Optimization for Machine Learning
CS-439

Lecture 7: Newton's and Quasi-Newton Methods

Nicolas Flammarion

EPFL – github.com/epfml/OptML_course

April 18, 2021

Chapter 8

Newton's Method

1-dimensional case: Newton-Raphson method

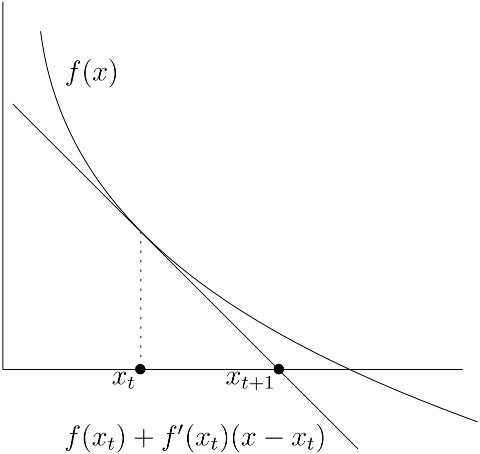
Goal: find a zero of differentiable $f : \mathbb{R} \to \mathbb{R}$.

Method:

$$x_{t+1} := x_t - \frac{f(x_t)}{f'(x_t)}, \quad t \geq 0.$$

x_{t+1} solves

$$f(x_t) + f'(x_t)(x - x_t) = 0,$$



The Babylonian method

Computing square roots: find a zero of $f(x) = x^2 - R, R \in \mathbb{R}_+$.

Newton-Raphson step:

$$x_{t+1} = x_t - \frac{f(x_t)}{f'(x_t)} = x_t - \frac{x_t^2 - R}{2x_t} = \frac{1}{2}\left(x_t + \frac{R}{x_t}\right).$$

Starting from $x_0 > 0$, we have

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

Starting from $x_0 = R \geq 1$, it takes $O(\log R)$ steps to get $x_t - \sqrt{R} < 1/2$ (Exercise 43).

The Babylonian method - Takeoff

Suppose $x_0 - \sqrt{R} < 1/2$ (achievable after $O(\log R)$ steps).

$$x_{t+1} - \sqrt{R} = \frac{1}{2}\left(x_t + \frac{R}{x_t}\right) - \sqrt{R} = \frac{x_t}{2} + \frac{R}{2x_t} - \sqrt{R} = \frac{1}{2x_t}\left(x_t - \sqrt{R}\right)^2.$$

Assume $R \geq 1/4$.Then all iterates have value at least $\sqrt{R} \geq 1/2$. Hence we get

$$x_{t+1} - \sqrt{R} \leq \left(x_t - \sqrt{R}\right)^2.$$

$$x_T - \sqrt{R} \leq \left(x_0 - \sqrt{R}\right)^{2^T} < \left(\frac{1}{2}\right)^{2^T}, \quad T \geq 0.$$

To get $x_T - \sqrt{R} < \varepsilon$, we only need $T = \log\log(\frac{1}{\varepsilon})$ steps!

The Babylonian method - Example

$R = 1000$, IEEE 754 double arithmetic

- 7 steps to get $x_7 - \sqrt{1000} < 1/2$
- 3 more steps to get x_{10} equal to $\sqrt{1000}$ up to machine precision (53 binary digits).
- First phase: $\approx$ one more correct digit per iteration
- Last phase, $\approx$ double the number of correct digits in each iteration!

Once you're close, you're there...

Newton's method for optimization

1-dimensional case: Find a global minimum $x^\star$ of a differentiable convex function $f : \mathbb{R} \to \mathbb{R}$.

Can equivalently search for a zero of the derivative f': Apply the Newton-Raphson method to f'.

Update step:

$$x_{t+1} := x_t - \frac{f'(x_t)}{f''(x_t)} = x_t - f''(x_t)^{-1} f'(x_t)$$

(needs f twice differentiable).

d-dimensional case: Newton's method for minimizing a convex function $f : \mathbb{R}^d \to \mathbb{R}$:

$$\mathbf{x}_{t+1} := \mathbf{x}_t - \nabla^2 f(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t)$$

Newton's method = adaptive gradient descent

General update scheme:

$$\mathbf{x}_{t+1} = \mathbf{x}_t - H(\mathbf{x}_t)\nabla f(\mathbf{x}_t),$$

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

Newton's method: $H = \nabla^2 f(\mathbf{x}_t)^{-1}$.

Gradient descent: $H = \gamma I$.

