

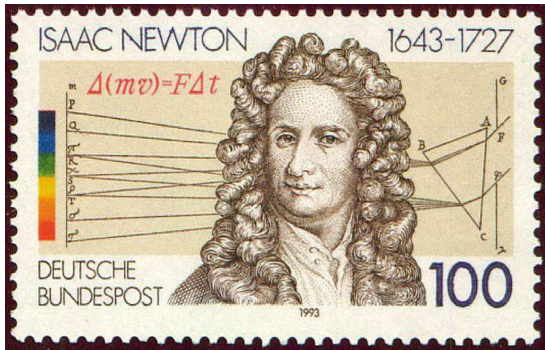
Newton's Method: Universality and Geometry

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Rutgers University

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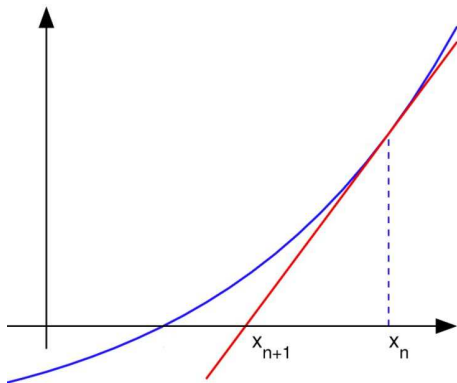


- 1 Introduction
- 2 Universality: Every iteration, away from its fixed points, is Newton
- 3 The logistic iteration: Chaos is just a ping-pong game
- 4 The geometry of the complex Newton method
- 5 Application to convex minimization
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Newton's method for $f(x) = 0, f : \mathbb{R} \rightarrow \mathbb{R}$

$$x_{n+1} := x_n - \frac{f(x_n)}{f'(x_n)}, \quad n = 0, 1, \dots$$



Theorem 1

Assume that f is twice differentiable on an open interval (a, b) , and that there exists $x^* \in (a, b)$ with $f'(x^*) \neq 0$.

Define Newton's method by the sequence

$$x_{k+1} := x_k - \frac{f(x_k)}{f'(x_k)}, \quad k = 1, 2, \dots$$

and assume that $\{x_k\}$ converges to x^* as $k \rightarrow \infty$.

Then, for k sufficiently large,

$$|x_{k+1} - x^*| \leq M |x_k - x^*|^2 \quad \text{if} \quad M > \frac{|f''(x^*)|}{2|f'(x^*)|}$$

Thus, $\{x_k\}$ converges to x^* **quadratically**.

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Newton's method for system of equations $\mathbf{f}(\mathbf{x}) = \mathbf{0}$

Let $\mathbf{f}: \mathbb{R}^n \rightarrow \mathbb{R}^m$ and consider the system

$$\mathbf{f}(\mathbf{x}) = \mathbf{0}, \quad \text{standing for } f_i(x_1, \dots, x_n) = 0, \quad i = 1, \dots, m$$

If $m = n$, the Newton iteration is

$$\mathbf{x}_+ := \mathbf{x} - (J\mathbf{f}(\mathbf{x}))^{-1} \mathbf{f}(\mathbf{x}), \quad J\mathbf{f} = \left(\frac{\partial f_i}{\partial x_j} \right) \text{ is the **Jacobian**}$$

If $m \neq n$ or the Jacobian is singular, ([2],[9]),

$$\mathbf{x}_+ := \mathbf{x} - (J\mathbf{f}(\mathbf{x}))^\dagger \mathbf{f}(\mathbf{x}), \quad \dagger \text{ is the **Moore–Penrose inverse**}$$

Converging to a stationary point of $\|\mathbf{f}(\mathbf{x})\|^2 = \sum_{i=1}^m f_i(\mathbf{x})^2$, since

$$\nabla \|\mathbf{f}(\mathbf{x})\|^2 = 2(J\mathbf{f}(\mathbf{x}))^* \mathbf{f}(\mathbf{x}), \quad \text{and } N(A^\dagger) = N(A^*), \quad \forall A.$$

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Definition 2

Let $f, u : \mathbb{R} \rightarrow \mathbb{R}$, and let f be differentiable in $S \subset \mathbb{R}$. If

$$u(x) = x - \frac{f(x)}{f'(x)}, \quad \forall x \in S,$$

then:

- (a) u is the **Newton transform** of f in S , denoted $u = \mathbf{N}f$, and
- (b) f is called the **inverse Newton transform** of u in S , denoted $f = \mathbf{N}^{-1}u$.

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The Newton transform

The **Newton transform** $\mathbf{N}f$ of a differentiable $f: \mathbb{R} \rightarrow \mathbb{R}$ is

$$(\mathbf{N}f)(x) := x - \frac{f(x)}{f'(x)}.$$

Maple

```
Newton:=proc(f,x); x-f/diff(f,x); end:
```

Example 3

$$(\mathbf{N}(x^{2/3} - 1)^{3/2})(x) = x^{1/3}$$

$$\text{simplify}(\text{Newton}((x^{(2/3)} - 1)^{(3/2)}, x)) \mapsto x^{1/3}$$

Example 4

$$(\mathbf{N}\exp\{-x\})(x) = x + 1$$

$$\text{Newton}(\exp(-x), x) \mapsto x + 1$$

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Example 5

$$\left(\mathbf{N} \left(\frac{x}{x-1} \right) \right) (x) = x^2$$

$$\text{Newton}(x/(x-1), x) \mapsto x^2$$

The iteration

$$x_+ := x^2$$

generates the same sequence as

$$x_+ := \mathbf{N} \left(\frac{x}{x-1} \right)$$

away from $x = 1$.

Example 5

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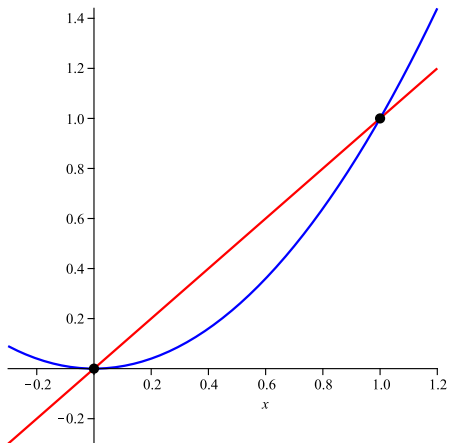
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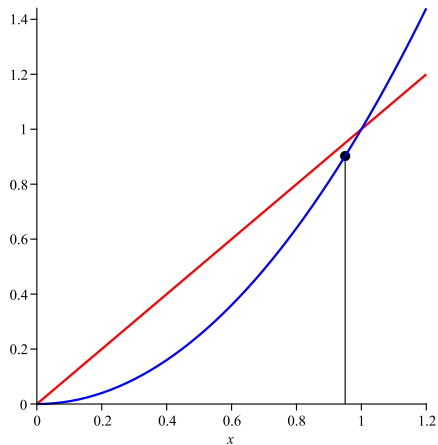
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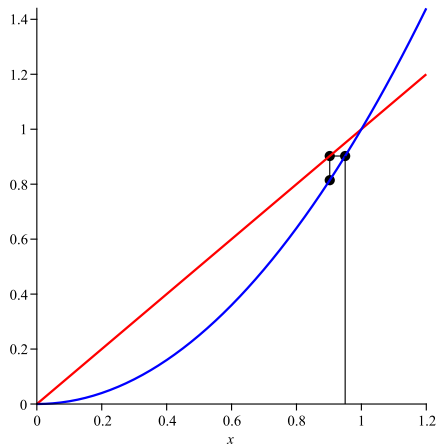
The fixed points of $u(x) := x^2$ are $\{0, 1\}$



