# Introduction to Optimization Introduction to Continuous Optimization II 

November 13, 2015
École Centrale Paris, Châtenay-Malabry, France

Dimo Brockhoff<br>INRIA Lille - Nord Europe

## Course Overview

| Date |  | Topic |
| :--- | :--- | :--- |
| Mon, 21.9.2015 |  | Introduction |
| Mon, 28.9.2015 | D | Basic Flavors of Complexity Theory |
| Mon, 5.10.2015 | D | Greedy algorithms |
| Mon, 12.10.2015 | D | Branch and bound (switched w/ dynamic programming) |
| Mon, 2.11.2015 | D | Dynamic programming [salle Proto] |
| Fri, 6.11.2015 | D | Approximation algorithms and heuristics [S205/S207] |
| Mon, 9.11.2015 | C | Introduction to Continuous Optimization I [S118] |
| Fri, 13.11.2015 | C | Introduction to Continuous Optimization II <br> [from here onwards always: S205/S207] |
| Fri, 20.11.2015 | C | Gradient-based Algorithms |
| Fri, 27.11.2015 | C | End of Gradient-based Algorithms + Linear Programming <br> Stochastic Optimization and Derivative Free Optimization I |
| Fri, 4.12.2015 | C | Stochastic Optimization and Derivative Free Optimization II |
| Tue, 15.12.2015 |  | Exam |

## Lecture Overview Continuous Optimization

## Introduction to Continuous Optimization

- examples (from ML / black-box problems)
- typical difficulties in optimization (e.g. constraints)

Mathematical Tools to Characterize Optima

- reminders about differentiability, gradient, Hessian matrix
- unconstrained optimization
- first and second order conditions
- convexity
- constrained optimization

Gradient-based Algorithms

- quasi-Newton method (BFGS)

Learning in Optimization / Stochastic Optimization

- CMA-ES (adaptive algorithms / Information Geometry)
- PhD thesis possible on this topic strongly related to ML, new promising research area, interesting open questions


## Mathematical Tools to Characterize Optima

## Mathematical Characterization of Optima

Objective: Derive general characterization of optima

Example: if $f: \mathbb{R} \rightarrow \mathbb{R}$ differentiable, $f^{\prime}(x)=0$ at optimal points


## Final Goal:

- generalization to $f: \mathbb{R}^{n} \rightarrow \mathbb{R}$
- generalization to constrained problems


## Reminder of Monday's Lecture

We have seen so far:

- continuity of a function
- differentiability in 1-D and n-D ("gradient")


## Gradient: Geometrical Interpretation

## Exercise:

Let $L_{c}=\left\{\boldsymbol{x} \in \mathbb{R}^{n} \mid f(\boldsymbol{x})=c\right\}$ be again a level set of a function $f(\boldsymbol{x})$. Let $\boldsymbol{x}_{0} \in L_{c} \neq \emptyset$.

Compute the level sets for $f_{1}(\boldsymbol{x})=\boldsymbol{a}^{T} \boldsymbol{x}$ and $f_{2}(\boldsymbol{x})=\|\boldsymbol{x}\|^{2}$ and the gradient in a chosen point $x_{0}$ and observe that $\nabla f\left(x_{0}\right)$ is orthogonal to the level set in $x_{0}$.

Again: if this seems too difficult, do it for two variables (and a concrete $\boldsymbol{a} \in \mathbb{R}^{2}$ and draw the level sets and the gradients.

More generally, the gradient of a differentiable function is orthogonal to its level sets.


## Differentiability in $\mathbb{R}^{n}$

## Taylor Formula - Order One

$$
f(\boldsymbol{x}+\boldsymbol{h})=f(\boldsymbol{x})+(\nabla f(\boldsymbol{x}))^{T} \boldsymbol{h}+o(\|\boldsymbol{h}\|)
$$

## Reminder: Second Order Differentiability in 1D

- Let $f: D \subseteq \mathbb{R} \rightarrow \mathbb{R}$ be a differentiable function and let $f^{\prime}: x \rightarrow$ $f^{\prime}(x)$ be its derivative.
- If $f^{\prime}$ is differentiable in $x$, then we denote its derivative as $f^{\prime \prime}(x)$
- $\quad f^{\prime \prime}(x)$ is called the second order derivative of $f$.


