Numerical Methods for Differential Equations

Mathematical and Computational Tools

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Contents

Part 1. Vector norms, matrix norms and logarithmic norms

1. Vector norms

Definition *A vector norm* $\|\cdot\| : \mathbb{X} \to \mathbb{R}$ *satisfies*

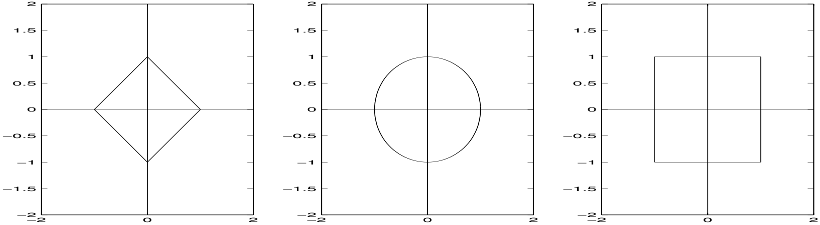
1. $\|u\| \geq 0\,;\qquad \|u\| = 0 \Leftrightarrow u = 0$
2. $\|\alpha u\| = |\alpha| \cdot \|u\|$
3. $\|u\| - \|v\| \leq \|u \pm v\| \leq \|u\| + \|v\|$

A norm generalizes the notion of *distance* between points

Vector norms

Definition *The* l^p *norms are defined* $\|x\|_p = \left(\sum_{k=1}^{N} |x_k|^p \right)^{1/p}$

Graph of the unit circle in $\mathbb{R}^2$ for l^p norms



Unit circles for $p = 1$, $p = 2$ *(Euclidean norm), and* $p = \infty$

2. Matrix norms

Definition *The operator norm associated with the vector norm* $\|\cdot\|$ *is defined by*

$$\|A\| = \sup_{x \neq 0} \frac{\|Ax\|}{\|x\|}$$

For every vector norm there is a corresponding matrix norm

Note

1. $\|Ax\| \leq \|A\| \cdot \|x\|$
2. $\|AB\| \leq \|A\| \cdot \|B\|$

Vector norm	Matrix norm
$\|x\|_1 = \sum_i \|x_i\|$	$\max_j \sum_i \|a_{ij}\|$
$\|x\|_2 = \sqrt{\sum_i \|x_i\|^2}$	$\sqrt{\rho[A^{\mathrm{H}} A]}$
$\|x\|_\infty = \max_i \|x_i\|$	$\max_i \sum_j \|a_{ij}\|$

Definition The *spectral radius* of a matrix is defined by

$$\rho[A] = \max |\lambda[A]|$$

3. Inner products

Definition A bilinear form $\langle \cdot, \cdot \rangle : \mathbb{X} \times \mathbb{X} \to \mathbb{C}$ satisfying

1. $\langle u, u \rangle \geq 0\,;\qquad \langle u, u \rangle = 0 \;\Leftrightarrow\; u = 0$
2. $\langle u, v \rangle = \overline{\langle v, u \rangle}$
3. $\langle u, \alpha v \rangle = \alpha \langle u, v \rangle$
4. $\langle u, v + w \rangle = \langle u, v \rangle + \langle u, w \rangle$

An inner product generates the Euclidean norm $\langle u, u \rangle = \|u\|^2$

An inner product generalizes the notion of scalar product

1. Scalar product in $\mathbb{R}^m$: $\langle u, v\rangle = u^{\mathrm{T}} v$

with corresponding Euclidean vector norm $\|u\|_2^2 = \sum_{k=1}^{N} |u_k|^2$

2. General inner product in $\mathbb{C}^m$: $\langle u, v\rangle_G = u^{\mathrm{H}} G v$ for any symmetric positive definite matrix G

3. Inner product in $L^2[0,1]$: $\langle u, v\rangle = \int_0^1 uv \, \mathrm{d}x$

with corresponding L^2 norm of functions $\|u\|_{L^2}^2 = \int_0^1 |u|^2 \, \mathrm{d}x$

Inner products and operator norms

Theorem *Cauchy–Schwarz inequality*

$$|\langle u, v\rangle| \leq \|u\| \cdot \|v\|$$

Note the absolute value!

