

Convex Optimization

CMU-10725

Newton Method

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MACHINE LEARNING DEPARTMENT



Administrivia

- ☐ Scribing
- ☐ Projects
- ☐ HW1 solutions
- ☐ Feedback about lectures / solutions on blackboard

Books to read

- **Boyd and Vandenberghe**: Convex Optimization, Chapters 9.5
- **Nesterov**: Introductory lectures on convex optimization
- **Bazaraa, Sherali, Shetty**: Nonlinear Programming
- **Dimitri P. Bestsekas**: Nonlinear Programming
- **Wikipedia**
- <http://www.chiark.greenend.org.uk/~sgtatham/newton/>

Goal of this lecture

Newton method

- ☐ Finding a root
- ☐ Unconstrained minimization
 - Motivation with quadratic approximation
 - Rate of Newton's method
- ☐ Newton fractals

Next lectures:

- ☐ Conjugate gradients
- ☐ Quasi Newton Methods

Newton method for finding a root

Newton method for finding a root

- ❑ Newton method: originally developed for finding a root of a function
- ❑ also known as the **Newton–Raphson method**

$$\phi : \mathbb{R} \rightarrow \mathbb{R}$$

$$\phi(x^*) = 0$$

$$x^* = ?$$

History

Finding \sqrt{S} is the same as solving the equation:

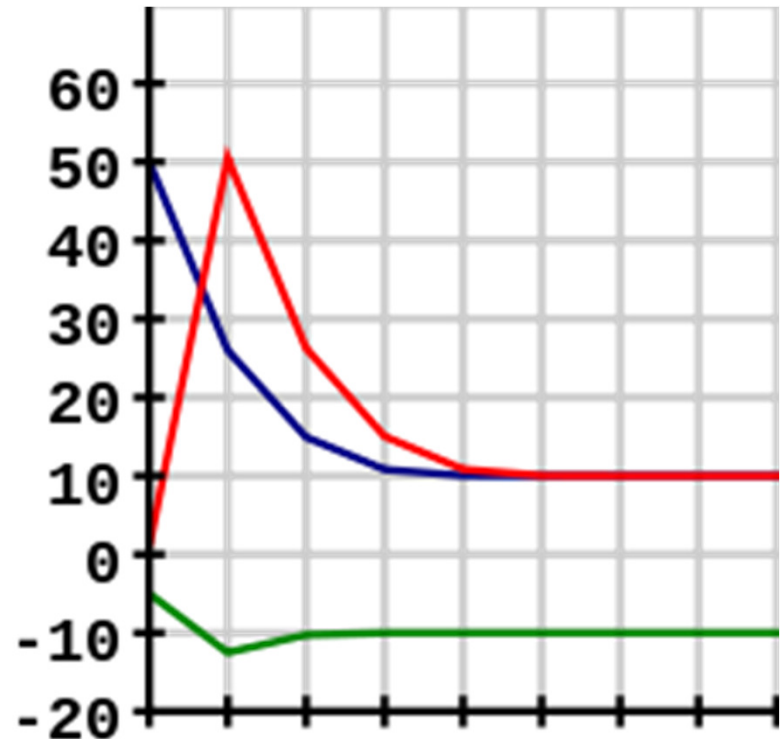
$$f(x) = x^2 - S = 0$$

Babylonian method:

$$x_{n+1} = \frac{1}{2} \left(x_n + \frac{S}{x_n} \right) = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^2 - S}{2x_n}$$

This is a special case of Newton's method

$S=100$. starting values $x_0 = 50$, $x_0 = 1$,
and $x_0 = -5$.



History

- ❑ **1669, Isaac Newton** [published in 1711]:
 - finding roots of polynomials
- ❑ **1690, Joseph Raphson**:
 - finding roots of polynomials
- ❑ **1740, Thomas Simpson**:
 - solving general nonlinear equation
 - generalization to systems of two equations
 - solving optimization problems (gradient = zero)
- ❑ **1879, Arthur Cayley**:
 - generalizing the Newton's method to finding complex roots of polynomials

Newton Method for Finding a Root

Goal: $\phi : \mathbb{R} \rightarrow \mathbb{R}$

$$\phi(x^*) = 0$$

$$x^* = ?$$

Linear Approximation (1st order Taylor approx):

$$\underbrace{\phi(\underbrace{x + \Delta x}_{x^*})}_{\phi(x^*) = 0} = \phi(x) + \phi'(x)\Delta x + \underbrace{o(|\Delta x|)}_{\text{NEGLECTABLE}}$$

Therefore,

$$0 \approx \phi(x) + \phi'(x)\Delta x$$

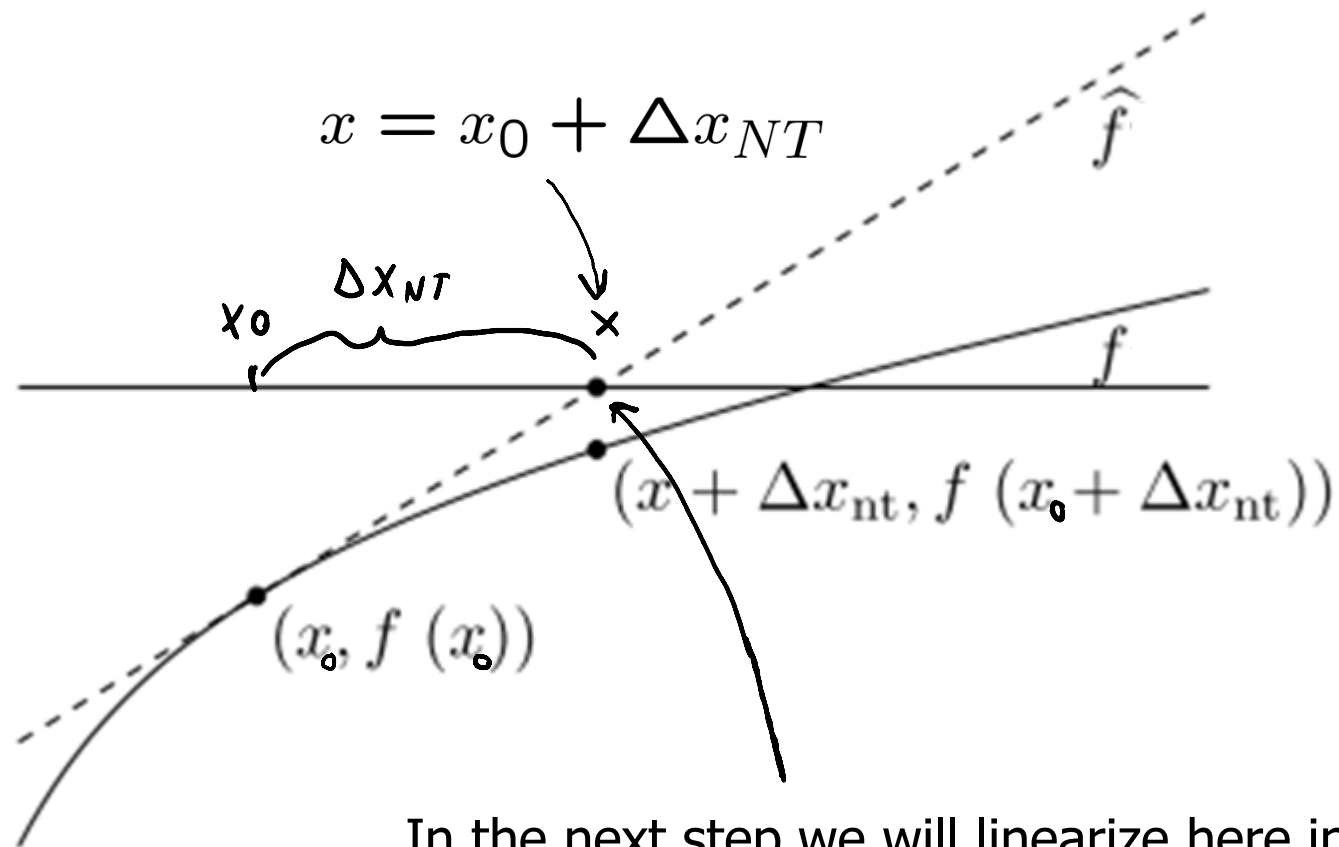
$$x^* - x = \Delta x = -\frac{\phi(x)}{\phi'(x)}$$