## Taylor Formula: Second Order Derivative

- If $f: \mathbb{R} \rightarrow \mathbb{R}$ is two times differentiable then

$$
f(x+h)=f(x)+f^{\prime}(x) h+f^{\prime \prime}(x) h^{2}+o\left(\|h\|^{2}\right)
$$

i.e. for $h$ small enough, $h \rightarrow f(x)+h f^{\prime}(x)+h^{2} f^{\prime \prime}(x)$ approximates $h+f(x+h)$

- $h \rightarrow f(x)+h f^{\prime}(x)+h^{2} f^{\prime \prime}(x)$ is a quadratic approximation (or order 2) of $f$ in a neighborhood of $x$

- The second derivative of $f: \mathbb{R} \rightarrow \mathbb{R}$ generalizes naturally to larger dimension.


## Hessian Matrix

In $\left(\mathbb{R}^{n},\langle x, y\rangle=x^{T} y\right), \nabla^{2} f(x)$ is represented by a symmetric matrix called the Hessian matrix. It can be computed as

$$
\nabla^{2}(f)=\left[\begin{array}{cccc}
\frac{\partial^{2} f}{\partial x_{1}^{2}} & \frac{\partial^{2} f}{\partial x_{1} \partial x_{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{1} \partial x_{n}} \\
\frac{\partial^{2} f}{\partial x_{2} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{2}^{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{2} \partial x_{n}} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial^{2} f}{\partial x_{n} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{n} \partial x_{2}} & \cdots & \frac{\partial^{2} f}{\partial x_{n}^{2}}
\end{array}\right]
$$

## Exercise on Hessian Matrix

## Exercise:

Let $f(\boldsymbol{x})=\frac{1}{2} \boldsymbol{x}^{T} A \boldsymbol{x}, \boldsymbol{x} \in \mathbb{R}^{n}$, and $A \in \mathbb{R}^{n \times n}$ symmetric.
Compute the Hessian matrix of $f$.
If it is too complex, consider $f:\left\{\begin{array}{c}\mathbb{R}^{2} \rightarrow \mathbb{R} \\ x \rightarrow \frac{1}{2} \boldsymbol{x}^{T} A \boldsymbol{x}\end{array}\right.$ with $A=\left(\begin{array}{ll}9 & 0 \\ 0 & 1\end{array}\right)$

## Second Order Differentiability in $\mathbb{R}^{n}$

## Taylor Formula - Order Two

$$
f(\boldsymbol{x}+\boldsymbol{h})=f(\boldsymbol{x})+(\nabla f(\boldsymbol{x}))^{T} \boldsymbol{h}+\frac{1}{2} \boldsymbol{h}^{T}\left(\nabla^{2} f(\boldsymbol{x})\right) \boldsymbol{h}+o\left(\|\boldsymbol{h}\|^{2}\right)
$$

## Back to III-Conditioned Problems

We have seen that for a convex quadratic function
$f(x)=\frac{1}{2}\left(x-x_{0}\right)^{T} A\left(x-x_{0}\right)+b$ of $x \in \mathbb{R}^{n}, A \in \mathbb{R}^{n \times n}, A \operatorname{SPD}, b \in \mathbb{R}^{n}$ :

1) The level sets are ellipsoids. The eigenvalues of $A$ determine the lengths of the principle axes of the ellipsoid.

2) The Hessian matrix of $f$ equals to $A$.

III-conditioned convex quadratic problems are problems with large ratio between largest and smallest eigenvalue of $A$ which means large ratio between longest and shortest axis of ellipsoid.

This corresponds to having an ill-conditioned Hessian matrix.

## Gradient Direction Vs. Newton Direction

Gradient direction: $\nabla f(x)$
Newton direction: $(H(x))^{-1} \cdot \nabla f(\boldsymbol{x})$
with $H(\boldsymbol{x})=\nabla^{2} f(\boldsymbol{x})$ being the Hessian at $\boldsymbol{x}$

## Exercise:

Let again $f(\boldsymbol{x})=\frac{1}{2} \boldsymbol{x}^{T} A \boldsymbol{x}, \boldsymbol{x} \in \mathbb{R}^{2}, A=\left(\begin{array}{ll}9 & 0 \\ 0 & 1\end{array}\right) \in \mathbb{R}^{2 \times 2}$.
Plot the gradient and Newton direction of $f$ in a point $x \in \mathbb{R}^{n}$ of your choice (which should not be on a coordinate axis) into the same plot with the level sets, we created before.