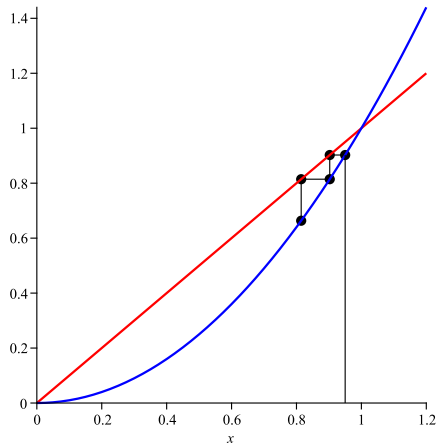
$x = 1$ is a repelling fixed point



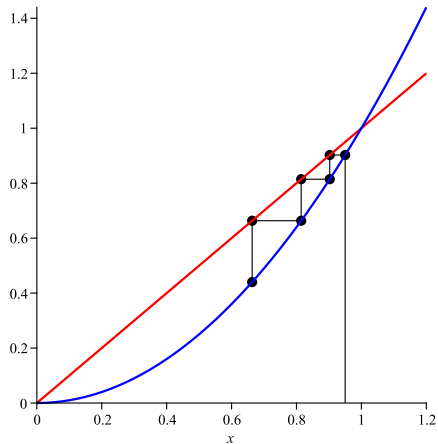
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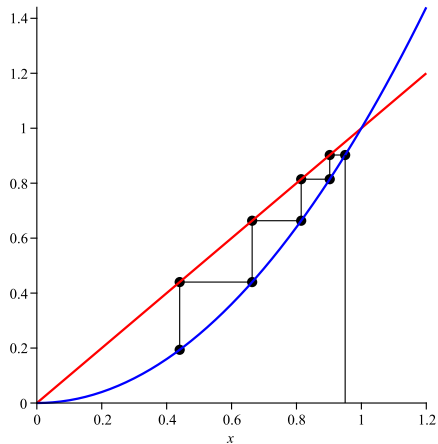
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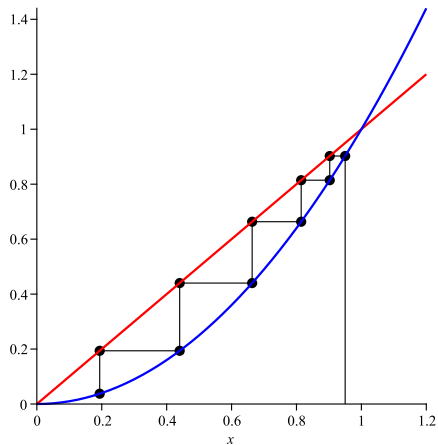
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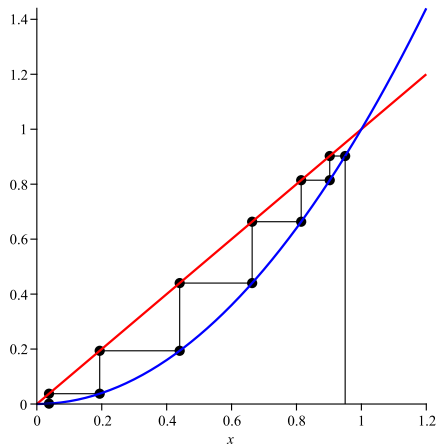
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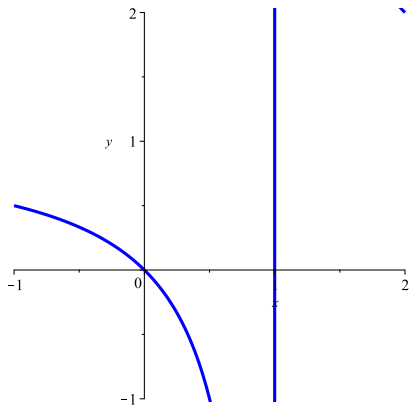
$x = 1$ is a repelling fixed point



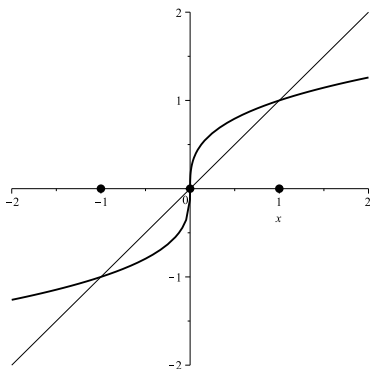
$x = 0$ is an attracting fixed point



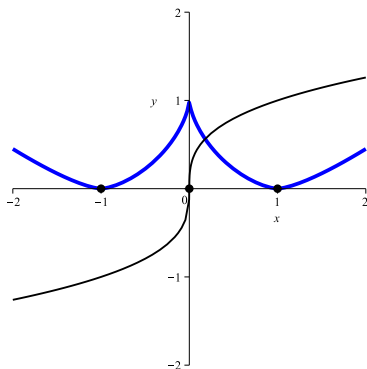
$$u(x) = x^2, \quad f(x) = (\mathbf{N}^{-1}u)(x) = \frac{x}{x-1}$$



$$\mathbf{u}(\mathbf{x}) := \mathbf{x}^{1/3}, \quad \mathbf{f}(\mathbf{x}) = (\mathbf{N}^{-1}\mathbf{u})(\mathbf{x}) = (\mathbf{x}^{2/3} - \mathbf{1})^{3/2}$$



Fixed points of $u(x)$ at $0, \pm 1$



Corresponding points of $f(x)$

$$f(x) = (\mathbf{N}^{-1}u)(x)$$

Questions:

Fixed points $\{u\} \stackrel{?}{=} \text{Zeros } \{f\} \cup \text{Singularities } \{f'\}$

Attracting fixed points $\{u\} \stackrel{?}{=} \text{Zeros } \{f\}$

Quadratic convergence of $u = \mathbf{N}f$?