$\Rightarrow \langle u, v\rangle \geq -\|u\| \cdot \|v\|$ on real vector spaces

Definition *The operator norm associated with $\langle \cdot, \cdot \rangle$ is*

$$\|A\|^2 = \sup_{x \neq 0} \frac{\langle Au, Au\rangle}{\|u\|^2}$$

Hence $\langle Au, Au\rangle \leq \|A\|^2 \|u\|^2$

Classical stability for ODEs

$$\dot{x} = Ax; \quad x(0) = x_0$$

Characterization *Elementary stability conditions*

- $\mathrm{Re}\,\lambda_k < 0 \quad (\Leftrightarrow \mathrm{e}^{tA} \to 0 \text{ as } t \to \infty)$
- $\|\mathrm{e}^{tA}\| \le C \quad \text{for all } t \ge 0$
- $\mathrm{d}\|\mathrm{e}^{tA}\|/\mathrm{d}t \le 0 \quad (\Leftrightarrow \|\mathrm{e}^{tA}\| \le 1 \text{ for all } t \ge 0)$

Time-dependent linear systems

Consider non-autonomus linear system

$$\dot{x} = A(t)x; \quad x(0) = x_0$$

Stability is no longer characterized by eigenvalues

Even with constant eigenvalues in the left half plane the system can be unstable (Petrowski & Hoppenstedt)

Problem *Under what conditions does* $\|x(t)\|$ *remain bounded as* $t \to \infty$*?*

Note that for an inner product norm,

$$\frac{\mathrm{d}\|x\|^2}{\mathrm{d}t} = \frac{\mathrm{d}\langle x, x\rangle}{\mathrm{d}t} = 2\mathrm{Re}\langle x, \dot{x}\rangle$$

and that if $\dot{x} = Ax$, then

$$\mathrm{Re}\,\langle x, \dot{x}\rangle = \mathrm{Re}\,\langle x, Ax\rangle \leq \mu[A] \cdot \langle x, x\rangle$$

Definition *The logarithmic norm is defined by*

$$\mu[A] = \sup_{x \neq 0} \frac{\mathrm{Re}\langle x, Ax\rangle}{\|x\|^2}$$

4. The logarithmic norm $\mu[A]$

Definition *For general matrix norms the logarithmic norm is defined by*

$$\mu[A] = \lim_{h \to 0+} \frac{\|I + hA\| - 1}{h}$$

If $\dot{x} = Ax$, the following differential inequality holds

$$\mathrm{d}\|x\|/\mathrm{d}t \ \leq \ \mu[A] \cdot \|x\|$$

Note The logarithmic norm may be *negative*. Solution bound

$$\|x(t)\| \leq \mathrm{e}^{t\mu[A]} \cdot \|x(0)\| \; ; \quad t \geq 0$$

Why the logarithmic norm?

Crude estimate

$$\frac{\mathrm{d}\|x\|}{\mathrm{d}t} \leq \|\dot{x}\| = \|Ax\| \leq \|A\| \cdot \|x\|$$

Exponentially growing bound

$$\|x(t)\| \leq \mathrm{e}^{t\|A\|} \cdot \|x(0)\|$$

Note *Because* $\mu[A] \leq \|A\|$ *we always have*

$$\mathrm{e}^{t\mu[A]} \leq \mathrm{e}^{t\|A\|}$$

Vector norm	Matrix norm	Log norm $\mu[A]$
$\|x\|_1 = \sum_i \|x_i\|$	$\max_j \sum_i \|a_{ij}\|$	$\max_j [\mathrm{Re}\, a_{jj} + \sum_i' \|a_{ij}\|]$
$\|x\|_2 = \sqrt{\sum_i \|x_i\|^2}$	$\sqrt{\rho[A^{\mathrm{H}}A]}$	$\alpha[(A + A^{\mathrm{H}})/2]$
$\|x\|_\infty = \max_i \|x_i\|$	$\max_i \sum_j \|a_{ij}\|$	$\max_i [\mathrm{Re}\, a_{ii} + \sum_j' \|a_{ij}\|]$