## Exercise: Comparing Gradient-Based Algorithms on Convex Quadratic Functions (Tasks 1. - 4.)

http://researchers.lille.inria.fr/ ~brockhof/optimizationSaclay/

## Optimality Conditions for Unconstrained Problems

## Optimality Conditions: First Order Necessary Cond.

For 1-dimensional optimization problems $f: \mathbb{R} \rightarrow \mathbb{R}$
Assume $f$ is differentiable

- $\boldsymbol{x}^{*}$ is a local optimum $\Rightarrow f^{\prime}\left(\boldsymbol{x}^{*}\right)=0$
not a sufficient condition: consider $f(x)=x^{3}$ proof via Taylor formula: $f\left(\boldsymbol{x}^{*}+\boldsymbol{h}\right)=f\left(\boldsymbol{x}^{*}\right)+f^{\prime}\left(\boldsymbol{x}^{*}\right) \boldsymbol{h}+o(\|\boldsymbol{h}\|)$
- points $\boldsymbol{y}$ such that $f^{\prime}(\boldsymbol{y})=0$ are called critical or stationary points

Generalization to $n$-dimensional functions
If $f: U \subset \mathbb{R}^{n} \mapsto \mathbb{R}$ is differentiable

- necessary condition: If $\boldsymbol{x}^{*}$ is a local optimum of $f$, then $\nabla f\left(\boldsymbol{x}^{*}\right)=0$
proof via Taylor formula


## Second Order Necessary and Sufficient Opt. Cond.

If $f$ is twice continuously differentiable

- Necessary condition: if $\boldsymbol{x}^{*}$ is a local minimum, then $\nabla f\left(\boldsymbol{x}^{*}\right)=0$ and $\nabla^{2} f\left(x^{*}\right)$ is positive semi-definite
proof via Taylor formula at order 2
- Sufficient condition: if $\nabla f\left(\boldsymbol{x}^{*}\right)=0$ and $\nabla^{2} f\left(\boldsymbol{x}^{*}\right)$ is positive definite, then $\boldsymbol{x}^{*}$ is a strict local minimum


## Proof of Sufficient Condition:

- Let $\lambda>0$ be the smallest eigenvalue of $\nabla^{2} f\left(x^{*}\right)$, using a second order Taylor expansion, we have for all $\boldsymbol{h}$ :
- $f\left(\boldsymbol{x}^{*}+\boldsymbol{h}\right)-f\left(\boldsymbol{x}^{*}\right)=\nabla f\left(\boldsymbol{x}^{*}\right)^{T} \boldsymbol{h}+\frac{1}{2} \boldsymbol{h}^{T} \nabla^{2} f\left(\boldsymbol{x}^{*}\right) \boldsymbol{h}+o\left(\|\boldsymbol{h}\|^{2}\right)$

$$
>\frac{\lambda}{2}\|\boldsymbol{h}\|^{2}+o\left(\|\boldsymbol{h}\|^{2}\right)=\left(\frac{\lambda}{2}+\frac{o\left(\|\boldsymbol{h}\|^{2}\right)}{\|\boldsymbol{h}\|^{2}}\right)\|\boldsymbol{h}\|^{2}
$$

## Convex Functions

Let $U$ be a convex open set of $\mathbb{R}^{n}$ and $f: U \rightarrow \mathbb{R}$. The function $f$ is said to be convex if for all $\boldsymbol{x}, \boldsymbol{y} \in U$ and for all $t \in[0,1]$

$$
f((1-t) \boldsymbol{x}+t \boldsymbol{y}) \leq(1-t) f(\boldsymbol{x})+t f(\boldsymbol{y})
$$

## Theorem

If $f$ is differentiable, then $f$ is convex if and only if for all $\boldsymbol{x}, \boldsymbol{y}$

$$
\begin{aligned}
f(\boldsymbol{y})-f(\boldsymbol{x}) & \geq(\nabla f(x))^{T}(\boldsymbol{y}-\boldsymbol{x}) \\
\text { if } n & =1, \text { the curve is on top of the tangent }
\end{aligned}
$$

If $f$ is twice continuously differentiable, then $f$ is convex if and only if $\nabla^{2} f(x)$ is positive semi-definite for all $\boldsymbol{x}$.