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Quadratic convergence of $u = \mathbf{N}f$?

(a) If f is twice differentiable, then

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

ζ is a **zero of order** $m > 0$ of f if

$$f(x) = (x - \zeta)^m g(x), \quad g(\zeta) \neq 0$$

(b) If ζ is a zero of f of order m , then

$$u'(x) = \frac{m(m-1)g(x)^2 + 2(x-\zeta)g'(x) + (x-\zeta)^2g''(x)}{m^2g(x)^2 + 2(x-\zeta)mg(x)g'(x) + (x-\zeta)^2g'(x)^2} \rightarrow \frac{m-1}{m},$$

as $x \rightarrow \zeta$, provided $\lim_{x \rightarrow \zeta} (x - \zeta)g'(x) = \lim_{x \rightarrow \zeta} (x - \zeta)^2g''(x) = 0$.

(c) If ζ is a zero of f of order $m < 1$, then f is not differentiable at ζ , but u may be, with $u'(\zeta) = \frac{m-1}{m}$.

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Theorem 6

Let f be differentiable at ζ , and in (a)–(c), $f'(\zeta) \neq 0$.

(a) ζ is a zero of f if, and only if, it is a fixed point of u .

(b) If ζ is a zero of f , f and u are twice differentiable at ζ , then ζ is a superattracting fixed point of u , and convergence is (at least) quadratic.

(c) If ζ is a zero of f of order $m > \frac{1}{2}$, and u is continuously differentiable at ζ , then ζ is an attracting fixed point of u .

(d) Let ζ have a neighborhood where u and f are continuously differentiable, and $f'(x) \neq 0$ except possibly at $x = \zeta$. If ζ is an attracting fixed point of u then it is a zero of f .

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An integral form of \mathbf{N}^{-1} , [4]

Theorem 7

Let u be a function: $\mathbb{R} \rightarrow \mathbb{R}$, D a region where

$$\frac{1}{x - u(x)}$$

is integrable. Then in D ,

$$(\mathbf{N}^{-1}u)(x) = C \cdot \exp \left\{ \int \frac{dx}{x - u(x)} \right\}, \quad C \neq 0.$$

Moreover, if $C > 0$ then $\mathbf{N}^{-1}u$ is

- (a) increasing if $x > u(x)$,
- (b) decreasing if $x < u(x)$,
- (c) convex if u is differentiable and increasing, or
- (d) concave if u is differentiable and decreasing.

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$$\frac{1}{x - u(x)}$$

is integrable. Then in D ,

$$(\mathbf{N}^{-1}u)(x) = C \cdot \exp \left\{ \int \frac{dx}{x - u(x)} \right\}, \quad C \neq 0.$$

Moreover, if $C > 0$ then $\mathbf{N}^{-1}u$ is

- (a) increasing if $x > u(x)$,
- (b) decreasing if $x < u(x)$,
- (c) convex if u is differentiable and increasing, or
- (d) concave if u is differentiable and decreasing.

An integral form of \mathbf{N}^{-1} , [4]

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$$(\mathbf{N}^{-1}\mathbf{u})(\mathbf{x}) = \mathbf{C} \cdot \exp \left\{ \int \frac{d\mathbf{x}}{\mathbf{x} - \mathbf{u}(\mathbf{x})} \right\}$$

Assuming $x \neq u(x)$,

$$u(x) = x - \frac{f(x)}{f'(x)} \quad \Longrightarrow \quad \frac{f'(x)}{f(x)} = \frac{1}{x - u(x)}$$

$$\therefore \ln f(x) = \int \frac{dx}{x - u(x)} + C$$

$$\therefore f(x) = C \exp \left\{ \int \frac{dx}{x - u(x)} \right\}$$

without loss of generality, $C = 1$.

$$(\mathbf{N}^{-1}\mathbf{u})(\mathbf{x}) = \mathbf{C} \cdot \exp \left\{ \int \frac{d\mathbf{x}}{\mathbf{x} - \mathbf{u}(\mathbf{x})} \right\}$$

$$\therefore f'(x) = \frac{1}{x - u(x)} \exp \left\{ \int \frac{dx}{x - u(x)} \right\}$$

$$\therefore f''(x) = \frac{u'(x)}{(x - u(x))^2} \exp \left\{ \int \frac{dx}{x - u(x)} \right\}$$

$$x > u(x) \implies f'(x) > 0$$

$$u'(x) > 0 \implies f''(x) > 0$$

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Maple

```
InverseNewton:=proc(u,x);  
simplify(exp(int(1/(x-u),x)));end:
```

Examples:

```
InverseNewton(Newton(f(x),x),x);  
f(x)
```

```
Newton(InverseNewton(u(x),x),x);  
u(x)
```

```
InverseNewton(x2,x);  
 $\frac{x}{x-1}$ 
```

$$(\mathbf{N}^{-1}\mathbf{u})(\mathbf{x}) = \exp \left\{ \int \frac{d\mathbf{x}}{\mathbf{x} - \mathbf{u}(\mathbf{x})} \right\}$$

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$$\mathbf{u}(\mathbf{x}) = \mathbf{x} - \frac{\mathbf{f}(\mathbf{x})}{\mathbf{f}'(\mathbf{x}) - \mathbf{a}(\mathbf{x})\mathbf{f}(\mathbf{x})}, \quad \mathbf{N}^{-1}\mathbf{u} = ?, [3]$$

InverseNewton($\mathbf{x} - \mathbf{f}(\mathbf{x}) / (\text{diff}(\mathbf{f}(\mathbf{x}), \mathbf{x}) - \mathbf{a}(\mathbf{x}) * \mathbf{f}(\mathbf{x}))$, \mathbf{x});

$$f(x) \exp \left\{ - \int a(x) dx \right\}$$

For the Halley method

$$H(x) := x - \frac{f(x)}{f'(x) - \frac{f''(x)f(x)}{2f'(x)}}$$

$$(\mathbf{N}^{-1}H)(x) = \frac{f(x)}{\sqrt{f'(x)}}$$

$$\mathbf{u}(\mathbf{x}) = \mathbf{x} - \frac{\mathbf{f}(\mathbf{x})}{\mathbf{f}'(\mathbf{x}) - \mathbf{a}(\mathbf{x})\mathbf{f}(\mathbf{x})}, \quad \mathbf{N}^{-1}\mathbf{u} = ?, [3]$$