Definition *Spectral abscissa* $\alpha[A] = \max \mathrm{Re}\, \lambda[A]$

5. Logarithmic norm properties

Theorem *The logarithmic norm has the following basic properties, which hold for all matrices* A and B

1. $\mu[A] \leq \|A\|$
2. $\mu[A + zI] = \mu[A] + \mathrm{Re}\, z$
3. $\mu[\alpha A] = \alpha\, \mu[A], \qquad \alpha \geq 0$
4. $\mu[A + B] \leq \mu[A] + \mu[B]$
5. $\|\mathrm{e}^{tA}\| \leq \mathrm{e}^{t\mu[A]}, \qquad t \geq 0$

Uniform Monotonicity Theorem

The condition $\mu[A] < 0$ is akin to A being *negative definite*. Then A has a bounded inverse. More precisely,

Theorem (Uniform Monotonicity Theorem) *If $\mu[A] < 0$ then A is nonsingular and*

$$\|A^{-1}\| \leq -1/\mu[A]$$

Proof (Here only for the Euclidean norm) Note that $\forall x$

$$x^{\mathrm{T}} A x \leq \mu_2[A] \cdot x^{\mathrm{T}} x$$

Suppose $\mu_2[A] < 0$. By the Cauchy-Schwarz inequality

$$-\|x\|_2 \cdot \|Ax\|_2 \leq x^{\mathrm{T}} Ax \leq \mu_2[A] \cdot \|x\|_2^2 < 0$$

for all $x \neq 0$. Hence $Ax \neq 0$, so A^{-1} exists! Put $x = A^{-1}y$ and rearrange to get

$$-\|y\|_2 \leq \mu_2[A] \cdot \|A^{-1}y\|_2 \quad \Rightarrow \quad \frac{\|A^{-1}y\|_2}{\|y\|_2} \leq -\frac{1}{\mu_2[A]}$$

Take maximum over y to see that $\|A^{-1}\|_2 \leq -1/\mu_2[A]$ $\square$

Consider Explicit Euler for $\dot{x} = Ax + f(t)$

$$x_{n+1} = x_n + hAx_n + hf(t_n)$$
$$x(t_{n+1}) = x(t_n) + hAx(t_n) + hf(t_n) - h^2 r_n$$

Global error $e_n = x_n - x(t_n)$

$$e_{n+1} = e_n + hAe_n + h^2 r_n \quad \Rightarrow$$

$$\|e_{n+1}\| \leq \|e_n\| + h\|A\| \cdot \|e_n\| + \|h^2 r_n\|$$

Classical convergence analysis

Recall (Chapter 1, p.15)

Lemma *If* $u_{n+1} \leq (1 + h\mu)u_n + ch^2$ *with* $u_0 = 0$, *then*

$$u_n \leq \frac{ch}{\mu}[(1 + h\mu)^n - 1] \leq ch\,\frac{\mathrm{e}^{\mu t_n} - 1}{\mu}$$

if $h\mu \geq 0$. *In case* $-1 < h\mu < 0$, *we have*

$$\max_n u_n \leq -\frac{ch}{\mu}$$

Classical convergence analysis . . .

$$\|e_{n+1}\| \leq (1 + h\|A\|) \cdot \|e_n\| + \|h^2 r_n\|$$

The lemma applies with $\mu = \|A\|$ and $c = \max_n \|r_n\|$

$$\|e_n\| \leq h \max_n \|r_n\| \, \frac{\mathrm{e}^{\|A\| t_n} - 1}{\|A\|}$$

"Convergence," but *exponentially growing bound*

(Hopeless!)

