity of linear systems

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$$

we seek an upper bound on the relative error $\frac{\|x-\tilde{x}\|}{\|x\|}$.
First result:

$$
\text { If } \frac{\|x-\tilde{x}\|}{\|x\|} \leq \theta<1 \text {, then } \frac{\|x-\tilde{x}\|}{\|\tilde{x}\|} \leq \frac{\theta}{1-\theta} \text {. }
$$

Second result: Set $E=A-\tilde{A}$ and use $A x=b=\tilde{A} \tilde{x}=A \tilde{x}+E \tilde{x}$ to get

$$
x-\tilde{x}=A^{-1} E \tilde{x} .
$$

Then,

$$
\frac{\|x-\tilde{x}\|}{\|\tilde{x}\|} \leq\left\|A^{-1} E\right\|=\left\|A^{-1} \tilde{A}-I\right\| \quad \Rightarrow \quad \frac{\|x-\tilde{x}\|}{\|x\|} \leq \frac{\left\|A^{-1} E\right\|}{1-\left\|A^{-1} E\right\|} .
$$

## Sensitivity of linear systems

Given invertible matrices $A$ and $\tilde{A}$ with vector $b$, and solutions $x$ and $\tilde{x}$ :

$$
A x=b, \quad \tilde{A} \tilde{x}=b,
$$

we seek an upper bound on the relative error $\frac{\|x-\tilde{x}\|}{\|x\|}$.
Use

$$
\left\|A^{-1} E\right\| \leq\left\|A^{-1}\right\|\|A\| \frac{\|E\|}{\|A\|}=\kappa(A) \frac{\|A-\tilde{A}\|}{\|A\|}
$$

where the condition number is $\kappa(A):=\left\|A^{-1}\right\|\|A\| \geq 1$, we have

$$
\frac{\|x-\tilde{x}\|}{\|x\|} \leq \frac{\kappa(A) \frac{\|A-\tilde{A}\|}{\|A\|}}{1-\kappa(A) \frac{\|E\|}{\|A\|}}=: c(E) \kappa(A) \frac{\|A-\tilde{A}\|}{\|A\|} .
$$

## Solving systems of equations

To solve

$$
A x=b, \text { where } A \in \mathbb{R}^{n \times n}, \quad b \in \mathbb{R}^{n},
$$

we have

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$$
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$$

we have

- Forward substitution if $A$ is lower triangular.
- Backward substitution if $A$ is upper triangular.
- Cholesky factorization $A=U^{T} U$ into upper triangular $U$ if $A$ is symmetric and positive definite (SPD). Then solve

$$
U x=y, \quad U^{T} y=b
$$

■ LU factorization $A=L U$ into lower tri. $L$ and upper tri. $U$ if $A$ is not SPD. Then solve

$$
U x=y, \quad L y=b
$$

■ LU with partial pivot in case the pivot at some stage is zero! This leads to the factorization

$$
P A=L U
$$

for some permutation matrix $P$.

## Non-square systems

If $A \in \mathbb{R}^{m \times n}, m \neq n$, then there may not be a solution/infinitely many solutions to

$$
A x=b \text { for } b \in \mathbb{R}^{m}, x \in \mathbb{R}^{n} .
$$

■ Overdetermined case $m>n$. Choose the solution $x_{*}$ with smallest error $\|A x-b\|_{2}$. The solution $x_{*}$ is given by the normal equation:

$$
x_{*}=\left(A^{T} A\right)^{-1} A^{T} b,
$$

obtained by differentiating

$$
\left.\frac{d}{d t} f\left(x_{*}+t y\right)\right|_{t=0}=0, \text { where } f(x)=\|A x-b\|_{2} .
$$

- Undetermined case $m<n$. Choose the solution $x^{*}$ with the smallest 2-norm amongst all other solutions. Obtained by differentiating the Lagrangian:

$$
L(x, \mu)=\|x\|_{2}^{2}-\mu^{T}(A x-b)
$$

and set all partial derivatives to zero. The solution is

$$
x^{*}=A^{T}\left(A A^{T}\right)^{-1} b .
$$

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To solve

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f(x)=0
$$

for some nonlinear function $f: \mathbb{R} \rightarrow \mathbb{R}$, we have

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To solve

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for some nonlinear function $f: \mathbb{R} \rightarrow \mathbb{R}$, we have