Newton's method: "adaptive gradient descent", adaptation is w.r.t. the local geometry of the function at $\mathbf{x}_t$.

Convergence in one step on quadratic functions

A nondegenerate quadratic function is a function of the form

$$f(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top M\mathbf{x} - \mathbf{q}^\top \mathbf{x} + c,$$

where $M \in \mathbb{R}^{d\times d}$ is an invertible symmetric matrix, $\mathbf{q} \in \mathbb{R}^d, c \in R$. Let $\mathbf{x}^\star = M^{-1}\mathbf{q}$ be the unique solution of $\nabla f(\mathbf{x}) = \mathbf{0}$.

- $\mathbf{x}^\star$ is the unique global minimum if f is convex.

Lemma

On nondegenerate quadratic functions, with any starting point $\mathbf{x}_0 \in \mathbb{R}^d$, Newton's method yields $\mathbf{x}_1 = \mathbf{x}^\star$.

Proof.

We have $\nabla f(\mathbf{x}) = M\mathbf{x} - \mathbf{q}$ (this implies $\mathbf{x}^\star = M^{-1}\mathbf{q}$) and $\nabla^2 f(\mathbf{x}) = M$. Hence,

$$\mathbf{x}_1 = \mathbf{x}_0 - \nabla^2 f(\mathbf{x}_0)^{-1}\nabla f(\mathbf{x}_0) = \mathbf{x}_0 - M^{-1}(M\mathbf{x}_0 - \mathbf{q}) = M^{-1}\mathbf{q} = \mathbf{x}^\star.$$

□

Affine Invariance

Newton's method is **affine invariant**
(invariant under any invertible affine transformation):

Lemma (Exercise 44)

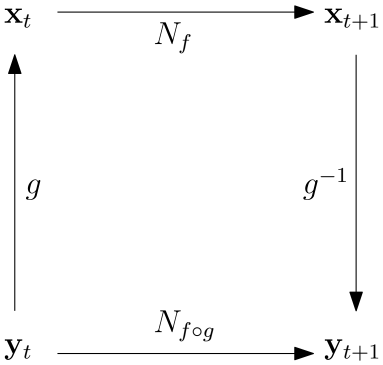
Let $f : \mathbb{R}^d \to \mathbb{R}$ *be twice differentiable,* $A \in \mathbb{R}^{d \times d}$ *an invertible matrix,* $\mathbf{b} \in \mathbb{R}^d$*. Let* $g : \mathbb{R}^d \to \mathbb{R}$ *be the (bijective) affine function* $g(\mathbf{y}) = A\mathbf{y} + \mathbf{b}, \mathbf{y} \in \mathbb{R}^d$*. Finally, for a twice differentiable function* $h : \mathbb{R}^d \to \mathbb{R}$*, let* $N_h : \mathbb{R}^d \to \mathbb{R}^d$ *denote the Newton step for* h*, i.e.*

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

whenever this is defined. Then we have $N_{f \circ g} = g^{-1} \circ N_f \circ g$*.*

Affine Invariance

Newton step for $f \circ g$ on $\mathbf{y}_t$: transform $\mathbf{y}_t$ to $\mathbf{x}_t = g(\mathbf{y}_t)$, perform the Newton step for f on $\mathbf{x}$ and transform the result $\mathbf{x}_{t+1}$ back to $\mathbf{y}_{t+1} = g^{-1}(\mathbf{x}_{t+1})$. This means, the following diagram commutes:



Gradient descent suffers if coordinates are at different scales; Newton's method doesn't.

Minimizing the second-order Taylor approximation

Alternative interpretation of Newton's method:

Each step minimizes the local second-order Taylor approximation.

Lemma (Exercise 47)

Let f be convex and twice differentiable at $\mathbf{x}_t \in \mathbf{dom}(f)$, with $\nabla^2 f(\mathbf{x}_t) \succ 0$ being invertible. The vector $\mathbf{x}_{t+1}$ resulting from the Netwon step satisfies

$$\mathbf{x}_{t+1} = \operatorname*{argmin}_{\mathbf{x} \in \mathbb{R}^d} f(\mathbf{x}_t) + \nabla f(\mathbf{x}_t)^\top (\mathbf{x} - \mathbf{x}_t) + \frac{1}{2}(\mathbf{x} - \mathbf{x}_t)^\top \nabla^2 f(\mathbf{x}_t)(\mathbf{x} - \mathbf{x}_t).$$

Local Convergence

We will prove: under suitable conditions, and starting close to the global minimum, Newton's method will reach distance at most ε to the minimum within $\log\log(1/\varepsilon)$ steps.