## Constrained Optimization

## Equality Constraint

## Objective:

Generalize the necessary condition of $\nabla f(x)=0$ at the optima of $\mathfrak{f}$ when $f$ is in $\mathcal{C}^{1}$, i.e. is differentiable and its derivative is continuous

## Theorem:

Be $U$ an open set of $(E,\| \|)$, and $f: U \rightarrow \mathbb{R}, g: U \rightarrow \mathbb{R}$ in $\mathcal{C}^{1}$.
Let $a \in E$ satisfy

$$
\left\{\begin{array}{c}
f(a)=\inf \left\{f(x) \mid x \in \mathbb{R}^{n}, g(x)=0\right\} \\
g(a)=0
\end{array}\right.
$$

i.e. $a$ is optimum of the problem

If $\nabla g(a) \neq 0$, then there exists a constant $\lambda \in \mathbb{R}$ called Lagrange multiplier, such that

$$
\nabla \underbrace{\nabla f(a)+\lambda \nabla g(a)=0}
$$

i.e. gradients of $f$ and $g$ in $a$ are colinear

Note: $a$ need not be a global minimum but a local one

## Geometrical Interpretation Using an Example

## Exercise:

Consider the problem

$$
\inf \left\{f(x, y) \mid(x, y) \in \mathbb{R}^{2}, g(x, y)=0\right\}
$$

$$
f(x, y)=y-x^{2} \quad g(x, y)=x^{2}+y^{2}-1
$$

1) Plot the level sets of $f$, plot $g=0$
2) Compute $\nabla f$ and $\nabla g$
3) Find the solutions with $\nabla f+\lambda \nabla g=0$
equation solving with 3 unknowns ( $x, y, \lambda$ )
4) Plot the solutions of 3 ) on top of the level set graph of 1 )

## Interpretation of Euler-Lagrange Equation

Intuitive way to retrieve the Euler-Lagrange equation:

- In a local minimum $a$ of a constrained problem, the hypersurfaces (or level sets) $f=f(a)$ and $g=0$ are necessarily tangent (otherwise we could decrease $f$ by moving along $g=0$ ).
- Since the gradients $\nabla f(a)$ and $\nabla g(a)$ are orthogonal to the level sets $f=f(a)$ and $g=0$, it follows that $\nabla f(a)$ and $\nabla g(a)$ are colinear.


## Generalization to More than One Constraint

## Theorem

- Assume $f: U \rightarrow \mathbb{R}$ and $g_{k}: U \rightarrow \mathbb{R}(1 \leq k \leq p)$ are $\mathcal{C}^{1}$.
- Let $a$ be such that

$$
\left\{\begin{array}{r}
f(a)=\inf \left\{f(x) \mid x \in \mathbb{R}^{n}, \quad g_{k}(x)=0, \quad 1 \leq k \leq p\right\} \\
g_{k}(a)=0 \text { for all } 1 \leq k \leq p
\end{array}\right.
$$

- If $\left(\nabla g_{k}(a)\right)_{1 \leq k \leq p}$ are linearly independent, then there exist $p$ real constants $\left(\lambda_{k}\right)_{1 \leq k \leq p}$ such that

$$
\nabla f(a)+\sum_{k=1 \uparrow}^{p} \lambda_{k} \nabla g_{k}(a)=0
$$

again: $a$ does not need to be global but local minimum

## The Lagrangian

- Define the Lagrangian on $\mathbb{R}^{n} \times \mathbb{R}^{p}$ as

$$
\mathcal{L}\left(x,\left\{\lambda_{k}\right\}\right)=f(x)+\sum_{k=1}^{p} \lambda_{k} g_{k}(x)
$$