- Bisection method
- Only needs $f(a) f(b)<0$ for some interval $[a, b]$ where $f$ is continuous.
- Always converges if $x_{0} \in(a, b)$.
- R-linear convergence.
- Newton's method
- Need $f$ to be differentiable and $f^{\prime}\left(x_{*}\right) \neq 0$.
- Converges if $x_{0}$ is close to $x_{*}$.
- Q-Quadratic convergence.
- Quasi-Newton methods

■ Replace $f^{\prime}\left(x_{k}\right)$ in Newton's method with simpler approximations.
■ Converges if $x_{0}$ is close to $x_{*}$.

- Q-linear convergence (Constant slope) or Order $p=\frac{1+\sqrt{5}}{2}$ (Secant method)


## Fixed-point iterative methods

Newton's method, constant slope method and Secant method are special cases of fixed point iterative methods:

$$
x_{k+1}=\varphi\left(x_{k}\right) \quad k=0,1,2, \ldots .
$$

## Fixed-point iterative methods

Newton's method, constant slope method and Secant method are special cases of fixed point iterative methods:

$$
x_{k+1}=\varphi\left(x_{k}\right) \quad k=0,1,2, \ldots .
$$

Main result for fixed-point iterative methods:

- If $\left|\varphi^{\prime}\left(x_{*}\right)\right|<1$, then there exists $\delta=\delta\left(x_{*}\right)$ such that if $x_{0} \in\left[x_{*}-\delta, x_{*}+\delta\right]$, the fixed-point iterative method converges.
- If $\varphi^{\prime}\left(x_{*}\right) \neq 0$, the convergence is Q -linear.
- If $\varphi^{\prime}\left(x_{*}\right)=\varphi^{\prime \prime}\left(x_{*}\right)=\cdots=\varphi^{(p-1)}\left(x_{*}\right)=0$ but $\varphi^{(p)}\left(x_{*}\right) \neq 0$, then the convergence is of order $p$.


## Systems of nonlinear equations

To solve the nonlinear system of equations

$$
F(x)=\left(\begin{array}{c}
f_{1}\left(x_{1}, \ldots, x_{n}\right) \\
\vdots \\
f_{n}\left(x_{1}, \ldots, x_{n}\right)
\end{array}\right)=0
$$

we have

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\vdots \\
f_{n}\left(x_{1}, \ldots, x_{n}\right)
\end{array}\right)=0
$$

we have

- Newton's method: (Quadratic local convergence)

$$
x_{k+1}=x_{k}-\left(D F\left(x_{k}\right)\right)^{-1} F\left(x_{k}\right) .
$$

- Broyden's method: (Linear local convergence)

$$
x_{k+1}=x_{k}-A_{k}^{-1} F\left(x_{k}\right) .
$$

- Steepest descent: (Linear global convergence)

$$
\begin{aligned}
x_{k+1} & =x_{k}-\alpha_{k} \nabla g\left(x_{k}\right), \quad g(x)=\frac{1}{2}\|F(x)\|_{2}^{2}, \\
\alpha_{k} & =\underset{s \geq 0}{\arg \min } g\left(x_{k}-s \nabla g\left(x_{k}\right)\right) .
\end{aligned}
$$

## Broyden's method

$$
x_{k+1}=x_{k}-A_{k}^{-1} F\left(x_{k}\right)
$$

Key properties of matrix $A_{k}$ :

- (Secant condition) $A_{k}\left(x_{k}-x_{k-1}\right)=F\left(x_{k}\right)-F\left(x_{k-1}\right)$.
- (Rank-one update) $A_{k}=A_{k-1}+p_{k} \otimes d_{k-1}, d_{k-1}=A_{k-1}^{-1} F\left(x_{k-1}\right)$.

■ (Orthogonal property) $A_{k} y=A_{k-1} y$ for all $y \cdot\left(x_{k}-x_{k-1}\right)=0$.