$$x_{k+1} = x_k - \frac{\phi(x)}{\phi'(x)}$$

Illustration of Newton's method

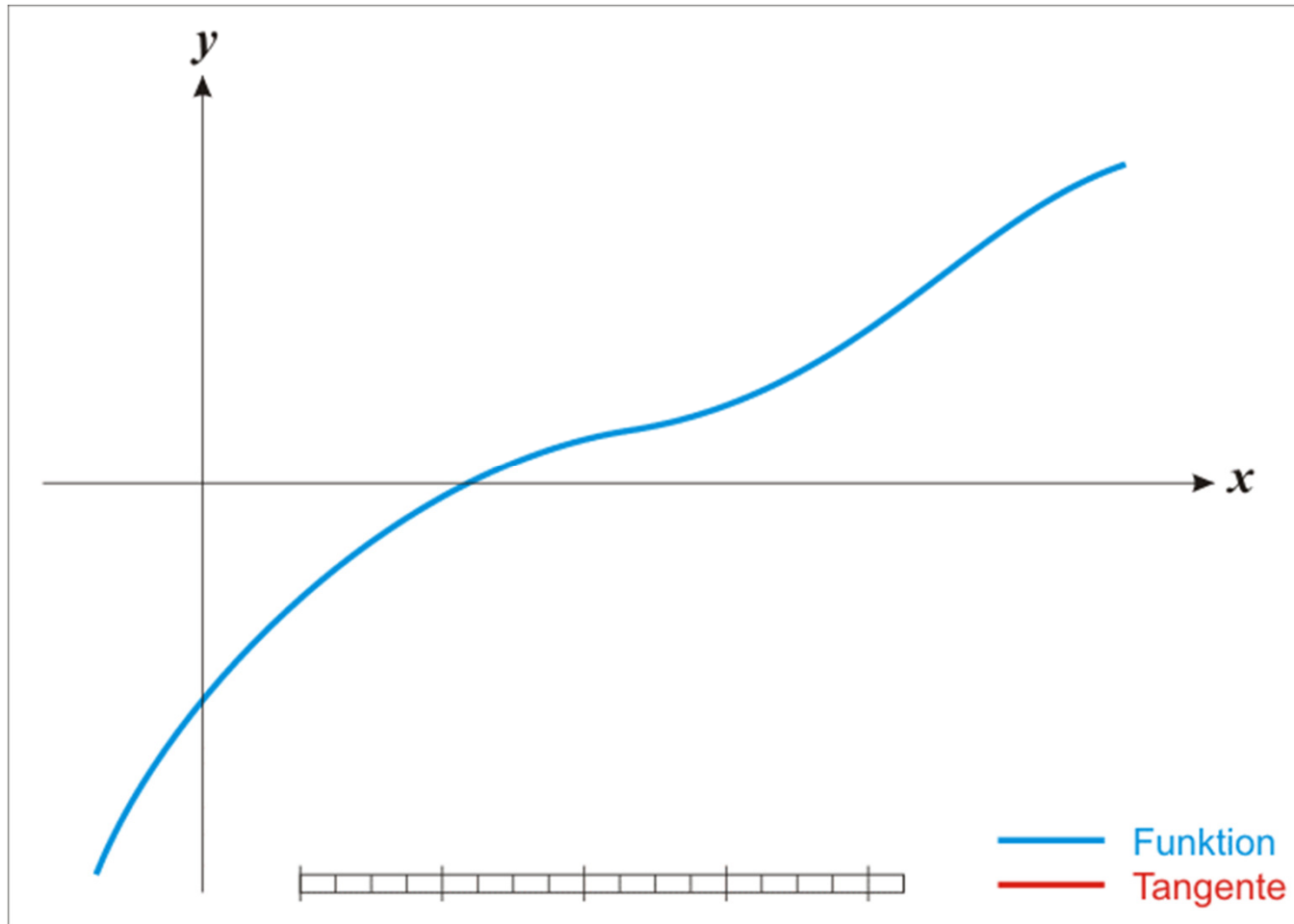
Goal: finding a root

$$\hat{f}(x) = f(x_0) + f'(x_0)(x - x_0)$$



In the next step we will linearize here in x

Example: Finding a Root



http://en.wikipedia.org/wiki/Newton%27s_method

Newton Method for Finding a Root

This can be generalized to multivariate functions

$$F : \mathbb{R}^n \rightarrow \mathbb{R}^m$$

$$0_m = F(x^*) = F(x + \Delta x) = F(x) + \underbrace{\nabla F(x)}_{\mathbb{R}^{m \times n}} \underbrace{\Delta x}_{\mathbb{R}^n} + o(|\Delta x|)$$

\uparrow
NEGLECT

Therefore,

$$0_m = F(x) + \nabla F(x) \Delta x$$

$$\Delta x = -[\nabla F(x)]^{-1} F(x)$$

[Pseudo inverse if there is no inverse]

$$\Delta x = x_{k+1} - x_k, \text{ and thus}$$

$$\underbrace{x_{k+1}}_{\mathbb{R}^n} = \underbrace{x_k}_{\mathbb{R}^n} - \underbrace{[\nabla F(x_k)]^{-1}}_{\mathbb{R}^{n \times m}} \underbrace{F(x_k)}_{\mathbb{R}^m}$$

Newton method: Start from x_0 and iterate.

Newton method for minimization

Newton method for minimization

$f : \mathbb{R}^n \rightarrow \mathbb{R}$, f is differentiable.

$$\min_{x \in \mathbb{R}^n} f(x)$$

We need to find the roots of $\nabla f(x) = 0_n$
 $\nabla f : \mathbb{R}^n \rightarrow \mathbb{R}^n$

Newton system: $\nabla f(x) + \nabla^2 f(x) \Delta x = 0_n$

Newton step: $\Delta x = x_{k+1} - x_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$

Iterate until convergence, or max number of iterations exceeded
(divergence, loops, division by zero might happen...)

How good is the Newton method?

Descent direction

Lemma [Descent direction]

If $\nabla^2 f \succ 0$, then Newton step is a descent direction.

Proof:

We know that if a vector has negative inner product with the gradient vector, then that direction is a descent direction

Newton step: $\Delta x = x_{k+1} - x_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$

$$\Rightarrow \nabla f(x_k)^T \Delta x = -\nabla f(x_k)^T [\nabla^2 f(x_k)]^{-1} \nabla f(x_k) < 0$$



Newton method properties

- ❑ Quadratic convergence in the neighborhood of a strict local minimum [under some conditions].
- ❑ It can break down if $f''(x_k)$ is degenerate.
[no inverse]
- ❑ It can diverge.
- ❑ It can be trapped in a loop.
- ❑ It can converge to a loop...

Motivation with Quadratic Approximation

Motivation with Quadratic Approximation

$f : \mathbb{R}^n \rightarrow \mathbb{R}$, f is differentiable.

Second order Taylor approximation:

Let $\phi(x) = f(x_k) + \nabla^T f(x_k)(x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k)$

Assume that

$\nabla^2 f(x_k) \succ 0$ [i.e. ϕ has strict global minimum]