- much faster than anything we have seen so far...
- ...but we need to start close to the minimum already.

This is a local convergence result.

Global convergence results that hold for every starting point were unknown for Newton's method until very recently [KSJ18].

Once you're close, you're there...

Theorem

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ *be convex with a unique global minimum* $\mathbf{x}^\star$*. Suppose there is a ball* $X \subseteq \mathbf{dom}(f)$ *with center* $\mathbf{x}^\star$*, s.t.*

(i) *Bounded inverse Hessians: There exists a real number* $\mu > 0$ *such that*

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

(ii) *Lipschitz continuous Hessians: There exists a real number* $B > 0$ *such that*

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

Then, for $\mathbf{x}_t \in X$ *and* $\mathbf{x}_{t+1}$ *resulting from the Newton step, we have*

$$\|\mathbf{x}_{t+1} - \mathbf{x}^\star\| \leq \frac{B}{2\mu}\|\mathbf{x}_t - \mathbf{x}^\star\|^2.$$

Super-exponentially fast

Corollary (Exercise 45)

With the assumptions and terminology of the convergence theorem, and if

$$\|\mathbf{x}_0 - \mathbf{x}^\star\| \leq \frac{\mu}{B},$$

then Newton's method yields

$$\|\mathbf{x}_T - \mathbf{x}^\star\| \leq \frac{\mu}{B} \left(\frac{1}{2}\right)^{2^T - 1}, \quad T \geq 0.$$

Starting close to the global minimum, we will reach distance at most ε to the minimum within $\mathcal{O}\big(\log\log(1/\varepsilon)\big)$ steps.

Bound as for the last phase of the Babylonian method.

Super-exponentially fast — intuitive reason

Almost constant Hessians close to optimality...

...so f behaves almost like a quadratic function which has truly constant Hessians and allows Newton's method to convergence in one step.

Lemma (Exercise 46)

With the assumptions and terminology of the convergence theorem, and if $\mathbf{x}_0 \in X$ *satisfies*

$$\|\mathbf{x}_0 - \mathbf{x}^\star\| \leq \frac{\mu}{B},$$

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

$$\frac{\left\|\nabla^2 f(\mathbf{x}_t) - \nabla f^2(\mathbf{x}^\star)\right\|}{\|\nabla f^2(\mathbf{x}^\star)\|} \leq \left(\frac{1}{2}\right)^{2^t - 1}, \quad t \geq 0.$$

Proof of convergence theorem

We abbreviate $H := \nabla^2 f$, $\mathbf{x} = \mathbf{x}_t, \mathbf{x}' = \mathbf{x}_{t+1}$. Subtracting $\mathbf{x}^\star$ from both sides of the Newton step definition:

$$\begin{aligned}
\mathbf{x}' - \mathbf{x}^\star &= \mathbf{x} - \mathbf{x}^\star - H(\mathbf{x})^{-1}\nabla f(\mathbf{x}) \\
&= \mathbf{x} - \mathbf{x}^\star + H(\mathbf{x})^{-1}(\nabla f(\mathbf{x}^\star) - \nabla f(\mathbf{x})) \\
&= \mathbf{x} - \mathbf{x}^\star + H(\mathbf{x})^{-1}\int_0^1 H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x}))(\mathbf{x}^\star - \mathbf{x})dt,
\end{aligned}$$

using the fundamental theorem of calculus

$$\int_a^b h'(t)dt = h(b) - h(a)$$

with

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

Proof of convergence theorem, II

We so far have

$$\mathbf{x}' - \mathbf{x}^\star = \mathbf{x} - \mathbf{x}^\star + H(\mathbf{x})^{-1} \int_0^1 H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x}))(\mathbf{x}^\star - \mathbf{x})dt.$$

With

$$\mathbf{x} - \mathbf{x}^\star = H(\mathbf{x})^{-1} H(\mathbf{x})(\mathbf{x} - \mathbf{x}^\star) = H(\mathbf{x})^{-1} \int_0^1 -H(\mathbf{x})(\mathbf{x}^\star - \mathbf{x})dt,$$

we further get

$$\mathbf{x}' - \mathbf{x}^\star = H(\mathbf{x})^{-1} \int_0^1 \big(H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x})) - H(\mathbf{x})\big)(\mathbf{x}^\star - \mathbf{x})dt.$$

Taking norms, we have

$$\|\mathbf{x}' - \mathbf{x}^\star\| \leq \|H(\mathbf{x})^{-1}\| \cdot \left\| \int_0^1 \big(H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x})) - H(\mathbf{x})\big)(\mathbf{x}^\star - \mathbf{x})dt \right\|,$$

because $\|A\mathbf{y}\| \leq \|A\| \cdot \|\mathbf{y}\|$ for any $A, \mathbf{y}$ (by def. of spectral norm).

