# Optimization for Machine Learning CS-439

Lecture 7: Newton's and Quasi-Newton Methods

Martin Jaggi

EPFL - github.com/epfml/0ptML\_course April 21, 2023

# Chapter 8

### **Newton's Method**

# 1-dimensional case: Newton-Raphson method

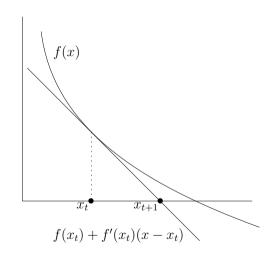
Goal: find a zero of differentiable  $f: \mathbb{R} \to \mathbb{R}$ .

#### Method:

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

 $x_{t+1}$  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

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

Starting from  $x_0 = R \ge 1$ , it takes  $O(\log R)$  steps to get  $x_t - \sqrt{R} < 1/2$  (Exercise 45).

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

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

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

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  $x^*$  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  $\mathbf{x}^* = M^{-1}\mathbf{q}$  be the unique solution of  $\nabla f(\mathbf{x}) = \mathbf{0}$ .

 $ightharpoonup \mathbf{x}^*$  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  $\mathbf{x}_1 = \mathbf{x}^*$ .

#### Proof.

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

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

#### **Affine Invariance**

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

## Lemma (Exercise 46)

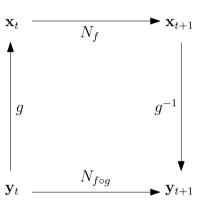
Let  $f: \mathbb{R}^d \to \mathbb{R}$  be twice differentiable,  $A \in \mathbb{R}^{d \times d}$  an invertible matrix,  $\mathbf{b} \in \mathbb{R}^d$ . Let  $g: \mathbb{R}^d \to \mathbb{R}$  be the (bijective) affine function  $g(\mathbf{y}) = A\mathbf{y} + \mathbf{b}, \mathbf{y} \in \mathbb{R}^d$ . 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 49)

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

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

## **Local Convergence**

We will prove: under suitable conditions, and starting close to the global minimum, Newton's method will reach distance at most  $\varepsilon$  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 twice differentiable with a critical point  $\mathbf{x}^*$ . Suppose there is a ball  $X \subseteq \mathbf{dom}(f)$  with center  $\mathbf{x}^*$ , s.t.

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

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

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

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

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

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

# **Super-exponentially fast**

#### Corollary (Exercise 47)

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

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

then Newton's method yields

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

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

Bound as for the last phase of the Babylonian method.

# Super-exponentially fast — intuitive reason

Almost constant Hessians close to optimality...

 $\dots$  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 48)

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

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

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

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

# **Proof of convergence theorem**

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

$$\mathbf{x}' - \mathbf{x}^* = \mathbf{x} - \mathbf{x}^* - H(\mathbf{x})^{-1} \nabla f(\mathbf{x})$$

$$= \mathbf{x} - \mathbf{x}^* + H(\mathbf{x})^{-1} (\nabla f(\mathbf{x}^*) - \nabla f(\mathbf{x}))$$

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

using the fundamental theorem of calculus

$$\int_{a}^{b} h'(t)dt = h(b) - h(a)$$

with

$$h(t) = \nabla f(\mathbf{x} + t(\mathbf{x}^* - \mathbf{x})),$$
  

$$h'(t) = \nabla^2 f(\mathbf{x} + t(\mathbf{x}^* - \mathbf{x}))(\mathbf{x}^* - \mathbf{x}).$$

# Proof of convergence theorem, II

We so far have

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

With

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

we further get

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

Taking norms, we have

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

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

# Proof of convergence theorem, III

We so far have

$$\|\mathbf{x}' - \mathbf{x}^{\star}\| \leq \|H(\mathbf{x})^{-1}\| \cdot \left\| \int_{0}^{1} \left( H(\mathbf{x} + t(\mathbf{x}^{\star} - \mathbf{x})) - H(\mathbf{x}) \right) (\mathbf{x}^{\star} - \mathbf{x}) dt \right\|$$

$$\leq \|H(\mathbf{x})^{-1}\| \int_{0}^{1} \left\| \left( H(\mathbf{x} + t(\mathbf{x}^{\star} - \mathbf{x})) - H(\mathbf{x}) \right) (\mathbf{x}^{\star} - \mathbf{x}) \right\| dt \quad (\mathsf{Ex. 51})$$

$$\leq \|H(\mathbf{x})^{-1}\| \int_{0}^{1} \left\| H(\mathbf{x} + t(\mathbf{x}^{\star} - \mathbf{x})) - H(\mathbf{x}) \right\| \cdot \|\mathbf{x}^{\star} - \mathbf{x}\| dt$$

$$= \|H(\mathbf{x})^{-1}\| \cdot \|\mathbf{x}^{\star} - \mathbf{x}\| \int_{0}^{1} \left\| H(\mathbf{x} + t(\mathbf{x}^{\star} - \mathbf{x})) - H(\mathbf{x}) \right\| dt.$$

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

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

# **Strong convexity** ⇒ **Bounded inverse Hessians**

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

## Lemma (Exercise 52)

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

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

Then  $\nabla^2 f(\mathbf{x})$  is invertible and  $\|\nabla^2 f(\mathbf{x})^{-1}\| \le 1/\mu$  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
- $lackbox{}$  or solve the linear system  $abla^2 f(\mathbf{x}_t) \Delta \mathbf{x} = -\nabla f(\mathbf{x}_t)$  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  $f'(x_t)$ :

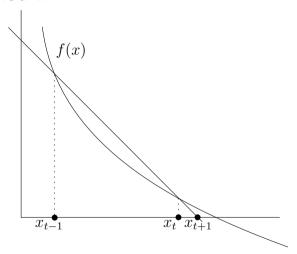
$$f'(x_t) \approx \frac{f(x_t) - f(x_{t-1})}{x_t - x_{t-1}}.$$

(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



- ightharpoonup construct the line through the two points  $(x_{t-1}, f(x_{t-1}))$  and  $(x_t, f(x_t))$ ;
- $\blacktriangleright$  next iterate  $x_{t+1}$  is where this line intersects the x-axis (Exercise 53)

#### 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),

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

the secant condition.

 $\Leftrightarrow$ 

▶ 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

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

EPFL Optimization for Machine Learning CS-439

## **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  $H_t \approx \nabla^2 f(\mathbf{x}_t) \dots$ 

... 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

- ightharpoonup Exercise 54: 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  ${\cal H}_t^{-1}$ .

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

Wanted: next matrix  $\boldsymbol{H}_t^{-1}$  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 $H_{t-1}^{-1} \rightarrow H_t^{-1}$

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:

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

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 $H_{t-1}^{-1} o H_t^{-1}$ II

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

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

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

 $\dots$  but mathematically (formula for E)

Minimize convex quadratic function subject to linear equations  $\rightarrow$  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.