# Newton's and Quasi-Newton Methods

Axel Böhm

September 28, 2021

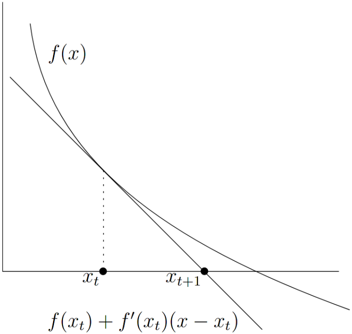
# 1-dimensional case: Newton-Raphson method

Objective: Find zero of differentiable $f : \mathbb{R} \to \mathbb{R}$.
Strategy: Solve

$$f(x_k) + f'(x_k)(x - x_k) = 0.$$

Method: Gives

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



# The Babylonian method

- compute square root of $R \in \mathbb{R}_+$
- find zero of $f(x) = x^2 - R$
- use Newton-Raphson:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} = x_k - \frac{x_k^2 - R}{2x_k} = \frac{1}{2}\left(x_k + \frac{R}{x_k}\right)$$

- Starting from $x_0 > 0$ we have

$$x_{k+1} = \frac{1}{2}\left(x_k + \frac{R}{x_k}\right) \geq \frac{x_k}{2}.$$

- Starting from $x_0 = R \geq 1$, it takes $\mathcal{O}(\log R)$ steps to get to $x_k - \sqrt{R} < \frac{1}{2}$.

## The Babylonian method - Takeoff

Note that

$$x_{k+1}-\sqrt{R} = \frac{1}{2}\left(x_k + \frac{R}{x_k}\right)-\sqrt{R} = \frac{x_k}{2}+\frac{R}{2x_k}-\sqrt{R} = \frac{1}{2x_k}\left(x_k - \sqrt{R}\right)^2$$

For simplicity $R \geq 1/4$, then $x_k \geq \sqrt{R} \geq 1/2$. Hence

$$x_{k+1} - \sqrt{R} = \frac{1}{2x_k}\left(x_k - \sqrt{R}\right)^2 \leq \left(x_k - \sqrt{R}\right)^2$$

If $x_0 - \sqrt{R} < \frac{1}{2}$ (ensured after $\mathcal{O}(\log R)$ steps).

$$x_k - \sqrt{R} \leq \left(x_0 - \sqrt{R}\right)^{2^k} \leq \left(\frac{1}{2}\right)^{2^k}$$

To achieve $x_k - \sqrt{R} < \epsilon$ we only need $k = \log\log(\epsilon^{-1})$ steps!

# The Babylonian method - Example

$R = 1000$, in double arithmetic

- 7 steps to get to $x_7 - \sqrt{1000} < 1/2$
- 3 steps to get to $\sqrt{1000}$ up to *machine precision*
- First phase: $\approx$ one more correct digit per iteration
- Second phase: $\approx$ double the number of correct digits per iteration

In practice: $\log \log x \leq 5$.

# Newton's method for optimization

Goal: Find global minimum $x^*$ of convex, differentiable function $f$.
Strategy: Search for zero of derivative.
1-**dimensional case:** Apply Newton-Raphson method to $f'$:

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

(requires twice differentiable and $f'' > 0$)
$d$-**dimensional case:** Newtons methods for minimizing convex $f : \mathbb{R}^d \to \mathbb{R}$:

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

## Newton's method as adaptive gradient descent

General update scheme:

$$x_{k+1} = x_k - H(x_k)\nabla f(x_k)$$

for some matrix $H(x) \in \mathbb{R}^{d\times d}$.

- Newton's method: $H = \nabla^2 f(x_k)^{-1}$.
- Gradient descent: $H = \alpha \, \mathrm{Id}$

Newton's methods **adapts** to the local geometry of $f$ at $x_k$
$\rightarrow$ *no need for choosing a stepsize.*

# Convergence in one step on quadratic functions

A quadratic function

$$f(x) = \frac{1}{2}x^T Mx + q^T x + c$$

is called *nondegenerate* if $M \in \mathbb{R}^{d\times d}$ is invertible.

- $x^* := M^{-1}q$ is the unique solution of $\nabla f(x) = 0$
- $x^*$ is the unique global minimum if $f$ is convex

## Lemma

*On nondegenerate quadratic functions with arbitrary starting point $x_0$, Newtons method yields $x_1 = x^*$*

## Proof.

We have $\nabla f(x) = Mx - q$ and $\nabla^2 f(x) = M$. Therefore

$$x_1 = x_0 - \nabla^2 f(x_0)\nabla f(x_0) = x_0 - M^{-1}(Mx_0 - q) = M^{-1}q = x^*.$$

# Affine Invariance

Newton's method is affine invariant (invariant under any invertible affine transformation): Denote the Newton step for $h$ by

$$N_h(x) := x - \nabla^2 h^{-1} \nabla h(x).$$

## Lemma

*Let $f : \mathbb{R}^d \to \mathbb{R}$ be twice differentiable, $A \in \mathbb{R}^{d \times d}$ an invertible matrix and $b \in \mathbb{R}^d$.*

$$g(x) = Ax + b.$$

*Then*

$$N_{f \circ g} = g^{-1} \circ N_f \circ g$$

$$
\begin{tikzcd}
\mathbf{x}_t \arrow[r, "N_f"'] & \mathbf{x}_{t+1} \arrow[d, "g^{-1}"'] \\
\mathbf{y}_t \arrow[u, "g"'] \arrow[r, "N_{f\circ g}"] & \mathbf{y}_{t+1}
\end{tikzcd}
$$

# Minimizing the second-order Taylor approximation

Alternative interpretation of Newton's method: Minimize (local) quadratic model of $f$.