- To find optimal solutions, we can solve the optimality system
$\left\{\right.$ Find $\left(x,\left\{\lambda_{k}\right\}\right) \in \mathbb{R}^{n} \times \mathbb{R}^{p}$ such that $\nabla f(x)+\sum_{k=1}^{p} \lambda_{k} \nabla g_{k}(x)=0$

$$
g_{k}(x)=0 \text { for all } 1 \leq k \leq p
$$

$$
\Leftrightarrow\left\{\begin{array}{c}
\text { Find }\left(x,\left\{\lambda_{k}\right\}\right) \in \mathbb{R}^{n} \times \mathbb{R}^{p} \text { such that } \nabla_{x} \mathcal{L}\left(x,\left\{\lambda_{k}\right\}\right)=0 \\
\nabla_{\lambda_{k}} \mathcal{L}\left(x,\left\{\lambda_{k}\right\}\right)(x)=0 \text { for all } 1 \leq k \leq p
\end{array}\right.
$$

## Inequality Constraints: Definitions

Let $U=\left\{x \in \mathbb{R}^{n} \mid g_{k}(x)=0\right.$ (for $k \in E$ ), $g_{k}(x) \leq 0$ (for $k \in I$ ) $\}$.

## Definition:

The points in $\mathbb{R}^{n}$ that satisfy the constraints are also called feasible points.

## Definition:

Let $a \in U$, we say that the constraint $g_{k}(x) \leq 0$ (for $k \in I$ ) is active in $a$ if $g_{k}(a)=0$.

## Inequality Constraint: Karush-Kuhn-Tucker Theorem

Theorem (Karush-Kuhn-Tucker, KKT):
Let $U$ be an open set of $(E,\| \|)$ and $f: U \rightarrow \mathbb{R}, g_{k}: U \rightarrow \mathbb{R}$, all $\mathcal{C}^{1}$
Furthermore, let $a \in U$ satisfy
$\left\{\begin{aligned} f(a)=\inf \left(f(x) \mid x \in \mathbb{R}^{n}, g_{k}(x)=0(\text { for } k \in E),\right. & g_{k}(x) \leq 0(\text { for } k \in \mathrm{I}) \\ g_{k}(a)=0(\text { for } k \in E) & \text { also works again for } a \\ g_{k}(a) \leq 0(\text { for } k \in I) & \text { being a local minimum }\end{aligned}\right.$
Let $I_{a}^{0}$ be the set of constraints that are active in $a$. Assume that $\left(\nabla g_{k}(a)\right)_{k \in E \cup I_{a}^{0}}$ are linearly independent.
Then there exist $\left(\lambda_{k}\right)_{1 \leq k \leq p}$ that satisfy

$$
\left\{\begin{array}{c}
\nabla f(a)+\sum_{k=1}^{p} \lambda_{k} \nabla g_{k}(a)=0 \\
g_{k}(a)=0(\text { for } k \in E) \\
g_{k}(a) \leq 0(\text { for } k \in I) \\
\lambda_{k} \geq 0\left(\text { for } k \in I_{a}^{0}\right) \\
\lambda_{k} g_{k}(a)=0(\text { for } k \in E \cup I)
\end{array}\right.
$$

## Inequality Constraint: Karush-Kuhn-Tucker Theorem

Theorem (Karush-Kuhn-Tucker, KKT):
Let $U$ be an open set of $(E,\| \|)$ and $f: U \rightarrow \mathbb{R}, g_{k}: U \rightarrow \mathbb{R}$, all $\mathcal{C}^{1}$
Furthermore, let $a \in U$ satisfy

$$
\left\{\begin{array}{c}
f(a)=\inf \left(f(x) \mid x \in \mathbb{R}^{n}, g_{k}(x)=0(\text { for } k \in E), g_{k}(x) \leq 0(\text { for } k \in \mathrm{I})\right. \\
g_{k}(a)=0(\text { for } k \in E) \\
g_{k}(a) \leq 0(\text { for } k \in I)
\end{array}\right.
$$