## Broyden's method

$$
x_{k+1}=x_{k}-A_{k}^{-1} F\left(x_{k}\right)
$$

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■ (Secant condition) $A_{k}\left(x_{k}-x_{k-1}\right)=F\left(x_{k}\right)-F\left(x_{k-1}\right)$.
■ (Rank-one update) $A_{k}=A_{k-1}+p_{k} \otimes d_{k-1}, d_{k-1}=A_{k-1}^{-1} F\left(x_{k-1}\right)$.
■ (Orthogonal property) $A_{k} y=A_{k-1} y$ for all $y \cdot\left(x_{k}-x_{k-1}\right)=0$.
The "good" Broyden method: Given $x_{0}$ and invertible $A_{0}$,

$$
\begin{aligned}
d_{k} & =A_{k}^{-1} F\left(x_{k}\right) \quad \mapsto \quad x_{k+1}=x_{k}+d_{k} \\
& \mapsto \quad A_{k+1}=A_{k}+\frac{F\left(x_{k}\right)-F\left(x_{k-1}\right)-A_{k} d_{k}}{d_{k} \cdot d_{k}} \otimes d_{k}
\end{aligned}
$$

## Broyden's method

$$
x_{k+1}=x_{k}-A_{k}^{-1} F\left(x_{k}\right)
$$

Key properties of matrix $A_{k}$ :
■ (Secant condition) $A_{k}\left(x_{k}-x_{k-1}\right)=F\left(x_{k}\right)-F\left(x_{k-1}\right)$.
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\end{aligned}
$$

The "bad" Broyden method employs the Sherman-Morrison formula to get $A_{k+1}^{-1}$ directly without inverting a matrix:

$$
\begin{aligned}
d_{k} & =A_{k}^{-1} F\left(x_{k}\right) \quad \mapsto \quad x_{k+1}=x_{k}+d_{k} \\
& \mapsto \quad A_{k+1}^{-1}=A_{k}^{-1}+\frac{A_{k}^{-1}\left(F\left(x_{k}\right) \otimes d_{k}\right) A_{k}^{-1}}{d_{k} \cdot d_{k}+d_{k} \cdot A_{k}^{-1} F\left(x_{k}\right)}
\end{aligned}
$$

## Steepest descent

Instead of solving $F(x)=0$, the Steepest descent method finds the minimum of $g(x)=\frac{1}{2}\|F(x)\|_{2}^{2}$.

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Procedure: Starting from $x_{0}$,

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Example

- One choice of search direction is the negative gradient $d_{k}=-\nabla g\left(x_{k}\right)$.
- One choice of search step is such that

$$
g\left(x_{k}+\alpha_{k} d_{k}\right) \leq g\left(x_{k}+s d_{k}\right) \text { for any } s \in \mathbb{R} .
$$

- If $\alpha_{k}$ is chosen as above, then $d_{k} \cdot d_{k+1}=0$ (Zig-zag motion).


## Outline

- Numerical integration
- Polynomial interpolation
- Linear systems of equations
- Nonlinear equations/systems
- Floating point arithmetic


## Scientific notation

A decimal can be represented as

$$
a= \pm r \times 10^{n},
$$

where

- $r \in[0.1,1)$ is the mantissa.
- $n \in \mathbb{Z}$ is the exponent.


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A binary number can be represented as

$$
a= \pm(q)_{2} \times 2^{\tilde{m}},
$$

where

- $q$ is the mantissa.
- $\tilde{m}$ is the exponent.


## Single/double precision format

The single precision floating point format with 32-bits for normalized binary numbers is

$$
s\left|m_{1} m_{2} \cdots m_{8}\right| f_{1} f_{2} \cdots f_{23} \quad \mapsto \quad a=(-1)^{s}\left(1 . f_{1} \ldots f_{23}\right)_{2} \times 2^{\left(m_{1} \ldots m_{8}\right)_{2}-127}
$$

- Biased exponent $\left(m_{1} \ldots m_{8}\right)_{2}-127$ is used to represent an equal number of non-negative and negative exponents.
- The cases $\left(m_{1} \ldots m_{8}\right)_{2}=(0 \ldots 0)_{2}$ or $(1 \ldots 1)_{2}$ are reserved for special values such as $0, \infty$ and NaN .
- Smallest positive normalized number $a_{\text {min }}$ and largest finite normalized number $a_{\max }$ are

$$
\begin{aligned}
& a_{\min } \mapsto 0|0 \cdots 01| 0 \cdots 0 \mapsto 2^{-126}, \\
& a_{\max } \mapsto 0|1 \cdots 10| 1 \cdots 1 \mapsto\left(2-2^{-23}\right) \times 2^{127} .
\end{aligned}
$$