Modern convergence analysis

Explicit Euler for $\dot{x} = Ax + f(t)$

$$x_{n+1} = x_n + hAx_n + hf(t_n)$$
$$x(t_{n+1}) = x(t_n) + hAx(t_n) + hf(t_n) - h^2 r_n$$

Global error $e_n = x_n - x(t_n)$

$$e_{n+1} = e_n + hAe_n + h^2 r_n = (I + hA)e_n + h^2 r_n \quad \Rightarrow$$

$$\|e_{n+1}\| \leq \|I + hA\| \cdot \|e_n\| + \|h^2 r_n\|$$

Modern convergence analysis ...

Note that, using the log norm,

$$\mu[A] = \lim_{h \to 0+} \frac{\|I + hA\| - 1}{h}$$

we have

$$\|I + hA\| = 1 + h\mu[A] + \mathrm{O}(h^2)$$

as $h\|A\| \to 0$

Modern convergence analysis . . .

Now the lemma applies with $\mu \approx \mu[A]$ and $c = \max_n \|r_n\|$

$$\|e_n\| \lessapprox h \max_n \|r_n\| \frac{\mathrm{e}^{\mu[A]t_n} - 1}{\mu[A]} ; \quad \mu[A] \geq 0$$

and in case $-1 < h\mu[A] < 0$ we have

$$\max_n \|e_n\| \lessapprox - \frac{h \max_n \|r_n\|}{\mu[A]}$$

Convergence, with *"realistic" error bound*, as $\mu[A] \leq \|A\|$

Consider Implicit Euler for $\dot{x} = Ax + f(t)$

$$x_{n+1} = x_n + hAx_{n+1} + hf(t_{n+1})$$
$$x(t_{n+1}) = x(t_n) + hAx(t_{n+1}) + hf(t_{n+1}) - h^2 r_n$$

When is it possible to solve $(I - hA)x_{n+1} = x_n + hf(t_{n+1})$?

Uniform monotonicity theorem guarantees unique solution if

$$\mu[hA - I] < 0 \Leftrightarrow \mu[hA] < 1$$

Easily satisfied, *even without bound on* $\|hA\|$

Part 2. Interpolation

1. What is interpolation?

Interpolation is "the opposite" of discretization

Problem Given a discrete grid function (a vector) $F = \{f_j\}_0^N$ defined on a grid $\{x_j\}_0^N$, find a continuous function $f(x)$ with the *interpolating property* $f(x_j) = f_j$

Compare digital–to–analog conversion

Typically the function *f is sought among polynomials* or among trigonometric functions (Fourier analysis)

Naïve polynomial interpolation

$$P_n(x) = c_0 + c_1 x + c_2 x^2 + \cdots + c_n x^n$$

$n + 1$ coefficients, $n + 1$ interpolation conditions $P_n(x_j) = f_j$

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \ldots & x_0^n \\ 1 & x_1 & x_1^2 & \ldots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \ldots & x_n^n \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{pmatrix} = \begin{pmatrix} f_0 \\ f_1 \\ \vdots \\ f_n \end{pmatrix}$$

Vandermonde matrix, nonsingular if $x_i \neq x_j$, unique solution

Tedious and often ill-conditioned approach

On a grid $\{x_0, x_1, \ldots, x_k\}$ construct a degree k polynomial basis

$$\{\varphi_i(x)\}_{i=0}^{k}$$

such that $\varphi_i(x_j) = \delta_{ij}$ (the Kronecker delta)