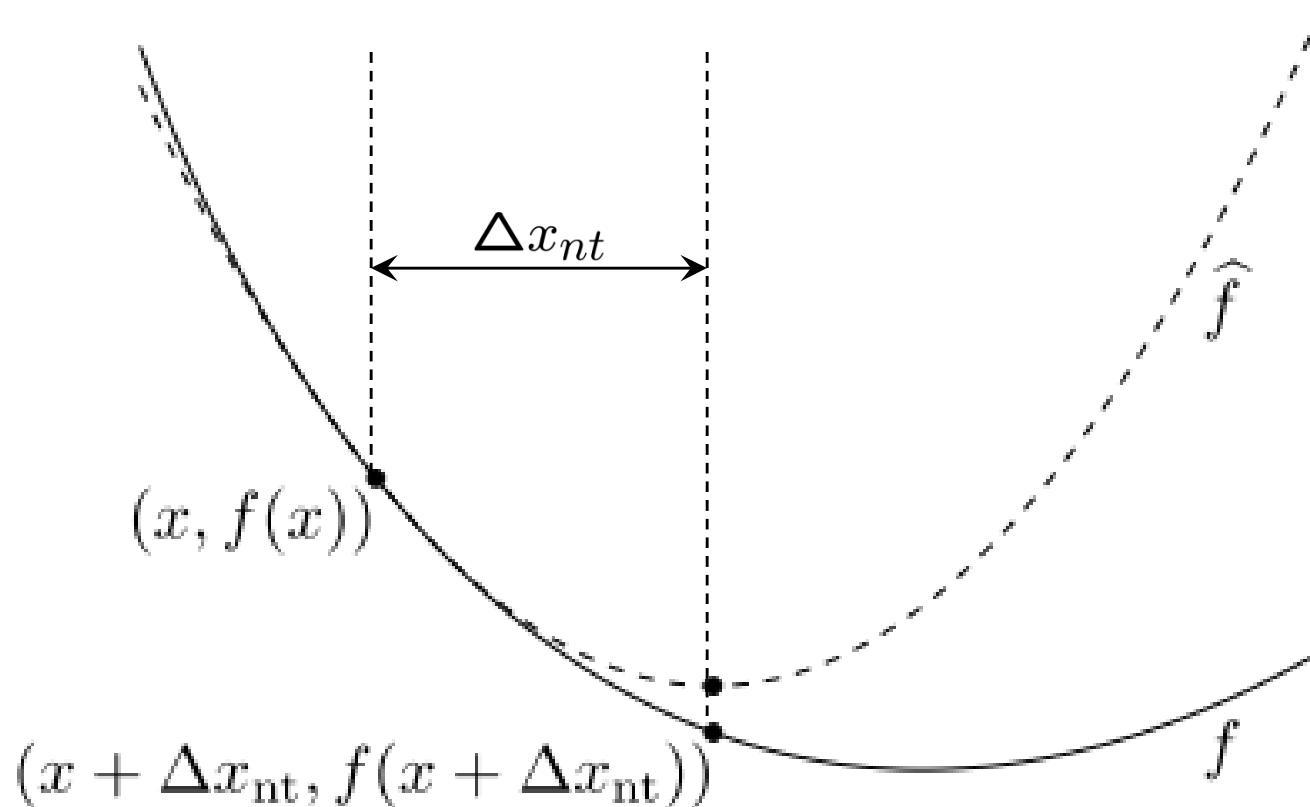
Now, if x_{k+1} is the global minimum of the quadratic function ϕ , then

$$0_n = \nabla \phi(x_{k+1}) = \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k)$$

Newton step:

$$\Delta x = x_{k+1} - x_k = -[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

Motivation with Quadratic Approximation



Quadratic approximation is good, when x is close to x^*

$$\hat{f}(z) = f(x) + \nabla^T f(x)(z - x) + \frac{1}{2}(z - x)^T \nabla^2 f(x)(z - x)$$

Convergence rate ($f: \mathbb{R} \rightarrow \mathbb{R}$ case)

Rates

A sequence $\{s_i\}$ exhibits linear convergence if $\lim_{i \rightarrow \infty} s_i = \bar{s}$, and

$$\lim_{i \rightarrow \infty} \frac{|s_{i+1} - \bar{s}|}{|s_i - \bar{s}|} = \delta < 1 \quad \text{Example:} \quad s_i = cq^i, \quad 0 < q < 1$$

$$\frac{|s_{i+1} - \bar{s}|}{|s_i - \bar{s}|} = \frac{cq^{i+1}}{cq^i} = q < 1$$

Superlinear rate: $\delta = 0$ Example: $s_i = \frac{c}{i!}$

$$\frac{|s_{i+1} - \bar{s}|}{|s_i - \bar{s}|} = \frac{ci!}{c(i+1)!} = \frac{1}{i+1} \rightarrow 0$$

Sublinear rate: $\delta = 1$ Example: $s_i = \frac{c}{i^a}, \quad a > 0$

$$\frac{|s_{i+1} - \bar{s}|}{|s_i - \bar{s}|} = \frac{ci^a}{c(i+1)^a} = \left(\frac{i}{i+1}\right)^a \rightarrow 1$$

Quadratic rate:

$$\lim_{i \rightarrow \infty} \frac{|s_{i+1} - \bar{s}|}{|s_i - \bar{s}|^2} < \infty \quad \text{Example:} \quad s_i = q^{2^i}, \quad 0 < q < 1$$

Finding a root: Convergence rate

Goal: Find x^* s.t. $f(x^*) = 0$, where $f : \mathbb{R} \rightarrow \mathbb{R}$

Assumption: f has continuous second derivative in x^*

Taylor theorem: For a ξ_n between x_n and x^* , we have

$$0 = f(x^*) = f(x_n) + \nabla f(x_n)(x^* - x_n) + \frac{1}{2} \nabla^2 f(\xi_n)(x^* - x_n)^2$$

Therefore, assuming $\exists [\nabla f(x_n)]^{-1}$

$$0 = [\nabla f(x_n)]^{-1} f(x_n) + (x^* - x_n) + \frac{1}{2} [\nabla f(x_n)]^{-1} \nabla^2 f(\xi_n)(x^* - x_n)^2$$

$$\underbrace{[\nabla f(x_n)]^{-1} f(x_n) + (x^* - x_n)}_{\substack{x^* - x_{n+1} \\ \epsilon_{n+1}}} = -\frac{1}{2} [\nabla f(x_n)]^{-1} \nabla^2 f(\xi_n) \underbrace{(x^* - x_n)^2}_{\epsilon_n^2}$$

$$\Rightarrow \epsilon_{n+1} = -\frac{1}{2} [\nabla f(x_n)]^{-1} \nabla^2 f(\xi_n) \epsilon_n^2$$

Finding a root: Convergence rate

We have seen that

$$\epsilon_{n+1} = -\frac{\overbrace{1 \nabla^2 f(\xi_n)}^M}{2 \nabla f(x_n)} \epsilon_n^2$$

Assume that $M = \sup_x \frac{1}{2} \frac{|\nabla^2 f(x)|}{|\nabla f(x)|} < \infty$

$$\Rightarrow |\epsilon_{n+1}| \leq M \epsilon_n^2 \quad \text{sup } \frac{1}{2} \frac{|\nabla^2 f(x)|}{|\nabla f(x)|} < \infty$$

Assume that $|\epsilon_0| = |x^* - x_0| < \frac{1}{M}$

\Rightarrow Quadratic convergence

Problematic cases

Finding a root: chaotic behavior

Let $f(x) = x^3 - 2x^2 - 11x + 12$

$$x^3 - 2x^2 - 11x + 12$$

Goal: find the roots, $(-3, 1, 4)$, using Newton's method

$x_0 = 2.35287527$ converges to 4;

· 2.35284172 converges to -3 ;

2.35283735 converges to 4;

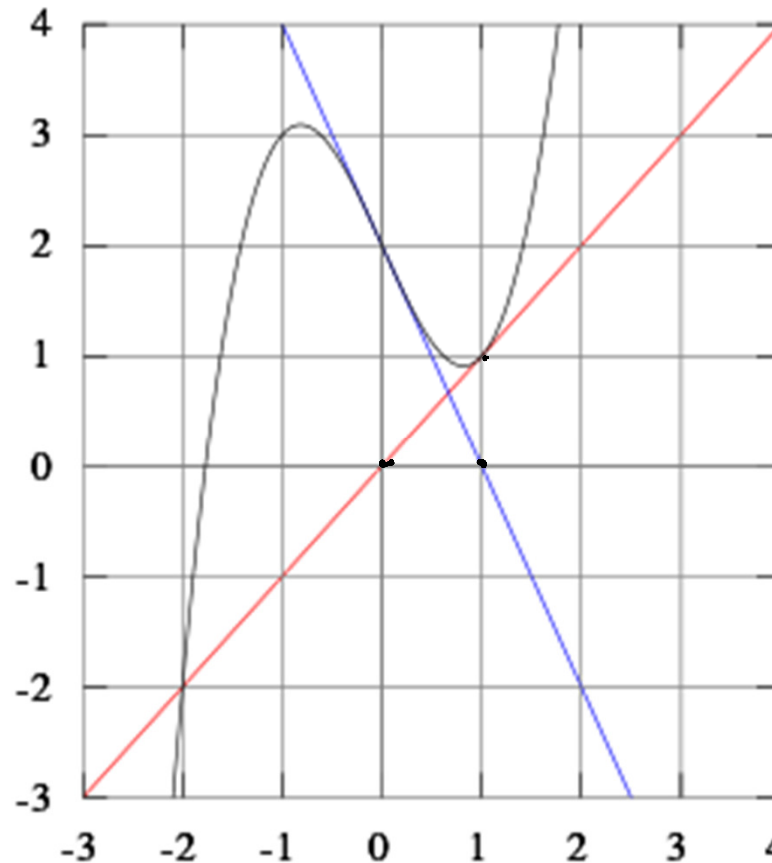
2.352836327 converges to -3 ;

2.352836323 converges to 1.