**Lemma**

*Let $f$ be conve, twice differentiable and $\nabla^2 f(x) \succ 0$. Then $x_{k+1}$ resulting from **Newton's step** satisfies*

$$x_{k+1} = \arg\min_{x \in \mathbb{R}^d} f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle x - x_k, \nabla^2 f(x_k)(x - x_k) \rangle$$

# Local Convergence

We will prove:
Under suitable conditions on $f$ and close to the minimum Newton's method approximates solution up to an error $\epsilon$ in $\log\log(1/\epsilon)$ iterations.

- much faster than anything so far..
- only locally

We call this a local convergence result.
Global convergence statements are more difficult to obtain (some only recently).

# Theorem + Technical conditions

## Theorem

*Let $f$ be convex with unique global minimum $x^*$, and $X$ a ball around $x^*$ s.t.*

1. *Bounded inverse Hessians: There exists $\mu > 0$*

$$\|\nabla^2 f(x)^{-1}\| \leq \frac{1}{\mu}, \quad \forall x \in X$$

2. *Lipschitz continuous Hessians: There exists $B > 0$*

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq B\|x - y\|, \quad \forall x, y \in X$$

*Then, for $x_{k+1} = N_f(x_k)$ we have*

$$\|x_{k+1} - x^*\| \leq \frac{B}{2\mu}\|x_k - x^*\|^2$$

# Super-exponential speed

## Corollary

*In the setting of previous theorem, if*

$$\|x_k - x^*\| \leq \frac{\mu}{B},$$

*then*

$$\|x_k - x^*\| \leq \frac{\mu}{B}\left(\frac{1}{2}\right)^{2^k-1}$$

Close to the global minimum, we will reach distance to the minumum less than $\epsilon$ in at most $\log\log(1/\epsilon)$ steps.
As for the last phase of Babylonian method.

# Super-exponential speed - intuition

- Almost constant Hessians close to optimality...
- so $f$ behaves almost like a quadratic
- on which Newton's converge in one step

## Lemma

*If*

$$\|x_0 - x^*\| \leq \frac{\mu}{B}$$

*the Hessians in Newton's method satisfy the relative error bound*

$$\frac{\|\nabla^2 f(x_k) - \nabla^2 f(x^*)\|}{\|\nabla^2 f(x^*)\|} \leq \left(\frac{1}{2}\right)^{2^k - 1}.$$

# Proof of convergence theorem

We abbreviate $H = \nabla^2 f(x_k)$, $x = x_k$, $x^+ = x_{k+1}$

$$\begin{aligned}
x^+ - x^* &= x - x^* - H^{-1}\nabla f(x) \\
&= x - x^* + H^{-1}(\nabla f(x^*) - \nabla f(x)) \\
&= x - x^* + H^{-1}\int_0^1 H(x + t(x^* - x))(x^* - x)\,\mathrm{d}t,
\end{aligned}$$

where we used the fundamental theorem of calculus

$$\int_a^b h'(t)\,\mathrm{d}t$$

with

$$\begin{aligned}
h(t) &= \nabla f(x + t(x^* - x)) \\
h'(t) &= \nabla^2 f(x + t(x^* - x))(x^* - x).
\end{aligned}$$

# Proof of convergence theorem

We abbreviate $H = \nabla^2 f(x_k)$, $x = x_k$, $x^+ = x_{k+1}$

$$\begin{aligned} x^+ - x^* &= x - x^* - H^{-1}\nabla f(x) \\ &= x - x^* + H^{-1}(\nabla f(x^*) - \nabla f(x)) \\ &= x - x^* + H^{-1}\int_0^1 H(x + t(x^* - x))(x^* - x)\,\mathrm{d}t, \end{aligned}$$

where we used the fundamental theorem of calculus

$$\int_a^b h'(t)\,\mathrm{d}t$$

with

$$\begin{aligned} h(t) &= \nabla f(x + t(x^* - x)) \\ h'(t) &= \nabla^2 f(x + t(x^* - x))(x^* - x). \end{aligned}$$

## Downside of Newton's method

Computational bottleneck in every step:

- compute Hessian
- invert Hessian or solve $\nabla^2 f(x_k)\Delta x = -\nabla f(x_k)$

Matrix has size $d \times d$, taking $\mathcal{O}(d^3)$ to invert.
In many applications the dimension $d$ is large (too large to even store Hessian).

# The secant method

Another iterative method for finding zeros in 1-d. Recall Newton-Raphson:

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

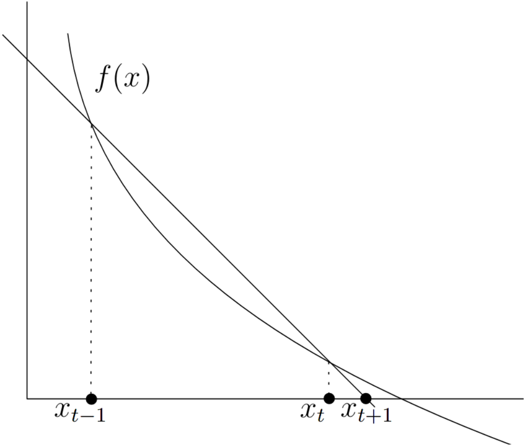
Use finite difference approximation of $f'(x_k)$:

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

We obtain the **secant method**:

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

# The secant method




Constructs the line through $(x_{k-1}, f(x_{k-1}))$ and $(x_k, f(x_k))$