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For the **Halley method**

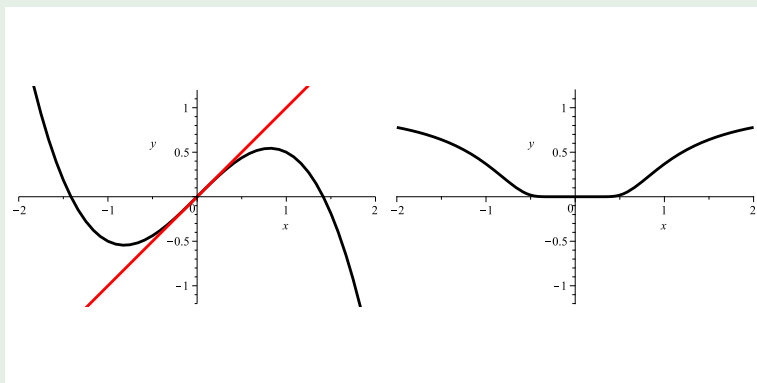
$$H(x) := x - \frac{f(x)}{f'(x) - \frac{f''(x)f(x)}{2f'(x)}}$$

$$(\mathbf{N}^{-1}H)(x) = \frac{f(x)}{\sqrt{f'x}}$$

Example of slow convergence

Example 8

$$\mathbf{u}(\mathbf{x}) := \mathbf{x} - \frac{1}{2}\mathbf{x}^3, \quad \mathbf{f}(\mathbf{x}) = (\mathbf{N}^{-1}\mathbf{u})(\mathbf{x}) = \exp\left\{-\frac{1}{\mathbf{x}^2}\right\}$$

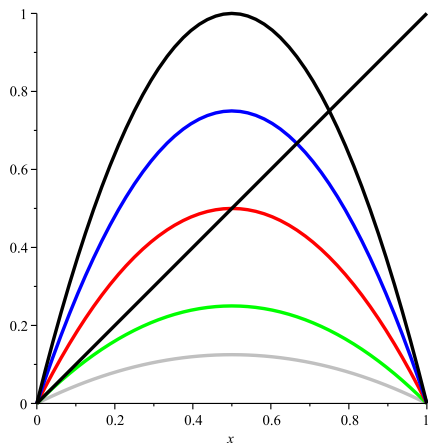


u has attracting fixed point at 0 $f^{(k)}(0) = 0, \forall k$

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The logistic iteration

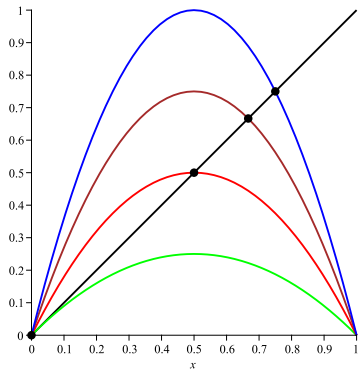
$$u(x) = \mu x(1-x), \quad 0 \leq x \leq 1, \quad 0 \leq \mu \leq 4$$



The logistic function with $\mu = 0.5, 1, 2, 3, 4$

The logistic iteration $u(x) = \mu x(1-x)$

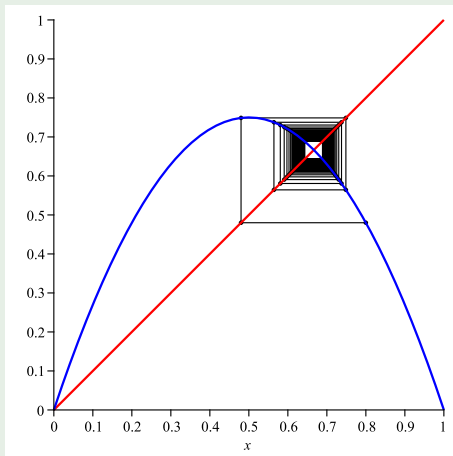
Fixed points $\left\{0, \frac{\mu-1}{\mu}\right\}$



$$u'(0) = \mu, \quad u'\left(\frac{\mu-1}{\mu}\right) = 2 - \mu$$

$$u(x) = 3x(1-x)$$

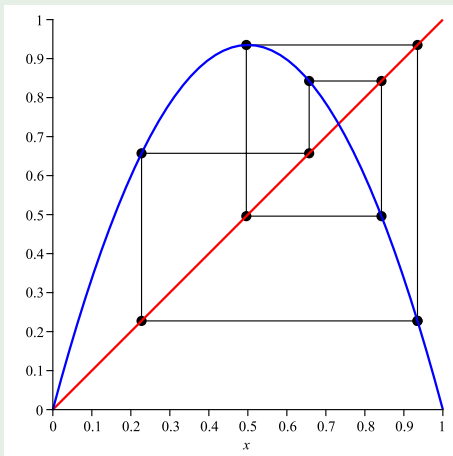
Example 9



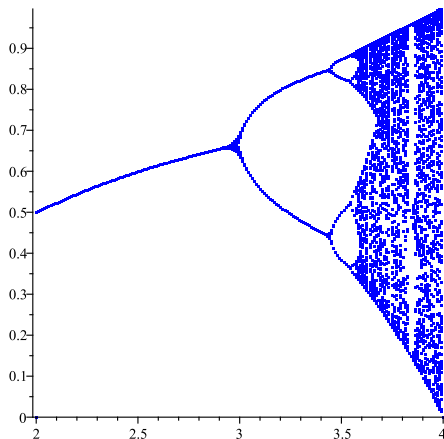
100 iterations, $x_0 = 0.8$

$$u(x) = 3.74x(1-x)$$

Example 10



5 cycle, $x_0 = 0.934945$



100 iterates of the logistic function for selected values of
 $2 \leq \mu \leq 4$

The logistic iteration

$$u(x) = \mu x(1-x), \quad 0 \leq x \leq 1, \quad 1 \leq \mu \leq 4$$

`expand(InverseNewton($\mu * x * (1-x)$, x));`

$$\frac{(1 - \mu + \mu x)^{(-1+\mu)^{-1}}}{x^{(-1+\mu)^{-1}}}$$

$$(a) \therefore f(x) = (\mathbf{N}^{-1}u)(x) = \left(\frac{x - \frac{\mu-1}{\mu}}{x} \right)^{\frac{1}{\mu-1}}$$

$$(b) \text{ Fixed points } \{u\} = \left\{ 0, \frac{\mu-1}{\mu} \right\}$$

(c) The fixed point $\frac{\mu-1}{\mu}$ is attracting for $1 \leq \mu < 3$

(d) $f(x)$ is convex [concave] for $x < \frac{1}{2}$ [$x > \frac{1}{2}$]

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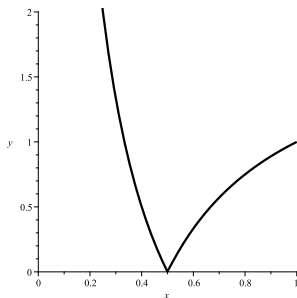
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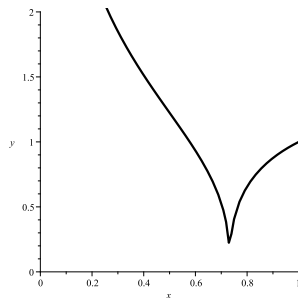
Chaos explained