Finding a root: Cycle

$$f(x) = x^3 - 2x + 2$$

Goal: find its roots



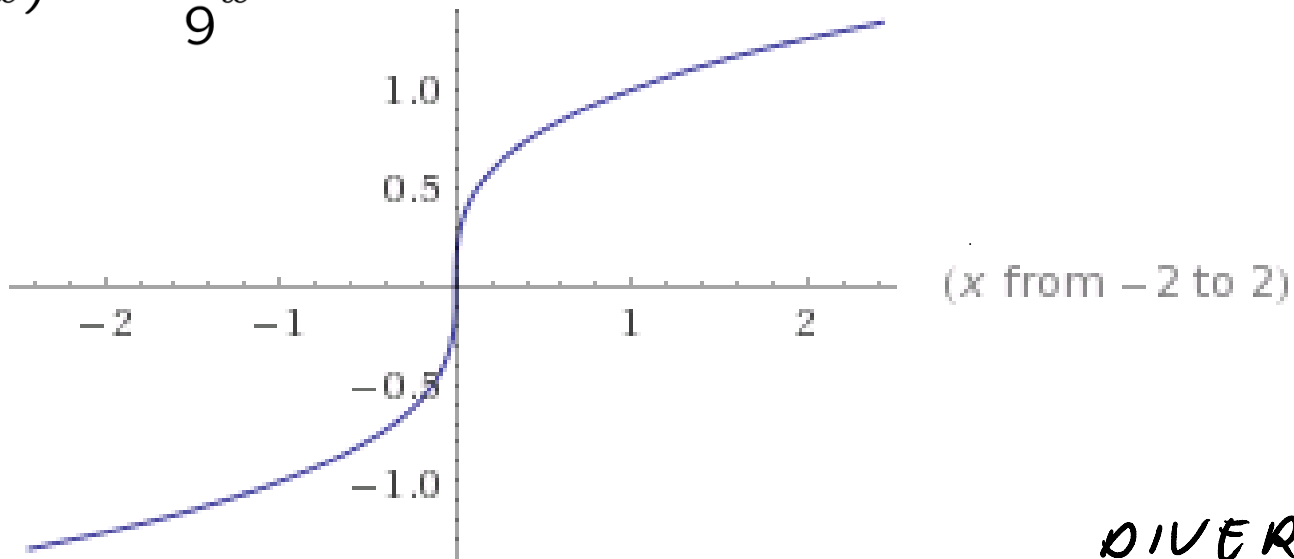
$x_0 = 0 \quad x_1 = 1, x_2 = 0, x_3 = 1, x_4 = 0 \dots \Rightarrow 2\text{-cycle}$

Stating point is important!

Finding a root: divergence everywhere (except in the root)

Newton's method might never converge (except in the root)!

$$f(x) = \sqrt[3]{x}$$
$$\nabla f(x) = \frac{1}{3}x^{-2/3}$$
$$\nabla^2 f(x) = -\frac{2}{9}x^{-5/3}$$
$$\lim_{x \rightarrow 0} \frac{1}{2} \frac{|\nabla^2 f(x)|}{|\nabla f(x)|} = \lim_{x \rightarrow 0} \frac{c}{|x|} = \infty$$



DIVERGENCE!

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n^{\frac{1}{3}}}{\frac{1}{3}x_n^{\frac{1}{3}-1}} = x_n - 3x_n = -2x_n$$

Finding a root: Linear convergence only

If the first derivative is zero at the root, then convergence might be only linear (not quadratic)

$$f(x) = x^2$$

$$\nabla f(x) = 2x$$

$$\nabla^2 f(x) = 2$$

$$\lim_{x \rightarrow 0} \frac{1}{2} \frac{|\nabla^2 f(x)|}{|\nabla f(x)|} = \lim_{x \rightarrow 0} \frac{1}{|x|} = \infty$$

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} = x_n - x_n^2 / (2x_n) = x_n / 2$$

Linear convergence only!

Difficulties in minimization

$$f(x) = 7x - \ln(x)$$

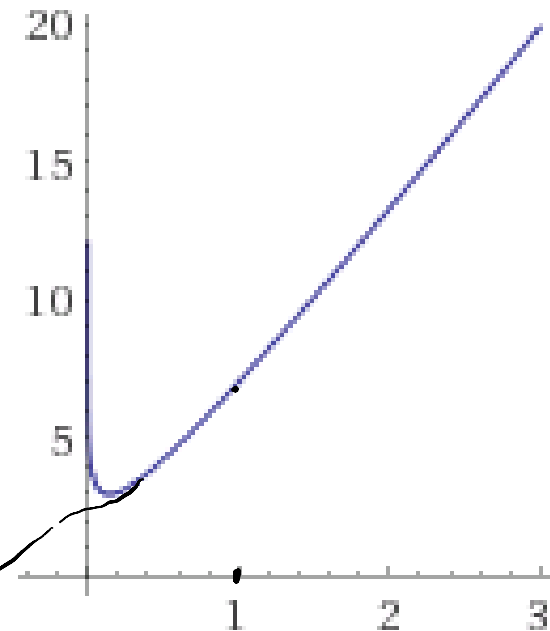
$$x^* = \frac{1}{7} = 0.142857143$$

$$f'(x) = 7 - \frac{1}{x}$$

$$f''(x) = \frac{1}{x^2}$$

$$x^{k+1} = x^k + (x^k - 7(x^k)^2) = 2x^k - 7(x^k)^2$$

| k | x^k | x^k | x^k | x^k |
|-----|--------------------------|-------|-------------|-------------|
| 0 | 1.0 | 0 | 0.1 | 0.01 |
| 1 | -5.0 | 0 | 0.13 | 0.0193 |
| 2 | -185.0 | 0 | 0.1417 | 0.03599257 |
| 3 | -239,945.0 | 0 | 0.14284777 | 0.062916884 |
| 4 | -4.0302×10^{11} | 0 | 0.142857142 | 0.098124028 |
| 5 | -1.1370×10^{24} | 0 | 0.142857143 | 0.128849782 |
| 6 | -9.0486×10^{48} | 0 | 0.142857143 | 0.1414837 |
| 7 | -5.7314×10^{98} | 0 | 0.142857143 | 0.142843938 |
| 8 | $-\infty$ | 0 | 0.142857143 | 0.142857142 |
| 9 | $-\infty$ | 0 | 0.142857143 | 0.142857143 |
| 10 | $-\infty$ | 0 | 0.142857143 | 0.142857143 |