## Single/double precision format

The double precision floating point format with 64 -bits for normalized binary numbers is
$s\left|m_{1} m_{2} \cdots m_{11}\right| f_{1} f_{2} \cdots f_{52} \quad \mapsto \quad a=(-1)^{s}\left(1 . f_{1} \ldots f_{52}\right)_{2} \times 2^{\left(m_{1} \ldots m_{11}\right)_{2}-1023}$

- Double precision is used if we need to have twice as much accuracy than single precision.
- Smallest positive normalized number $a_{\text {min }}$ and largest finite normalized number $a_{\max }$ are

$$
\begin{aligned}
& a_{\min } \mapsto 0|0 \cdots 01| 0 \cdots 0 \mapsto 2^{-1022}, \\
& a_{\max } \mapsto 0|1 \cdots 10| 1 \cdots 1 \mapsto\left(2-2^{-52}\right) \times 2^{1023} .
\end{aligned}
$$

## Rounding/Chopping

Two ways to obtain from a decimal number $x=x_{0} \cdot x_{1} \ldots x_{m}$ with $m$ digits to a decimal number with $n<m$ digits:

- Rounding:

$$
x_{r}= \begin{cases}x_{0} \cdot x_{1} \ldots x_{n} & \text { if } x_{n+1} \in\{0,1,2,3,4\}, \\ x_{0} \cdot x_{1} \ldots x_{n}+10^{-n} & \text { if } x_{n+1} \in\{5,6,7,8,9\} .\end{cases}
$$

- Chopping:

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x_{c}=x_{0} \cdot x_{1} \ldots x_{n}
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- Chopping:

$$
x_{c}=x_{0} \cdot x_{1} \ldots x_{n}
$$

Estimates on relative errors:

$$
\frac{\left|x-x_{r}\right|}{|x|} \leq \frac{1}{2} \times 10^{-n}, \quad \frac{\left|x-x_{c}\right|}{|x|} \leq 10^{-n}
$$

Similar when rounding/chopping binary numbers.

## Machine precision

The machine precision/machine epsilon $\varepsilon_{M}$ can be defined in two ways:

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- The upper bound on the relative error of rounding a number a in between $a_{\min }$ and $a_{\min , 2}$ (or $a_{\max , 2}$ and $a_{\max }$ ):

$$
\frac{\left|a_{\min }-a\right|}{|a|} \leq \varepsilon_{M} .
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$$

Easier way: The machine epsilon is $\varepsilon_{M}=2^{-y}$ where $y$ is the number of bits reserved for the manitssa.

## Loss of significance

Any instance of creating a number $x$ where

- $x<a_{\text {min }}$ leads to underflow, and $x$ is set to zero.
- $x>a_{\max }$ leads to overflow, and the computation is halted.


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$\sqrt{101}-\sqrt{100}=0.0499000$ (computed from rounding $\sqrt{101}$ to 6 sign. digits),
$\sqrt{101}-\sqrt{100}=0.0498756$ (true value to 6 sign. digits)
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$\sqrt{101}-\sqrt{100}=0.0498756$ (true value to 6 sign. digits)
leading to a loss of 4 digits of accuracy.
Remedy? Rewrite expression that does not involve subtraction/use double precision.

## Error analysis

For a non-machine number $x$, its closest machine number $f(x)$ satisfies

$$
f \prime(x)=x(1+\varepsilon) \text { for }|\varepsilon| \leq \varepsilon_{M} .
$$

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$$
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$$

This relation is used to analyse the relative errors we make when performing computer arithmetic that do not obey the usual rules of arithmetic due to rounding.

- Forward error analysis measures the relative error between $x \odot y$ and $f l(f l(x) \odot f l(y)):$

$$
\frac{|x \odot y-f|(f \mid(x) \odot f l(y)) \mid}{|x \odot y|} \leq C \varepsilon_{M} .
$$

- Backward error analysis is concerned with showing the computed value $\hat{z}$ of $x \odot y$ is an exact calculation with perturbed data:

$$
\hat{z}=\left(x+\delta_{x}\right) \odot\left(y+\delta_{y}\right) \text { with }\left|\delta_{x}\right|,\left|\delta_{y}\right| \leq \varepsilon_{M}
$$