Theorem *If the values* $f_j = f(x_j)$ *are known for the function* $f(x)$*, then the degree* k *polynomial*

$$P(x) = \sum_{j=0}^{k} \varphi_j(x)\, f_j$$

interpolates $f(x)$ *on the grid:*

$$P(x_j) = f_j \quad \text{with} \quad P(x) \approx f(x) \quad \text{for all } x$$

$$\varphi_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

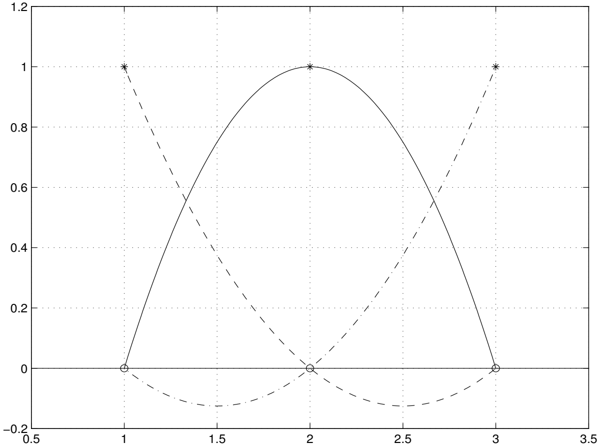


Table of Lagrange basis polynomials

x	φ_0	φ_1	φ_2	f	P_2
x_0	1	0	0	f_0	f_0
x_1	0	1	0	f_1	f_1
x_2	0	0	1	f_2	f_2

$$P_2(x) = f_0\,\varphi_0(x) + f_1\,\varphi_1(x) + f_2\,\varphi_2(x)$$

$$P_2(x) = f_0 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f_1 \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} + f_2 \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}$$

4. Numerical integration

Numerical integration is the approximation of definite integrals

$$I(f) = \int_a^b f(x)\,\mathrm{d}x$$

Problem For many functions *no primitive function is known.* The integral cannot be calculated analytically

Note For *polynomials* an integral $\int_a^b P(x)\mathrm{d}x$ can always be computed analytically

Idea Approximate $f(x) \approx P(x)$ and compute $\int_a^b P(x)\,\mathrm{d}x$

Numerical integration...

Approximate $f \approx P$ and substitute "infinite sum" by a finite sum

The integrand is sampled at a finite number of points

$$I(f) = \sum_{i=1}^{n} w_i f(x_i) + R_n$$

Here $R_n = I(f) - \sum_{i=0}^{n} w_i f(x_i)$ is the *integration error*

Numerical integration method

$$I(f) \approx \sum_{i=0}^{n} w_i f(x_i)$$

Approximate using Lagrange 2nd degree interpolant

$$\int_a^b f(x)\,\mathrm{d}x \approx \int_a^b \sum_{i=0}^{2} f(x_i)\varphi_i(x)\,\mathrm{d}x = \sum_{i=0}^{2} f(x_i) \int_a^b \varphi_i(x)\,\mathrm{d}x$$

Weights $w_i = \int_a^b \varphi_i(x)\,\mathrm{d}x$ can be computed once and for all

Numerical integration method

$$\int_a^b f(x)\,\mathrm{d}x \approx \sum_{i=0}^{2} w_i f(x_i)$$

Contents

1. Solving nonlinear equations $f(x) = 0$

We can have a single equation

$$x - \cos x = 0$$

but in general we have systems

$$4x^2 - y^2 = 0$$
$$4xy^2 - x = 1$$

Nonlinear equations may have

- no solution
- one solution
- any finite number of solutions
- infinitely many solutions

Nonlinear equations are solved by *iteration*, computing a *sequence* $\{x^{[k]}\}$ of approximations to the root x^*

Definition *The error is defined by* $e^{[k]} = x^{[k]} - x^*$

Definition *The method converges if* $\lim_{k\to\infty} \|e^{[k]}\| = 0$

Definition *The convergence is*

- *linear* if $\|e^{[k+1]}\| \le c \cdot \|e^{[k]}\|$ with $0 < c < 1$
- *quadratic* if $\|e^{[k+1]}\| \le c \cdot \|e^{[k]}\|^p$ with $p = 2$
- *superlinear* if $p > 1$;
- *cubic* if $p = 3$, etc.