The inverse Newton transform of $u(x) = \mu x(1-x)$

$$(\mathbf{N}^{-1}u)(x) = \left(\frac{x - \frac{\mu-1}{\mu}}{x} \right)^{\frac{1}{\mu-1}}$$

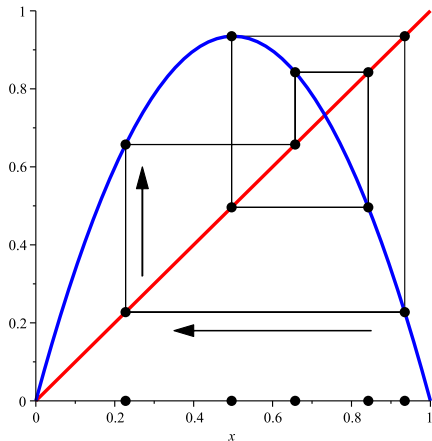


$\mu = 2.0$



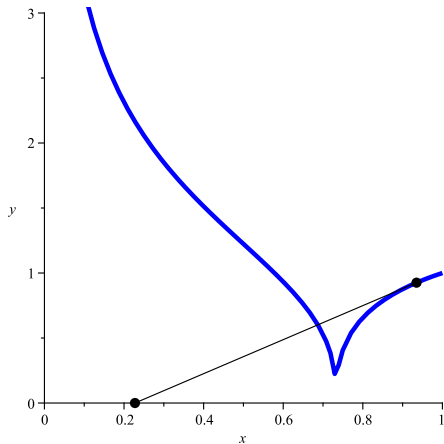
$\mu = 3.74$

5-cycle for $\mu = 3.74$

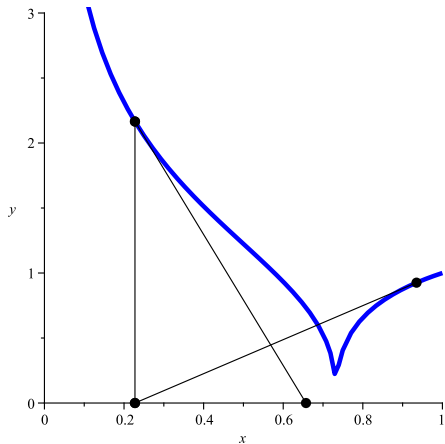


Starting at and returning to .9349453234

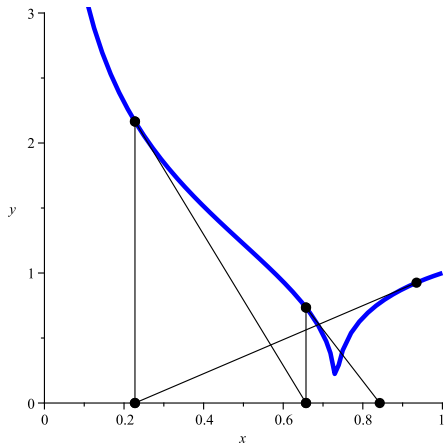
Ping pong-1



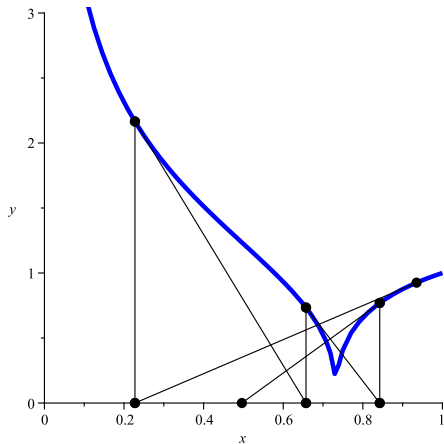
Ping pong-2



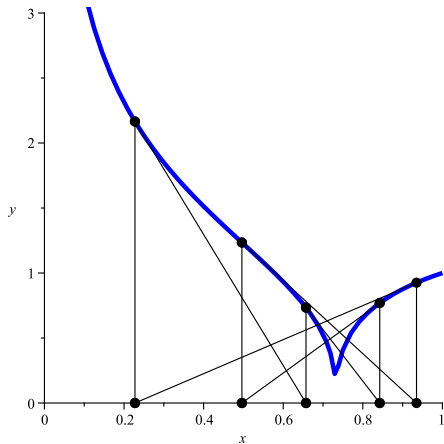
Ping pong-3



Ping pong-4



Ping pong-5



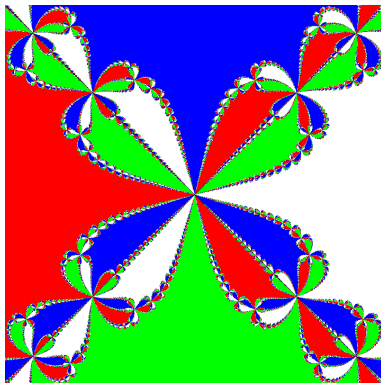
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The complex Newton method, [6]

$$z_+ := z - \frac{f(z)}{f'(z)}, f'(z) \neq 0$$

The complex Newton method

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

The geometry of the complex Newton method, [19]

$$z_+ := z - \frac{f(z)}{f'(z)}, f'(z) \neq 0$$

(a) Let

$$z = x + iy \longleftrightarrow (x, y)$$

be the natural correspondence between \mathbb{C} and \mathbb{R}^2 , and let

$$F(x, y) := |f(z)| \quad \text{for } z \longleftrightarrow (x, y).$$

(b) Let $\mathbf{T} \subset \mathbb{R}^3$ be the plane tangent to the graph of F at the point $(x, y, F(x, y))$, and let \mathbf{L} be the line of intersection of \mathbf{T} and the (x, y) -plane (\mathbf{L} is nonempty by the assumption that $f'(z) \neq 0$.)

(c) Then

$$z_+ \longleftrightarrow (x_+, y_+),$$

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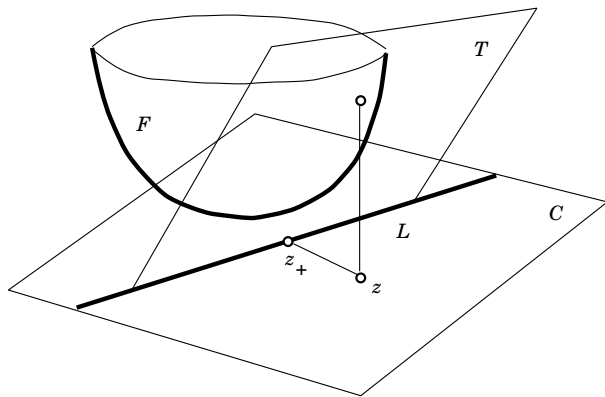
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The geometry of the complex Newton method



Outline of proof

The absolute value of $f = u + iv$

$$F(x, y) = |f(x + iy)| = \sqrt{u^2(x, y) + v^2(x, y)},$$

has gradient (where differentiable)

$$\nabla F(x, y) = \frac{1}{\sqrt{u^2 + v^2}} \begin{pmatrix} uu_x + vv_x \\ uu_y + vv_y \end{pmatrix}$$

where $u_x = \partial u / \partial x$, $u_y = \partial u / \partial y$, etc.