range of quadratic
convergence

$$x \in (0.0, 0.2857143)$$

Generalizations

□ **Newton method in Banach spaces**

- Newton method on the Banach space of functions
- We need Frechet derivatives

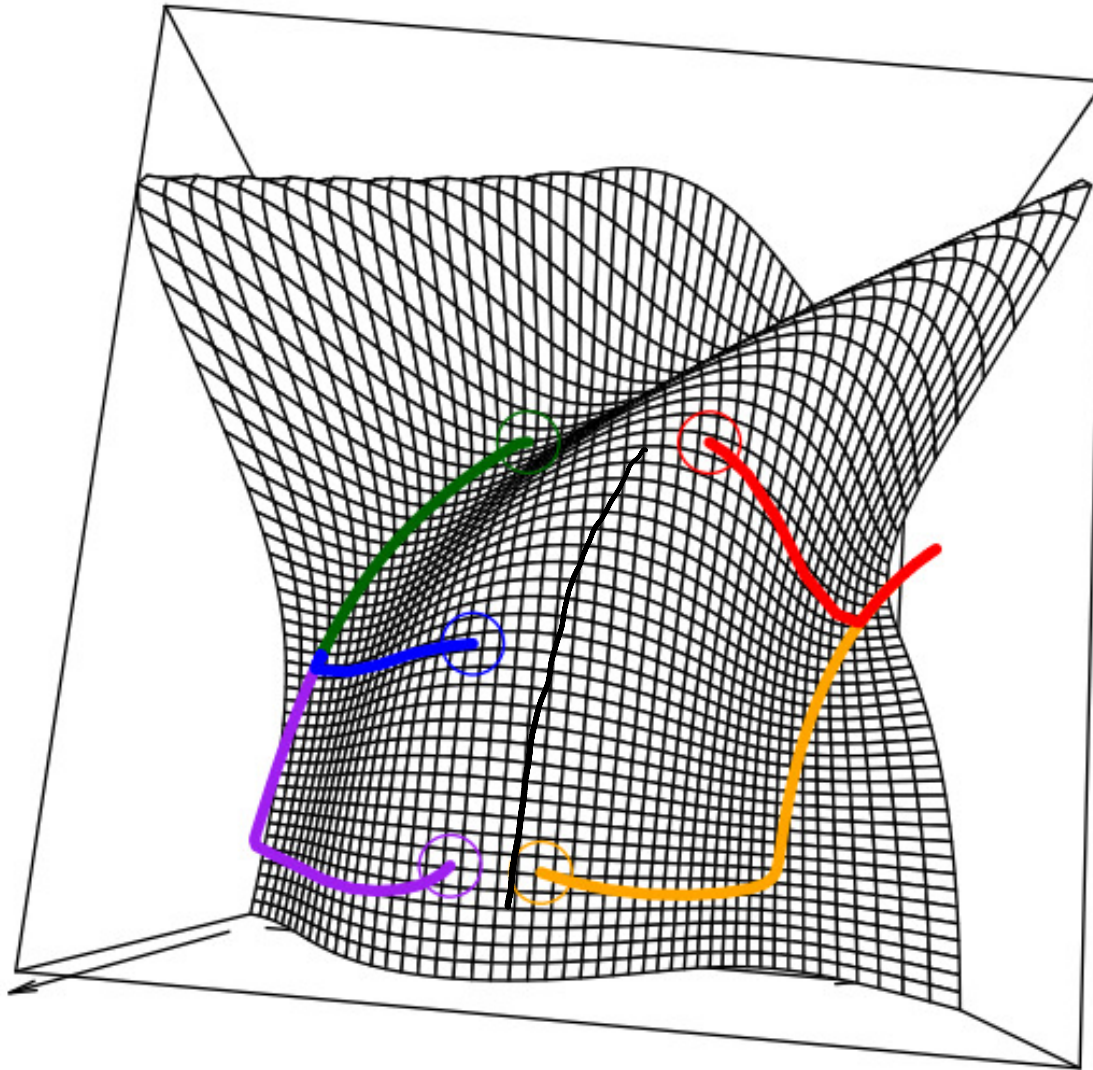
□ **Newton method on curved manifolds**

- E.g. on space of orthonormal matrices

□ **Newton method on complex numbers**

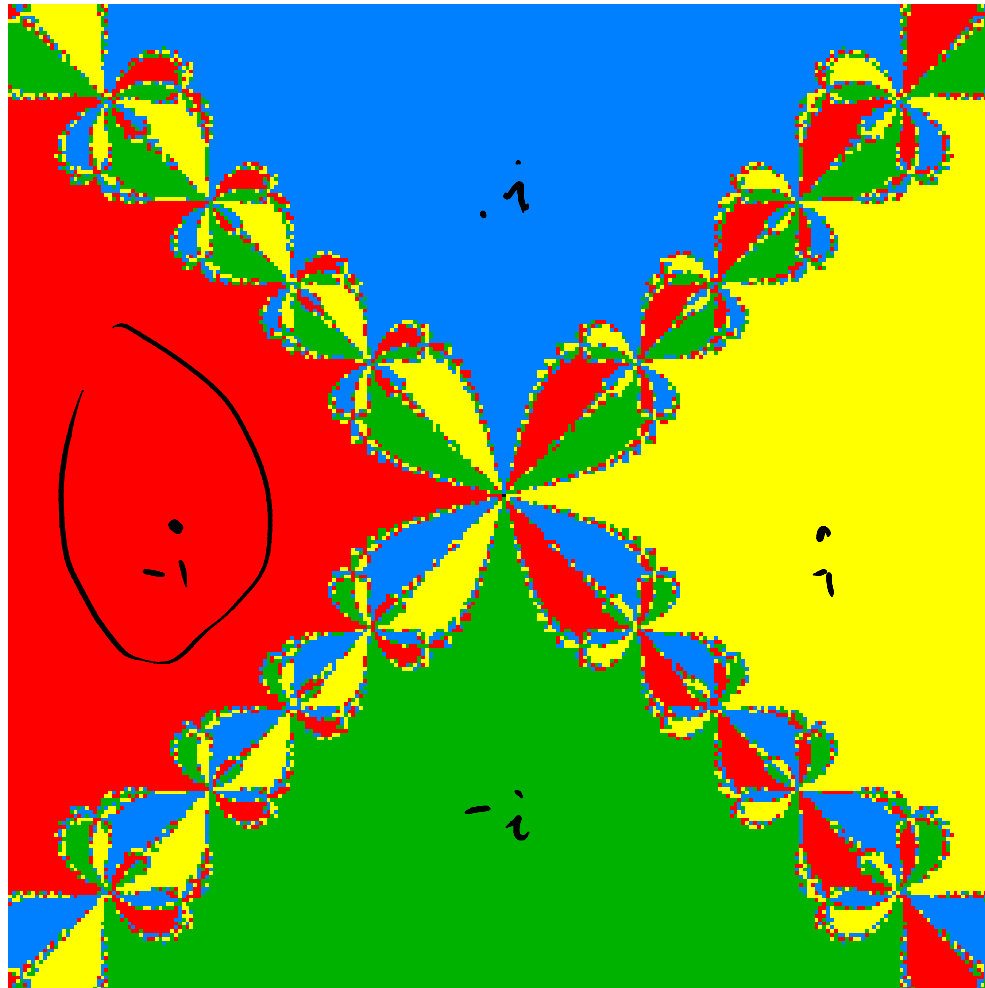
Newton Fractals

Gradient descent



Complex functions

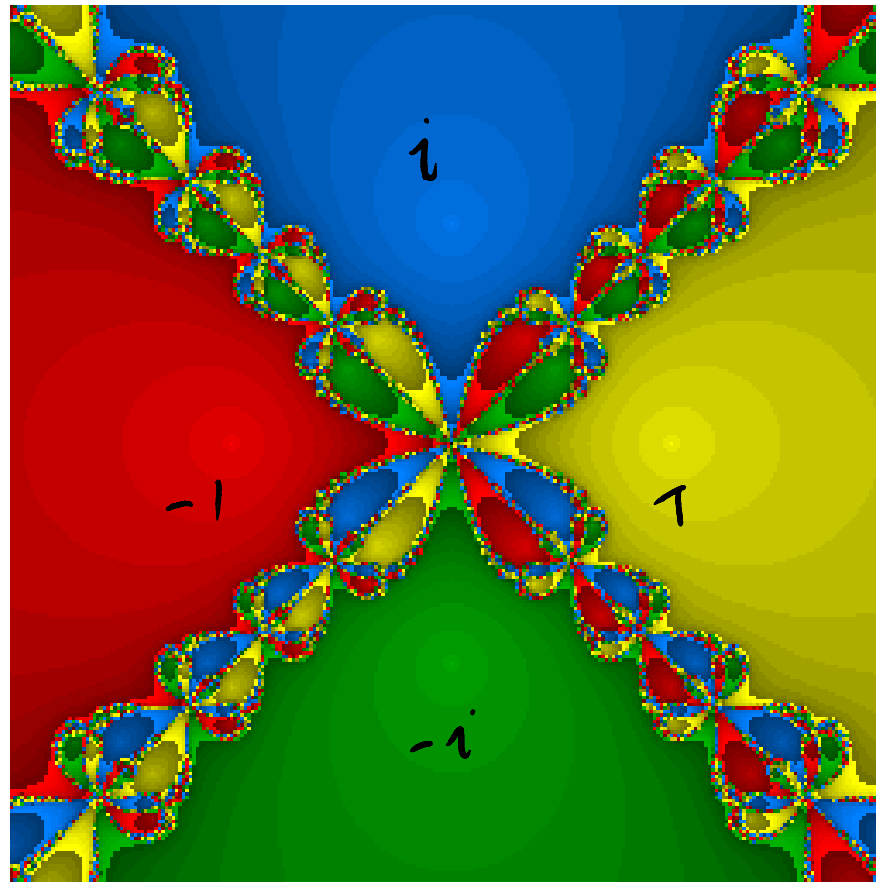
$f(z) = z^4 - 1$, Roots: $-1, +1, -i, +i$