2. Fixed points

Definition *x is called a fixed point of the function g if*

$$x = g(x)$$

Definition *A function g is called contractive if*

$$\|g(x) - g(y)\| \leq L[g] \cdot \|x - y\|$$

with $L[g] < 1$ *for all x, y in the domain of g*

A contraction map reduces the distance between points

Fixed Point Theorem

Theorem *Assume that g is Lipschitz continuous on the compact interval I. Further,*

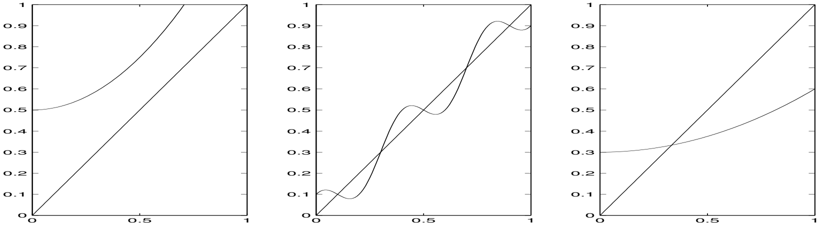
- *If $g : I \to I$ there exists an $x^* \in I$ such that $x^* = g(x^*)$*
- *If in addition $L[g] < 1$ on I, then x^* is unique, and*

$$x_{n+1} = g(x_n)$$

  converges to the fixed point x^* for all $x_0 \in I$

Note Both conditions are absolutely essential!

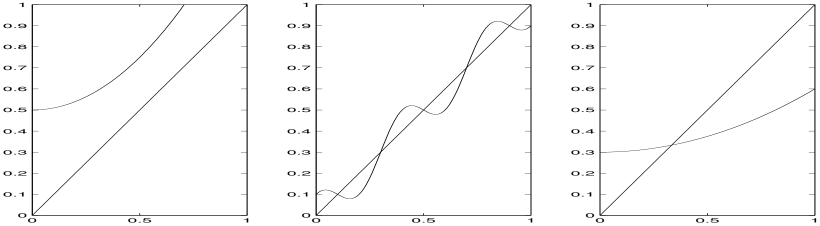
Fixed Point Theorem — *Existence and uniqueness*



Left	No condition satisfied – no x^*
Center	First condition satisfied – maybe multiple x^*
Right	Both conditions satisfied – unique x^*

Fixed Point Theorem

Existence and uniqueness



Left	No condition satisfied – no x^*
Center	First condition satisfied – maybe multiple x^*
Right	Both conditions satisfied – unique x^*
Exercise	Only second condition satisfied – ?

Error bound in fixed point iteration

By the Lipschitz condition

$$\begin{aligned} x^{[k+1]} - x^* &= g(x^{[k]}) - g(x^*) \\ &= g(x^{[k]}) - g(x^{[k+1]}) + g(x^{[k+1]}) - g(x^*) \end{aligned}$$

we have

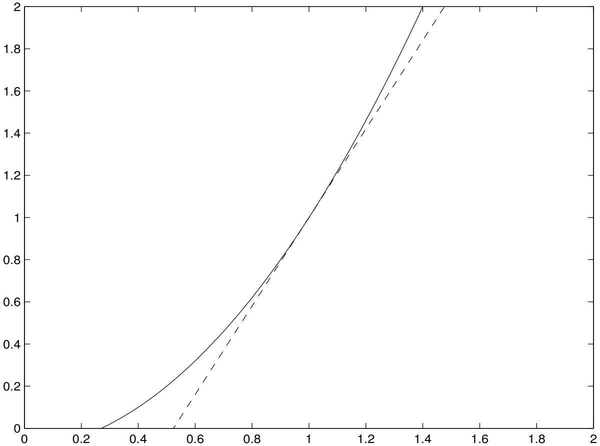
$$\|x^{[k+1]} - x^*\| \leq L[g] \cdot \|x^{[k]} - x^{[k+1]}\| + L[g] \cdot \|x^{[k+1]} - x^*\|$$

Theorem *If $L[g] < 1$, then the error in fixed point iteration is bounded by*

$$\|x^{[k+1]} - x^*\| \leq \frac{L[g]}{1 - L[g]} \|x^{[k]} - x^{[k+1]}\|$$

3. Newton's method

Newton's method solves $f(x) = 0$ using *repeated linearizations*.
Linearize at the point $(x^{[k]}, f(x^{[k]}))$



Newton's method ...