Using the **Cauchy-Riemann** conditions

$$u_x = v_y, \quad u_y = -v_x,$$

we get

$$\begin{aligned} \frac{f(z)}{f'(z)} &= \frac{u + iv}{u_x + iv_x} = \frac{(uu_x + vv_x) + i(uu_y + vv_y)}{u_x^2 + v_x^2} \\ &\longleftrightarrow \frac{1}{u_x^2 + v_x^2} \begin{pmatrix} uu_x + vv_x \\ uu_y + vv_y \end{pmatrix} = t \nabla F(x, y). \end{aligned}$$

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Outline of proof (contd.)

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The Newton method for f is thus a gradient method for $|f|$, i.e.,

$$\begin{pmatrix} x_+ \\ y_+ \end{pmatrix} := \begin{pmatrix} x \\ y \end{pmatrix} - t \nabla F(x,y) .$$

It remains to show that t is as claimed.

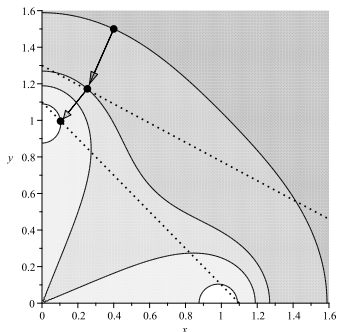
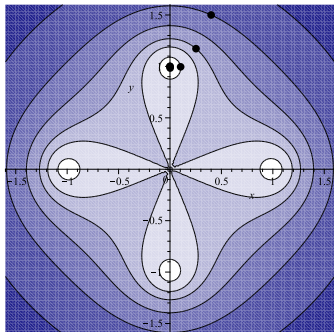
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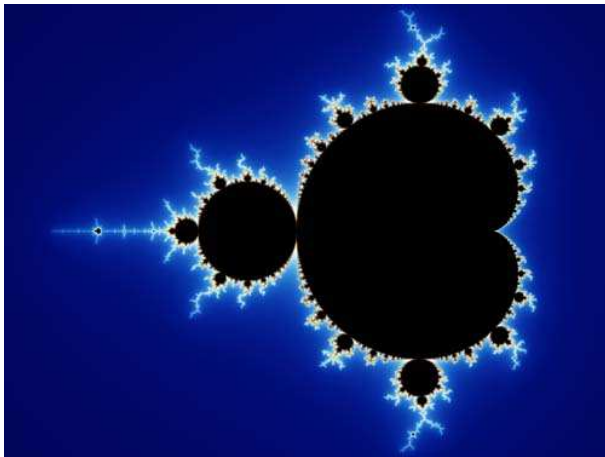
$$f(z) = z^4 - 1$$



Level sets of $|z^4 - 1|$ and iterates converging to i

The Mandelbrot set

$$M := \{c : \{z_n := z_{n-1}^2 + c, z_0 = 0\} \text{ bounded}\}$$



The Mandelbrot set

$$M := \{c : \{z_n := z_{n-1}^2 + c, z_0 = 0\} \text{ bounded}\}$$

InverseNewton($z^2 + c, z$);

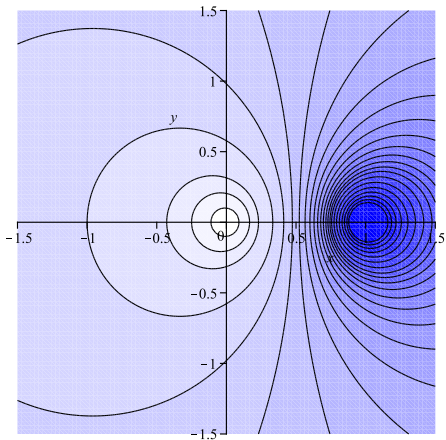
$$\exp \left\{ -\frac{2}{\sqrt{4c-1}} \arctan \left(\frac{2z-1}{\sqrt{4c-1}} \right) \right\}$$

InverseNewton($z^2 + (1/4), z$);

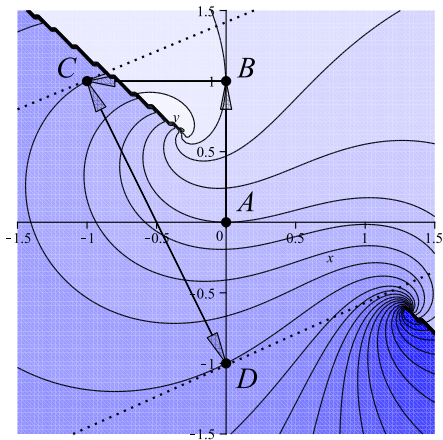
$$\exp \left\{ \frac{2}{2z-1} \right\}$$

InverseNewton(z^2, z);

$$\frac{z}{z-1}$$



Level sets of $|\mathbf{N}^{-1}(z^2)|$



Level sets of $|\mathbf{N}^{-1}(z^2 + i)|$

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Minimization of a convex $f : \mathbb{R} \rightarrow \mathbb{R}$, [12]

Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be convex, with an attained infimum f_{\min} .

A **bracket** is a closed interval $[L, U]$ with

$$L \leq f_{\min} \leq U.$$

The length of the bracket $[L, U]$ is denoted $\Delta := U - L$.

A **bracketing method** generates a sequence of nested brackets, shrinking to a point,

$$L \leq L_+ \leq f_{\min} \leq U_+ \leq U, \text{ and } \Delta_+ := U_+ - L_+ < \Delta.$$

At each iteration select a middle value

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The NB method

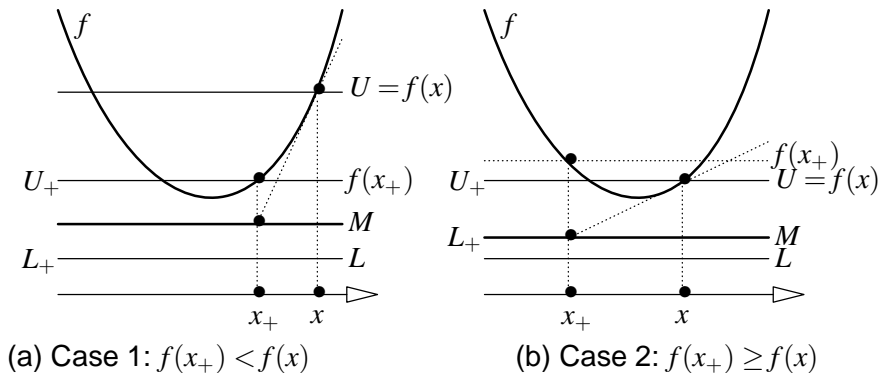


Figure: Illustration of the 2 cases of the NB method

0 Initialize.

x initial iterate

$U := f(x)$, upper bound

L , lower bound, must be less than f_{\min}

$\alpha \in (0, 1)$

$\varepsilon > 0$, tolerance.