Proof of convergence theorem, III

We so far have

$$\begin{aligned}
\|\mathbf{x}' - \mathbf{x}^\star\| &\leq \|H(\mathbf{x})^{-1}\| \cdot \left\| \int_0^1 \big(H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x})) - H(\mathbf{x})\big)(\mathbf{x}^\star - \mathbf{x}) dt \right\| \\
&\leq \|H(\mathbf{x})^{-1}\| \int_0^1 \left\| \big(H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x})) - H(\mathbf{x})\big)(\mathbf{x}^\star - \mathbf{x}) \right\| dt \quad \text{(Ex. 49)} \\
&\leq \|H(\mathbf{x})^{-1}\| \int_0^1 \left\| H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x})) - H(\mathbf{x}) \right\| \cdot \|\mathbf{x}^\star - \mathbf{x}\| dt \\
&= \|H(\mathbf{x})^{-1}\| \cdot \|\mathbf{x}^\star - \mathbf{x}\| \int_0^1 \left\| H(\mathbf{x} + t(\mathbf{x}^\star - \mathbf{x})) - H(\mathbf{x}) \right\| dt.
\end{aligned}$$

We can now use the properties (i) and (ii) (bounded inverse Hessians, Lipschitz continuous Hessians) to conclude that

$$\|\mathbf{x}' - \mathbf{x}^\star\| \leq \frac{1}{\mu} \|\mathbf{x}^\star - \mathbf{x}\| \int_0^1 B \|t(\mathbf{x}^\star - \mathbf{x})\| dt = \frac{B}{\mu} \|\mathbf{x}^\star - \mathbf{x}\|^2 \underbrace{\int_0^1 t dt}_{1/2} = \frac{B}{2\mu} \|\mathbf{x} - \mathbf{x}^\star\|^2.$$

□

Strong convexity $\Rightarrow$ Bounded inverse Hessians

One way to ensure bounded inverse Hessians is to require strong convexity over X.

Lemma (Exercise 50)

Let $f : \mathbf{dom}(f) \to \mathbb{R}$ be twice differentiable and strongly convex with parameter μ over an open convex subset $X \subseteq \mathbf{dom}(f)$ meaning that

$$f(\mathbf{y}) \geq f(\mathbf{x}) + \nabla f(\mathbf{x})^\top (\mathbf{y} - \mathbf{x}) + \frac{\mu}{2}\|\mathbf{x} - \mathbf{y}\|^2, \quad \forall \mathbf{x}, \mathbf{y} \in X.$$

Then $\nabla^2 f(\mathbf{x})$ is invertible and $\|\nabla^2 f(\mathbf{x})^{-1}\| \leq 1/\mu$ for all $\mathbf{x} \in X$, where $\|\cdot\|$ is the spectral norm.

Downside of Newton's method

Computational bottleneck in each step:

- compute and invert the Hessian matrix
- or solve the linear system $\nabla^2 f(\mathbf{x}_t)\Delta\mathbf{x} = -\nabla f(\mathbf{x}_t)$ for the next step $\Delta\mathbf{x}$.

Matrix / system has size $d \times d$, taking up to $\mathcal{O}(d^3)$ time to invert / solve.

In many applications, d is large...

The secant method

Another iterative method for finding zeros in dimension 1

Start from Newton-Raphson step

$$x_{t+1} := x_t - \frac{f(x_t)}{f'(x_t)},$$

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

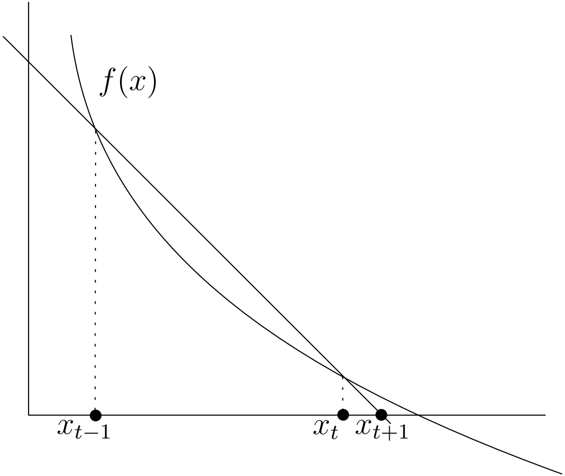
$$f'(x_t) \approx \frac{f(x_t) - f(x_{t-1})}{x_t - x_{t-1}}.$$