color the starting point according to *which* root it ended up

Basins of attraction

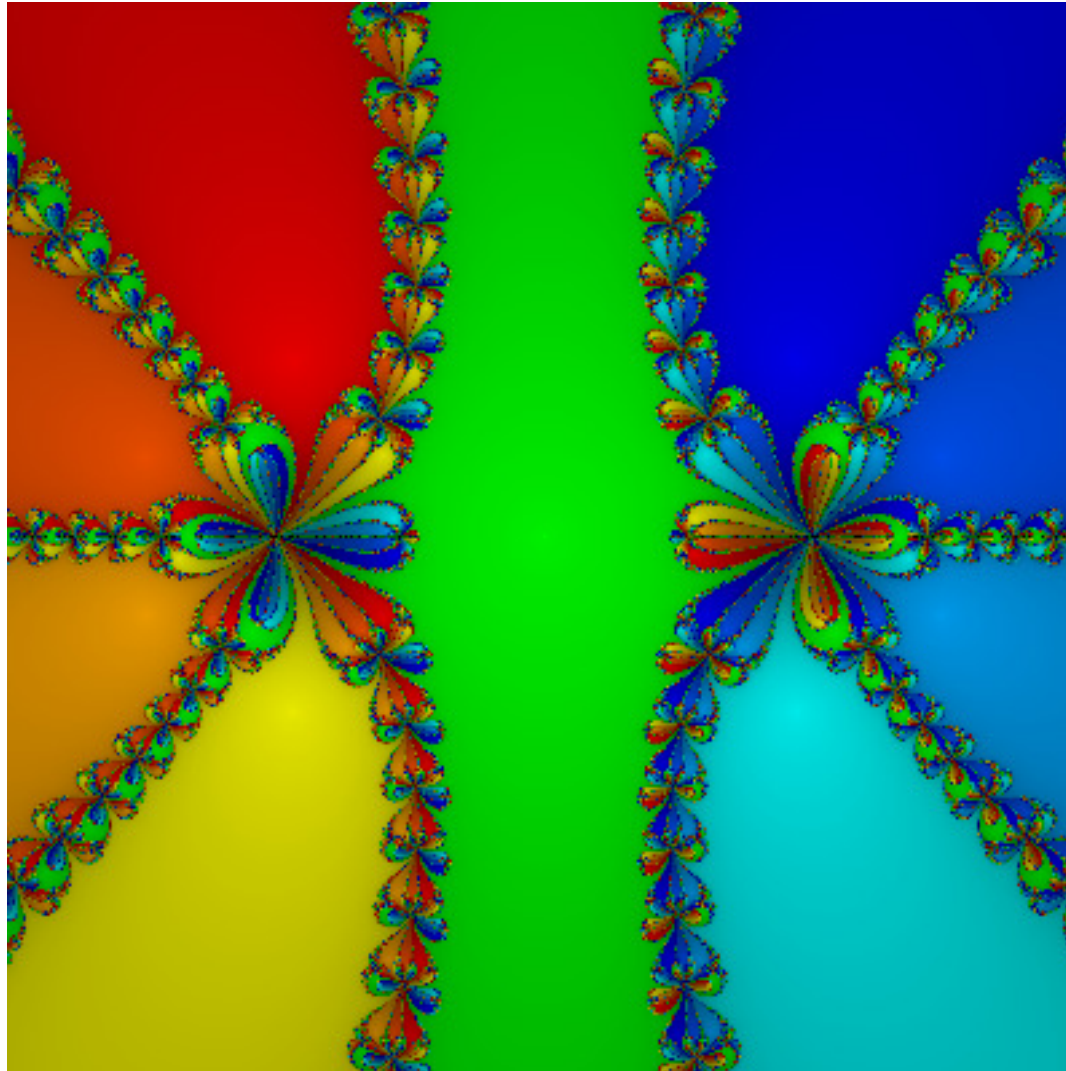
$f(z) = z^4 - 1$, Roots: $-1, +1, -i, +i$



Shading according to how many iterations it needed till convergence

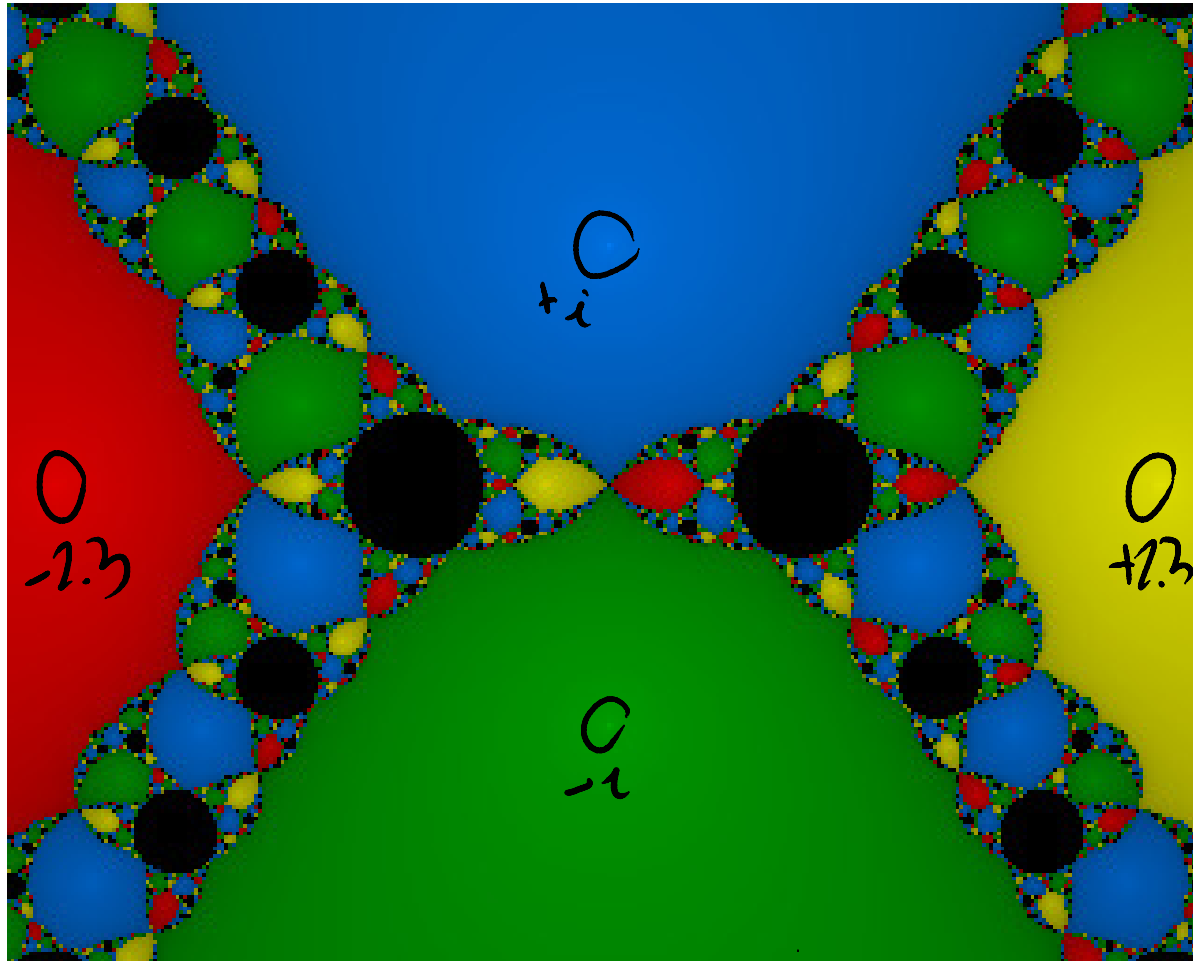
Basins of attraction

$$f'(z) = (z-1)^4(z+1)^4$$



No convergence

polynomial f , having the roots at $+i$, $-i$, -2.3 and $+2.3$



Black circles: no convergence, attracting cycle with period 2

Avoiding divergence

Damped Newton method

In order to avoid possible divergence
do line search with back tracking

$$x_{k+1} = x_k - \underline{h_k} [f''(x_k)]^{-1} f'(x_k)$$

Initial stage: back track line search for $0 < h_k \leq 1$.