1 **Stopping rule.** If $U - L < \varepsilon$, **stop** with x as solution.

2 Select a value $M := \alpha U + (1 - \alpha)L$, for some $0 < \alpha < 1$.

3 Do one Newton iteration $x_+ := x - \frac{f(x) - M}{f'(x)}$.

4 **Case 1:** If $f(x_+) < f(x)$ then update U : $U_+ := f(x_+)$
and leave $L_+ := L$. Go to 1.

5 **Case 2:** If $f(x_+) \geq f(x)$ then update L : $L_+ := M$
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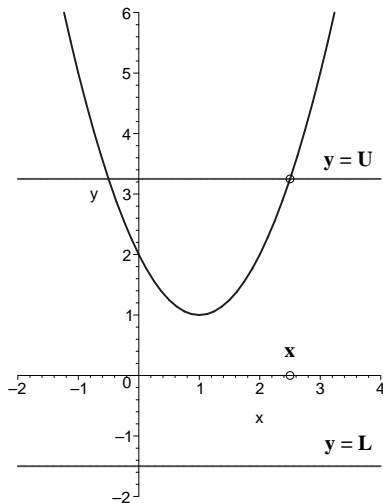
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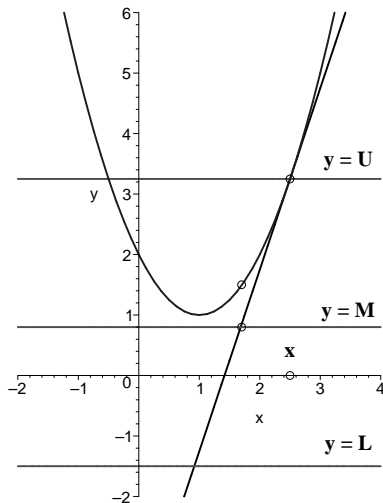
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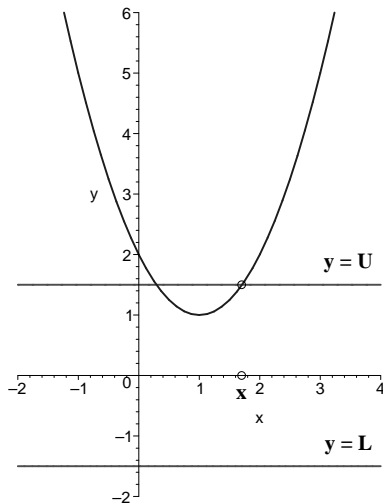
Example: Initialization