Straight line equation

$$y - f(x^{[k]}) = f'(x^{[k]}) \cdot (x - x^{[k]})$$

Define $x = x^{[k+1]} \;\Rightarrow\; y = 0$, *so that*

$$-f(x^{[k]}) = f'(x^{[k]}) \cdot (x^{[k+1]} - x^{[k]})$$

Solve for $x = x^{[k+1]}$, to get *Newton's method*

$$x^{[k+1]} = x^{[k]} - \frac{f(x^{[k]})}{f'(x^{[k]})}$$

Expand $f(x^{[k+1]})$ in a Taylor series around $x^{[k]}$

$$
\begin{aligned}
f(x^{[k+1]}) &= f(x^{[k]} + (x^{[k+1]} - x^{[k]})) \\
&\approx f(x^{[k]}) + f'(x^{[k]}) \cdot (x^{[k+1]} - x^{[k]}) := 0 \\
&\Rightarrow \\
x^{[k+1]} &= x^{[k]} - \left(f'(x^{[k]})\right)^{-1} f(x^{[k]})
\end{aligned}
$$

Definition $f'(x^{[k]})$ is the *Jacobian matrix* of f, defined by

$$f'(x) = \left\{ \frac{\partial f_i}{\partial x_j} \right\}$$

Write Newton's method as a fixed point iteration $x^{[k+1]} = g(x^{[k]})$ with iteration function

$$g(x) := x - f(x)/f'(x)$$

Note Newton's method *converges fast if* $f'(x^*) \neq 0$, because $g'(x^*) = f(x^*)f''(x^*)/f'(x^*)^2 = 0$

Expand $g(x)$ in a Taylor series around x^*

$$g(x^{[k]}) - g(x^*) \approx g'(x^*)(x^{[k]} - x^*) + \frac{g''(x^*)}{2}(x^{[k]} - x^*)^2$$

$$x^{[k+1]} - x^* \approx \frac{g''(x^*)}{2}(x^{[k]} - x^*)^2$$

Define the error by $\varepsilon^{[k]} = x^{[k]} - x^*$, then

$$\varepsilon^{[k+1]} \sim \left(\varepsilon^{[k]}\right)^2$$

Newton's method is *quadratically convergent*

Fixed point iterations are typically only linearly convergent

$$\varepsilon^{[k+1]} \approx g'(x^*) \cdot \varepsilon^{[k]}$$

A problem with Newton's method is that *starting values need to be close enough* to the root

Convergence order and rate

Definition *The convergence order is p with (asymptotic) error constant C_p, if*

$$0 < \lim_{k\to\infty} \frac{\|\varepsilon^{[k+1]}\|}{\|\varepsilon^{[k]}\|^p} = C_p < \infty$$

Special cases

$p = 1$ Linear convergence
Fixed point iteration $C_p = |f'(x^*)|$

$p = 2$ Quadratic convergence
Newton iteration $C_p = \left|\frac{f''(x^*)}{2f'(x^*)}\right|$

As $y_{n+1} = y_n + hf(y_{n+1})$ we need to solve an equation

$$y = hf(y) + \psi$$

Note All implicit methods lead to an equation of this form

Theorem *Fixed point iterations converge if* $L[hf] < 1$, *restricting the step size to* $h < 1/L[f]$

Note For stiff equations $L[hf] \gg 1$ so fixed point iterations will not converge; it is *necessary to use Newton's method*