(for $|x_t - x_{t-1}|$ small)

Obtain the **secant method**:

$$x_{t+1} := x_t - f(x_t)\frac{x_t - x_{t-1}}{f(x_t) - f(x_{t-1})}$$

The secant method II



- construct the line through the two points $(x_{t-1}, f(x_{t-1}))$ and $(x_t, f(x_t))$;
- next iterate x_{t+1} is where this line intersects the x-axis (Exercise 51)

The secant method III

We now have a derivative-free version of the Newton-Raphson method.

Secant method for optimization: Can we also optimize a differentiable univariate function f?— Yes, apply the secant method to f':

$$x_{t+1} := x_t - f'(x_t)\frac{x_t - x_{t-1}}{f'(x_t) - f'(x_{t-1})}$$

- a second-derivative-free version of Newton's method for optimization.

Can we generalize this to higher dimensions to obtain a Hessian-free version of Newton's method on $\mathbb{R}^d$?

The secant condition

Apply finite difference approximation to f'' (still 1-dim),

$$H_t := \frac{f'(x_t) - f'(x_{t-1})}{x_t - x_{t-1}} \approx f''(x_t)$$

$\Leftrightarrow$

$$f'(x_t) - f'(x_{t-1}) = H_t(x_t - x_{t-1}),$$

the secant condition.

- Newton's method: $x_{t+1} := x_t - f''(x_t)^{-1} f'(x_t)$
- Secant method: $x_{t+1} := x_t - H_t^{-1} f'(x_t)$

In higher dimensions: Let $H_t \in \mathbb{R}^{d\times d}$ be a symmetric matrix satisfying the d-dimensional secant condition

$$\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}) = H_t(\mathbf{x}_t - \mathbf{x}_{t-1}).$$

The secant method step then becomes

$$\mathbf{x}_{t+1} := \mathbf{x}_t - H_t^{-1}\nabla f(\mathbf{x}_t). \tag{1}$$

Quasi-Newton methods

Newton: $\mathbf{x}_{t+1} := \mathbf{x}_t - \nabla^2 f(\mathbf{x}_t)^{-1} \nabla f(\mathbf{x}_t)$
Secant $\mathbf{x}_{t+1} := \mathbf{x}_t - H_t^{-1} \nabla f(\mathbf{x}_t)$, where $\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}) = H_t(\mathbf{x}_t - \mathbf{x}_{t-1})$

If f is twice differentiable, secant condition and first-order approximation of $\nabla f(\mathbf{x})$ at $\mathbf{x}_t$ yield:

$$\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}) = H_t(\mathbf{x}_t - \mathbf{x}_{t-1}) \approx \nabla^2 f(\mathbf{x}_t)(\mathbf{x}_t - \mathbf{x}_{t-1}).$$

Might therefore hope that $H_t \approx \nabla^2 f(\mathbf{x}_t)$...
...meaning that the secant method approximates Newton's method.

- $d = 1$: unique number H_t satisfying the secant condition
- $d > 1$: Secant condition $\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1}) = H_t(\mathbf{x}_t - \mathbf{x}_{t-1})$ has infinitely many symmetric solutions H_t (underdetermined linear system).

Any scheme of choosing in each step of the secant method a symmetric H_t that satisfies the secant condition defines a **Quasi-Newton method**.

Quasi-Newton methods II

- Exercise 52: Newton's method is a Quasi-Newton method if and only if f is a nondegenerate quadratic function.
- Hence, Quasi-Newton methods do not generalize Newton's method but form a family of related algorithms.
- The first Quasi-Newton method was developed by William C. Davidon in 1956; he desperately needed iterations that were faster than those of Newton's method in order obtain results in the short time spans between expected failures of the room-sized computer that he used to run his computations on.
- But the paper he wrote about his new method got rejected for lacking a convergence analysis, and for allegedly dubious notation. It became a very influential Technical Report in 1959 [Dav59] and was finally officially published in 1991, with a foreword giving the historical context [Dav91]. Ironically, Quasi-Newton methods are today the methods of choice in a number of relevant machine learning applications.
- Here: no convergence analysis (for a change), we focus on development of algorithms from first principles.