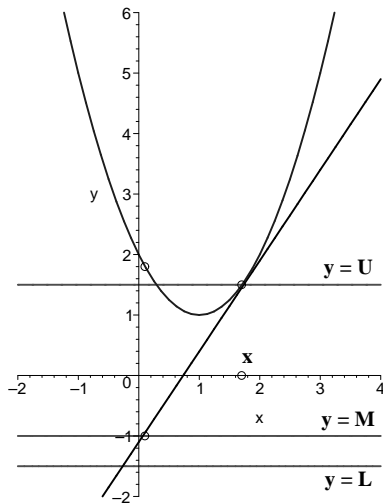
Iteration 1: Newton step



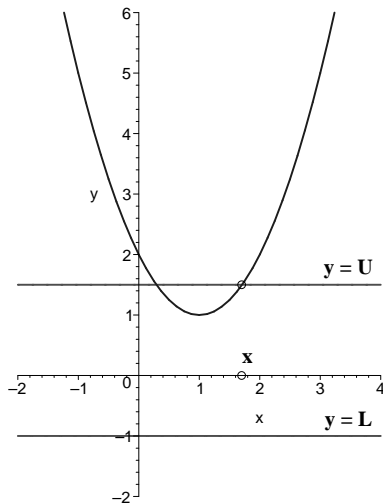
Iteration 1: New bracket



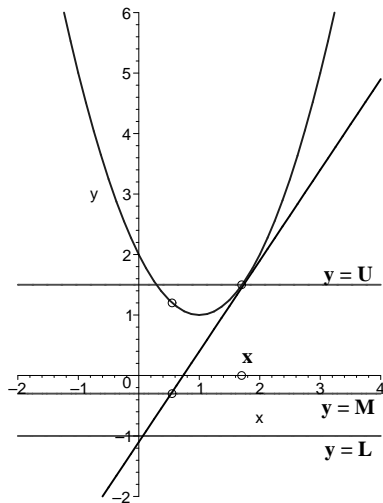
Iteration 2: Newton step



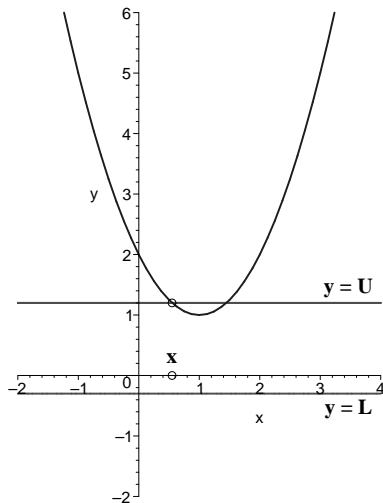
Iteration 2: New bracket



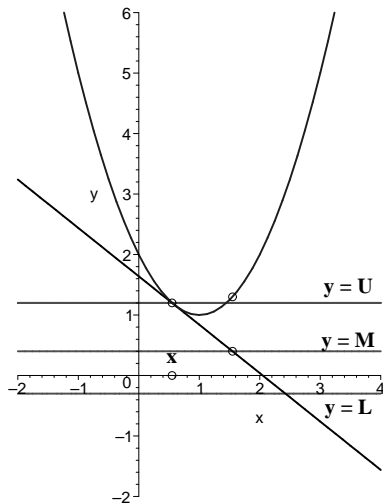
Iteration 3: Newton step



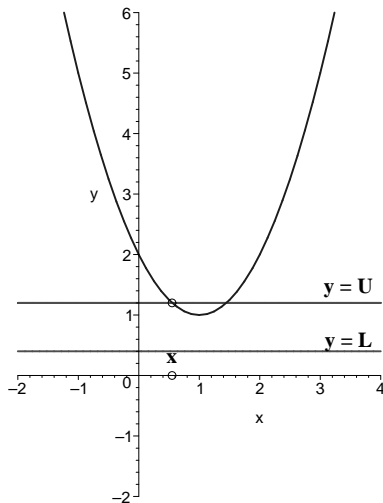
Iteration 3: New bracket



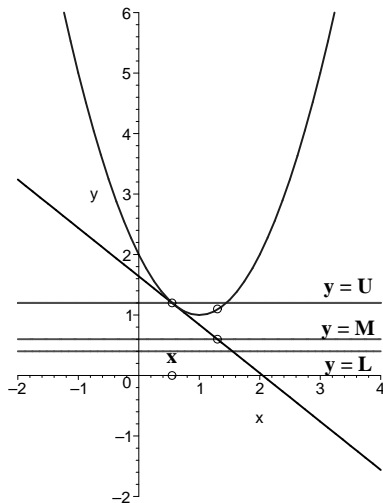
Iteration 4: Newton step



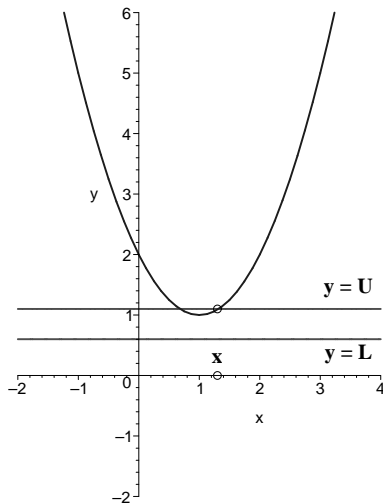
Iteration 4: New bracket



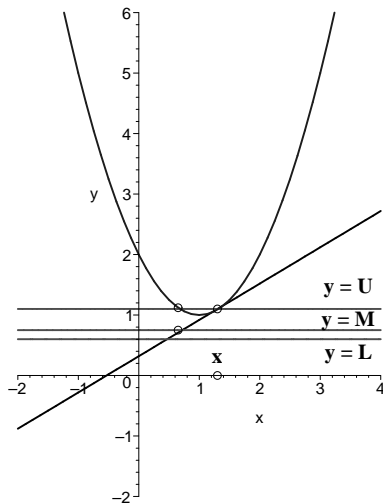
Iteration 5: Newton step



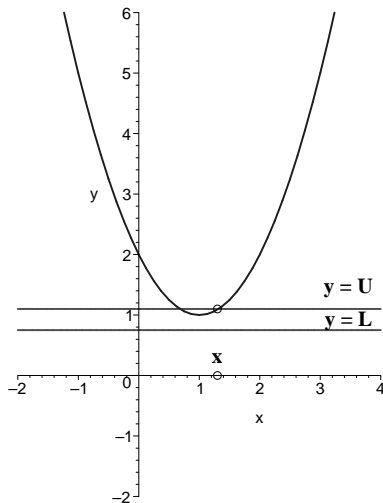
Iteration 5: New bracket



Iteration 6: Newton step



Iteration 6: New bracket



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The NB method is **valid** if

$$L \leq f_{\min} \leq U$$

holds throughout the iterations. This is guaranteed for $n = 1$.

Sufficient validity conditions for $n > 1$ were given in [12], in particular, the method is valid for the quadratic function,

$$f(\mathbf{x}) = \frac{1}{2} \mathbf{x}^T Q \mathbf{x} + \mathbf{c}^T \mathbf{x} + \gamma, \quad Q \text{ positive definite,}$$

if Q is well-conditioned,

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Application: The Fermat–Weber location problem

Find $\mathbf{x} \in \mathbb{R}^n$ minimizing the sum of Euclidean distances

$$f(\mathbf{x}) = \sum_{i=1}^m \|\mathbf{a}_i - \mathbf{x}\|$$

from m given points $\{\mathbf{a}_i : i = 1, \dots, m\} \subset \mathbb{R}^n$.

Gradient methods, such as the **Weiszfeld method** ([18], [1]) suffer from slow convergence and the lack of a natural stopping criterion.

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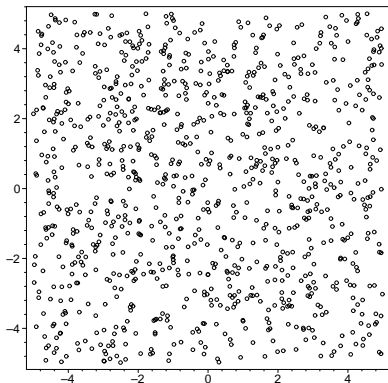
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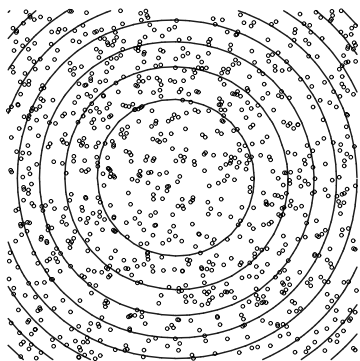
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1000 points $\{\mathbf{a}_i\}$ and level sets of $\sum_{i=1}^m \|\mathbf{a}_i - \mathbf{x}\|$



(a) Points



(b) Level sets

Figure: 1,000 random points in $[-5,5]^2$

Numerical results for 1000 random points in $[-5,5]^2$

Iteration	0	1	2	3	4	5	6
α	0.95	0.95	0.95	0.88	0.95	0.95	0.95
Case	1	1	2	1	1	2	2
Δ	3809.9	3771.1	188.5	172.3	167.3	8.37	0.418
Reduction		0.989	0.05	0.914	0.971	0.05	0.05

Iteration	7	8	9	10	11	12
α	0.83	0.95	0.95	0.89	0.95	0.95
Case	1	1	2	1	1	2
Δ	0.367	0.355	0.018	0.0163	0.016	0.0008
Reduction	0.881	0.945	0.05	0.905	0.981	0.05

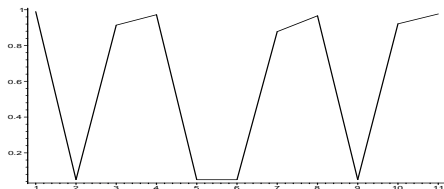


Figure: Reduction per iteration

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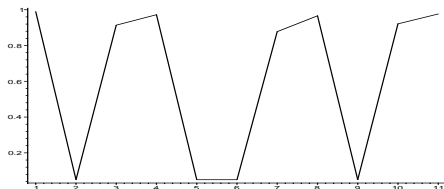


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THANKS FOR YOUR ATTENTION