Final stage: $h_k = 1$ [Full Newton step].

We already know that the Newton direction is descent direction

Classes of differentiable functions

Classes of Differentiable functions

- Any continuous (but otherwise ugly, nondifferentiable) function can be approximated arbitrarily well with smooth (k times differentiable) function
- Assuming smoothness only is not enough to talk about rates...
- We need stronger assumptions on the derivatives. [e.g. their magnitudes behaves nicely]

The $C_L^{k,p}(Q)$ Class

Definition

$$\begin{aligned} C_L^{k,p}(Q) = \{ & f : Q \rightarrow \mathbb{R} \\ & f \text{ is } k\text{-times continuously differentiable on } Q \subseteq \mathbb{R}^n \\ & k \geq p \\ & \|f^{(p)}(x) - f^{(p)}(y)\| \leq L\|x - y\|, \forall x, y \in Q \\ & \} \end{aligned}$$

[Lipschitz continuous pth order derivative]

Notation

$$\begin{aligned} C^k(Q) = \{ & f : Q \rightarrow \mathbb{R} \\ & f \text{ is } k\text{-times continuously differentiable on } Q \subseteq \mathbb{R}^n \} \end{aligned}$$

Trivial Lemmas

Lemma [Linear combinations]

$$\left. \begin{array}{l} f_1 \in C_{L_1}^{k,p}(Q) \\ f_2 \in C_{L_2}^{k,p}(Q) \\ \alpha, \beta \in \mathbb{R} \\ L_3 = |\alpha|L_1 + |\beta|L_2 \end{array} \right\} \Rightarrow \alpha f_1 + \beta f_2 \in C_{L_3}^{k,p}(Q)$$

Lemma [Class hierarchy]

If $q \geq r$, then $C_L^{q,p}(Q) \subseteq C_L^{r,p}(Q)$

$$\text{e.g. } C_L^{2,1}(Q) \subseteq C_L^{1,1}(Q)$$

Relation between 1st and 2nd derivatives

Lemma Let f be twice differentiable on \mathbb{R}^n

$$f'(x + \alpha(y - x)) - f'(x) = \int_0^\alpha f''(x + \tau(y - x))(y - x) d\tau$$

Proof Let $\phi(\tau) = f'(x + \tau(y - x))$. Now we have that

$$\phi(0) = f'(x)$$

$$\phi(\alpha) = f'(x + \alpha(y - x))$$

$$\phi'(\tau) = f''(x + \tau(y - x))(y - x)$$

Therefore,

$$f'(x + \alpha(y - x)) - f'(x) = \phi(\alpha) - \phi(0)$$

$$= \int_0^\alpha \phi'(\tau) d\tau$$

$$= \int_0^\alpha f''(x + \tau(y - x))(y - x) d\tau$$

Q.E.D

Special case,

$$f'(y) - f'(x) = \int_0^1 f''(x + \tau(y - x))(y - x) d\tau$$

$C_L^{2,1}(\mathbb{R}^n)$ and the norm of f''

Lemma [$C_L^{2,1}$ and the norm of f'']

Let f be twice differentiable on \mathbb{R}^n

Then $\|f''(x)\|_{op} \leq L \forall x \in \mathbb{R}^n \Leftrightarrow f \in C_L^{2,1}(\mathbb{R}^n)$

Proof

$$\begin{aligned} &\Rightarrow f'(y) - f'(x) = \int_0^1 f''(x + \tau(y - x))(y - x) d\tau \\ \Rightarrow \|f'(y) - f'(x)\| &\leq \int_0^1 \|f''(x + \tau(y - x))(y - x)\| d\tau \\ &\leq \int_0^1 \|f''(x + \tau(y - x))\|_{op} d\tau \|y - x\| \\ &\leq \|y - x\| \int_0^1 L d\tau = L\|y - x\| \\ &\Rightarrow f \in C_L^{2,1}(\mathbb{R}^n) \end{aligned}$$

Q.E.D

$C_L^{2,1}(\mathbb{R}^n)$ and the norm of f''

$$\|f''(x)\|_{op} \leq L \forall x \in \mathbb{R}^n \Leftrightarrow f \in C_L^{2,1}(\mathbb{R}^n)$$

Proving the other direction \Leftarrow

$$f \in C_L^{2,1}(\mathbb{R}^n) \Rightarrow$$

With $s = y - x$, we have seen that

$$f'(x + \alpha s) - f'(x) = \int_0^\alpha f''(x + \tau s) d\tau s$$

$$\Rightarrow \left\| \int_0^\alpha f''(x + \tau s) d\tau s \right\| = \|f'(x + \alpha s) - f'(x)\| \leq L \|\alpha s\|$$

$$\Rightarrow \frac{1}{\alpha} \left\| \int_0^\alpha f''(x + \tau s) d\tau s \right\| \leq L \|s\|$$

$f \in C_L^{2,1}(\mathbb{R}^n) \xrightarrow{\alpha \rightarrow 0} \forall s \in \mathbb{R}^n \forall \alpha > 0$

$$\xrightarrow{\alpha \rightarrow 0} \|f''(x) \cdot s\|$$

$$\Rightarrow \frac{\|f''(x)s\|}{\|s\|} \leq L$$

$$\Rightarrow \|f''(x)\|_{op} \leq L \quad \text{Q.E.D}$$

Examples

- $f(x) = \alpha + \langle a, x \rangle \in C_0^{'''}(\mathbb{R}^n)$
- $f(x) = \alpha + \langle a, x \rangle + \frac{1}{2} \langle Ax, x \rangle \in C_L^{'''}(\mathbb{R}^n)$
with $L = \|A\|$
- $f(x) = \sqrt{1+x^2} \in C_1^{'''}(\mathbb{R})$

Error of 1st order Taylor approx. in $C_L^{1,1}$

Lemma [1st order Taylor approximation in $C_L^{1,1}$]

$$\left. \begin{array}{l} f \in C_L^{1,1}(\mathbb{R}^n) \\ x, y \in \mathbb{R}^n \end{array} \right\} \Rightarrow |f(y) - f(x) - \langle f'(x), y - x \rangle| \leq \frac{L}{2} \|y - x\|^2$$

Proof

$$f(y) = f(x) + \int_0^1 \langle f'(x + \tau(y - x)), y - x \rangle d\tau$$

$$\begin{aligned} \Rightarrow |f(y) - f(x) - \langle f'(x), y - x \rangle| &= \left| \int_0^1 \langle f'(x + \tau(y - x)), y - x \rangle d\tau - \langle f'(x), y - x \rangle \right| \\ &= \left| \int_0^1 \langle f'(x + \tau(y - x)) - f'(x), y - x \rangle d\tau \right| \\ &\leq \int_0^1 |\langle f'(x + \tau(y - x)) - f'(x), y - x \rangle| d\tau \end{aligned}$$

Error of 1st order Taylor approx. in $C_L^{1,1}$

$$\begin{aligned} \Rightarrow |f(y) - f(x) - \langle f'(x), y - x \rangle| &\leq \int_0^1 |\langle f'(x + \tau(y - x)) - f'(x), y - x \rangle| d\tau \\ &\leq \int_0^1 \|f'(x + \tau(y - x)) - f'(x)\| \|y - x\| d\tau \end{aligned}$$

$$\wedge \quad L \| \tau(y-x) \| \quad f \in C_L^{1,1}(\mathbb{R}^n)$$

$$\leq \int_0^1 L\tau \|y - x\|^2 d\tau = \frac{L}{2} \|y - x\|^2$$

Q.E.D

Sandwiching with quadratic functions in $C_L^{1,1}$

We have proved:

$$f \in C_L^{1,1}(\mathbb{R}^n) \Rightarrow |f(y) - f(x) - \langle f'(x), y - x \rangle| \leq \frac{L}{2} \|y - x\|^2 \\ x, y \in \mathbb{R}^n$$