Developing a Quasi-Newton method

For efficieny reasons (want to avoid matrix inversions!), directly deal with the inverse matrices H_t^{-1}.

Given: iterates $\mathbf{x}_{t-1}, \mathbf{x}_t$ as well as the matrix H_{t-1}^{-1}.

Wanted: next matrix H_t^{-1} needed in next Quasi-Newton step

$$\mathbf{x}_{t+1} := \mathbf{x}_t - H_t^{-1} \nabla f(\mathbf{x}_t).$$

How should we choose H_t^{-1}?

Newton's method: $\nabla f^2(\mathbf{x}_t)$ fluctuates only very little in the region of extremely fast convergence.

Hence, in a Quasi-Newton method, it also makes sense to have that $H_t \approx H_{t-1}$, or $H_t^{-1} \approx H_{t-1}^{-1}$.

Greenstadt's family of Quasi-Newton methods

Given: iterates $\mathbf{x}_{t-1}, \mathbf{x}_t$ as well as the matrix H_{t-1}^{-1}.

Wanted: next matrix H_t^{-1} needed in next Quasi-Newton step

$$\mathbf{x}_{t+1} := \mathbf{x}_t - H_t^{-1} \nabla f(\mathbf{x}_t).$$

Greenstadt [Gre70]: Update

$$H_t^{-1} := H_{t-1}^{-1} + E_t,$$

E_t an error matrix.

Try to minimize the errror subject to H_t satisfying the secant condition!

Simple error measure: Frobenius norm

$$\|E\|_F^2 := \sum_{i=1}^{d} \sum_{j=1}^{d} E_{ij}^2.$$

Greenstadt's family of Quasi-Newton methods II

Greenstadt: minimizing $\|E\|_F$ gives just one method, this is "too specialized".

Greenstadt searched for a compromise between variability in the method and simplicity of the resulting formulas.

More general error measure

$$\|AEA^\top\|_F^2,$$

where $A \in \mathbb{R}^{d\times d}$ is some fixed invertible transformation matrix.

$A = I$: squared Frobenius norm of E, the "specialized" method.

The Greenstadt Update $H_{t-1}^{-1} \to H_t^{-1}$

Secant condition in terms of H_t^{-1}:

$$H_t^{-1}(\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1})) = (\mathbf{x}_t - \mathbf{x}_{t-1}).$$

Fix t and simplify notation:

H	$:=$	H_{t-1}^{-1}	(old inverse)
H'	$:=$	H_t^{-1}	(new inverse)
E	$:=$	$E_t,$	(error matrix)
$\boldsymbol{\sigma}$	$:=$	$\mathbf{x}_t - \mathbf{x}_{t-1}$	(step in solutions)
$\mathbf{y}$	$=$	$\nabla f(\mathbf{x}_t) - \nabla f(\mathbf{x}_{t-1})$	(step in gradients)
$\mathbf{r}$	$=$	$\boldsymbol{\sigma} - H\mathbf{y}$	(error of old inverse in secant condition)

The update formula is

$$H' = H + E,$$

Secant condition becomes

$$H'\mathbf{y} = \boldsymbol{\sigma} \quad (\Leftrightarrow E\mathbf{y} = \mathbf{r}).$$

The Greenstadt Update $H_{t-1}^{-1} \to H_t^{-1}$ II

Minimizing the error becomes a convex constrained minimization problem in the d^2 variables E_{ij}:

$$
\begin{array}{lll}
\text{minimize} & \frac{1}{2}\|AEA^\top\|_F^2 & \text{(error function)} \\
\text{subject to} & E\mathbf{y} = \mathbf{r} & \text{(secant condition)} \\
 & E^\top - E = 0 & \text{(symmetry)}
\end{array}
$$

Don't need to solve it computationally (for numbers E_{ij}) ...

... but mathematically (formula for E)

Minimize convex quadratic function subject to linear equations $\to$ analytic formula for the minimizer from the **method of Lagrange multipliers**.

Bibliography

William C. Davidon.
Variable metric method for minimization.
Technical Report ANL-5990, AEC Research and Development, 1959.

William C. Davidon.
Variable metric method for minimization.
SIAM J. Optimization, 1(1):1–17, 1991.

J. Greenstadt.
Variations on variable-metric methods.
Mathematics of Computation, 24(109):1–22, 1970.

Sai Praneeth Karimireddy, Sebastian U Stich, and Martin Jaggi.
Global linear convergence of Newton's method without strong-convexity or Lipschitz gradients.
arXiv, 2018.