Corollary [Sandwiching $C_L^{1,1}$ functions with quadratic functions]

$$f \in C_L^{1,1}(\mathbb{R}^n) \Rightarrow f(x_0) + \langle f'(x_0), x - x_0 \rangle - \frac{L}{2} \|x - x_0\|^2 \leq f(x) \\ f(x) \leq f(x_0) + \langle f'(x_0), x - x_0 \rangle + \frac{L}{2} \|x - x_0\|^2$$

Function f can be lower and upper bounded with quadratic functions

$C_L^{2,2}(\mathbb{R}^n)$ Class

Lemma [Properties of $C_L^{2,2}$ Class]

$$\left. \begin{array}{l} f \in C_L^{2,2}(\mathbb{R}^n) \\ x, y \in \mathbb{R}^n \end{array} \right\} \Rightarrow$$

$$\|f''(x) - f''(y)\|_{op} \leq L\|y - x\| \quad (*1)$$

$$\|f'(y) - f'(x) - f''(x)(y - x)\| \leq \frac{L}{2}\|y - x\|^2 \quad (*2)$$

[Error of the 1st order approximation of f']

$$\|f(y) - f(x) - f'(x)^T(y - x) - \frac{1}{2}(y - x)^T f''(x)(y - x)\| \leq \frac{L}{6}\|y - x\|^3 \quad (*3)$$

[Error of the 2nd order approximation of f]

Proof (*1) Definition

(*2) Same as previous lemma [f' instead of f]

(*3) Similar [Homework]

Sandwiching $f''(y)$ in $C_L^{2,2}(\mathbb{R}^n)$

By definition

$$\left. \begin{array}{l} f \in C_L^{2,2}(\mathbb{R}^n) \\ x, y \in \mathbb{R}^n \end{array} \right\} \Rightarrow \|f''(x) - f''(y)\|_{op} \leq L\|y - x\| \quad (*1)$$

Corollary [Sandwiching $f''(y)$ matrix]

$$\left. \begin{array}{l} f \in C_L^{2,2}(\mathbb{R}^n) \\ \|x - y\| = r \end{array} \right\} \Rightarrow f''(x) - Lr\mathbf{I}_n \preceq f''(y) \preceq f''(x) + Lr\mathbf{I}_n$$

Proof

$$f \in C_L^{2,2}(\mathbb{R}^n) \Rightarrow \|\overbrace{f''(x) - f''(y)}^G\|_{op} \leq L\|y - x\| = Lr$$

$$\Rightarrow |\lambda_i(G)| \leq Lr \quad \forall i = 1, \dots, n$$

$$\Rightarrow \begin{cases} f''(x) - f''(y) = G \preceq Lr\mathbf{I}_n \\ f''(y) - f''(x) = -G \preceq Lr\mathbf{I}_n \end{cases}$$

Q.E.D

Convergence rate of Newton's method

Convergence rate of Newton's method

Assumptions

$$f \in C_L^{2,2}(\mathbb{R}^n)$$

\exists local minimum x^* of f with pos def Hessian in x^* :

$$f''(x^*) \succeq l\mathbf{I}_n \text{ for some } l > 0$$

x_0 is close enough to x^* [Local convergence only]

$$\text{Newton step: } x_{k+1} = x_k - [f''(x_k)]^{-1} f'(x_k)$$

Convergence rate of Newton's method

Newton step:

$$x_{k+1} - x^* = x_k - x^* - [f''(x_k)]^{-1} f'(x_k)$$

We already know:

$$f'(x_k) = f'(x_k) - f'(x^*) = \int_0^1 f''(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau$$

Therefore,

$$x_{k+1} - x^* = x_k - x^* - [f''(x_k)]^{-1} \int_0^1 f''(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau$$

$$\text{Trivial identity: } x_k - x^* = [f''(x_k)]^{-1} \int_0^1 f''(x_k)(x_k - x^*) d\tau$$

$$\Rightarrow x_{k+1} - x^* = [f''(x_k)]^{-1} G_k(x_k - x^*)$$

$$\text{where } G_k = \int_0^1 [f''(x_k) - f''(x^* + \tau(x_k - x^*))] d\tau$$

Convergence rate of Newton's method

$$G_k = \int_0^1 [f''(x_k) - f''(x^* + \tau(x_k - x^*))] d\tau$$

$$\Rightarrow \|G_k\|_{op} \leq \int_0^1 \|f''(x_k) - f''(x^* + \tau(x_k - x^*))\|_{op} d\tau$$

$$\begin{array}{c} \nearrow \\ \leq \int_0^1 L \|x_k - x^* - \tau(x_k - x^*)\| d\tau \end{array}$$

$$f \in C_L^{2,2}(\mathbb{R}^n)$$

$$= \int_0^1 L(1 - \tau) \|x_k - x^*\| d\tau = \int_0^1 L(1 - \tau) r_k d\tau \leq \frac{Lr_k}{2}$$

$$\Rightarrow \|G_k\|_{op} \leq \frac{Lr_k}{2}$$

Convergence rate of Newton's method

We have already proved:

$$\left. \begin{array}{l} f \in C_L^{2,2}(\mathbb{R}^n) \\ \|x - y\| = r \end{array} \right\} \Rightarrow f''(x) - Lr\mathbf{I}_n \preceq f''(y) \preceq f''(x) + Lr\mathbf{I}_n$$

Therefore,

$$f''(x_k) \succeq f''(x^*) - Lr_k\mathbf{I}_n \succeq l\mathbf{I}_n - Lr_k\mathbf{I}_n = (l - Lr_k)\mathbf{I}_n$$

$\forall l\mathbf{I}_n$ ASSUMPTION

and thus,

$$\text{If } l - Lr_k > 0, \text{ then } \left\{ \begin{array}{l} f''(x_k) \text{ is positive definite} \\ \|[f''(x_k)]^{-1}\|_{op} \leq \frac{1}{l - Lr_k} \end{array} \right.$$

Convergence rate of Newton's method

We already know:

$$\begin{aligned} r_{k+1} &= \|x_{k+1} - x^*\| = \|[f''(x_k)]^{-1}G_k(x_k - x^*)\| \\ &\leq \|[f''(x_k)]^{-1}\|_{op} \|G_k\|_{op} \|(x_k - x^*)\| \\ &\quad \begin{array}{ccc} \nearrow & \uparrow & \nearrow \\ \leq (l - Lr_k)^{-1} & \leq \frac{r_k}{2}L & = r_k \end{array} \end{aligned}$$

$$\Rightarrow r_{k+1} \leq \frac{Lr_k^2}{2(l - Lr_k)}$$

Convergence rate of Newton's method

$$\Rightarrow r_{k+1} \leq \frac{Lr_k^2}{2(l-Lr_k)}$$

Now, we have that

$$\left. \begin{array}{l} \text{If } l > Lr_k \\ 2l > 3Lr_k \end{array} \right\} \Rightarrow r_{k+1} \leq \frac{Lr_k^2}{2(l-Lr_k)} = \frac{Lr_k^2}{2l-2Lr_k} < \frac{Lr_k^2}{3Lr_k-2Lr_k} = r_k$$

The error doesn't increase!

Convergence rate of Newton's method

We have proved the following theorem

Theorem [Rate of Newton's method]

Let f satisfy the above assumptions $\left. \begin{array}{l} \\ \bar{r} \doteq \|x_0 - x^*\| \leq \frac{2l}{3L} \end{array} \right\} \Rightarrow$

$$\Rightarrow \left\{ \begin{array}{l} \|x_k - x^*\| \leq \bar{r} \quad \forall k \\ \|x_{k+1} - x^*\| \leq \frac{L\|x_k - x^*\|^2}{2(l - L\|x_k - x^*\|)} \leq \left\{ \begin{array}{l} c\|x_k - x^*\|^2 \\ \|x_k - x^*\| \end{array} \right.$$

\Rightarrow **Quadratic rate!**

Summary

Newton method

- ☐ Finding a root
- ☐ Unconstrained minimization
 - Motivation with quadratic approximation
 - Rate of Newton's method
- ☐ Newton fractals

Classes of differentiable functions