Let $I_{a}^{0}$ be the set of constraints that are active in $a$. Assume that $\left(\nabla g_{k}(a)\right)_{k \in E \cup I_{a}^{0}}$ are linearly independent.
Then there exist $\left(\lambda_{k}\right)_{1 \leq k \leq p}$ that satisfy

$$
\left\{\begin{array}{c}
\nabla f(a)+\sum_{k=1}^{p} \lambda_{k} \nabla g_{k}(a)=0 \\
g_{k}(a)=0(\text { for } k \in E) \\
g_{k}(a) \leq 0(\text { for } k \in I) \\
\lambda_{k} \geq 0\left(\text { for } k \in I_{a}^{0}\right) \\
\lambda_{k} g_{k}(a)=0(\text { for } k \in E \cup I)
\end{array}\right.
$$

either active constraint or $\lambda_{k}=0$

## Descent Methods

## Descent Methods

## General principle

(1) choose an initial point $x_{0}$, set $t=1$
(2) while not happy

- choose a descent direction $\boldsymbol{d}_{t} \neq 0$
- line search:
- choose a step size $\sigma_{t}>0$
- set $\boldsymbol{x}_{t+1}=\boldsymbol{x}_{t}+\sigma_{t} \boldsymbol{d}_{t}$
- set $t=t+1$


## Remaining questions

- how to choose $\boldsymbol{d}_{t}$ ?
- how to choose $\sigma_{t}$ ?


## Gradient Descent

Rationale: $\boldsymbol{d}_{t}=-\nabla f\left(\boldsymbol{x}_{t}\right)$ is a descent direction indeed for $f$ differentiable

$$
\begin{aligned}
f(x-\sigma \nabla f(x)) & =f(x)-\sigma\|\nabla f(x)\|^{2}+o(\sigma\|\nabla f(x)\|) \\
< & f(x) \text { for } \sigma \text { small enough }
\end{aligned}
$$

## Step-size

- optimal step-size: $\sigma_{t}=\operatorname{argmin} f\left(\boldsymbol{x}_{t}-\sigma \nabla f\left(\boldsymbol{x}_{t}\right)\right)$
- Line Search: total or partial optimization w.r.t. $\sigma$ Total is however often too "expensive" (needs to be performed at each iteration step)
Partial optimization: execute a limited number of trial steps until a loose approximation of the optimum is found. Typical rule for partial optimization: Armijo rule


## Stopping criteria:

norm of gradient smaller than $\epsilon$

## The Armijo-Goldstein Rule

Choosing the step size:

- Only to decrease $f$-value not enough to converge (quickly)
- Want to have a reasonably large decrease in $f$


## Armijo-Goldstein rule:

- also known as backtracking line search
- starts with a (too) large estimate of $\sigma$ and reduces it until $f$ is reduced enough
- what is enough?
- assuming a linear $f$ e.g. $m_{k}(x)=f\left(x_{k}\right)+\nabla f\left(x_{k}\right)^{T}\left(x-x_{k}\right)$
- expected decrease if step of $\sigma_{k}$ is done in direction $\boldsymbol{d}$ : $\sigma_{k} \nabla f\left(x_{k}\right)^{T} \boldsymbol{d}$
- actual decrease: $f\left(x_{k}\right)-f\left(x_{k}+\sigma_{k} \boldsymbol{d}\right)$
- stop if actual decrease is at least constant times expected decrease (constant typically chosen in $[0,1]$ )


## The Armijo-Goldstein Rule

## The Actual Algorithm:

Input: descent direction d, point $\mathbf{x}$, objective function $f(\mathbf{x})$ and its gradient $\nabla f(\mathbf{x})$, parameters $\sigma_{0}=10, \theta \in[0,1]$ and $\beta \in(0,1)$
Output: step-size $\sigma$
Initialize $\sigma: \sigma \leftarrow \sigma_{0}$
while $f(\mathbf{x}+\sigma \mathbf{d})>f(\mathbf{x})+\theta \sigma \nabla f(\mathbf{x})^{T} \mathbf{d}$ do
$\sigma \leftarrow \beta \sigma$
end while

Armijo, in his original publication chose $\beta=\theta=0.5$.
Choosing $\theta=0$ means the algorithm accepts any decrease.

## The Armijo-Goldstein Rule

## Graphical Interpretation


linear approximation
(expected decrease)

## The Armijo-Goldstein Rule

## Graphical Interpretation


linear approximation
(expected decrease)

## The Armijo-Goldstein Rule

## Graphical Interpretation


linear approximation
(expected decrease)

## Gradient Descent: Simple Theoretical Analysis

Assume $f$ is twice continuously differentiable, convex and that $\mu I_{d} \preccurlyeq \nabla^{2} f(x) \preccurlyeq L I_{d}$ with $\mu>0$ holds, assume a fixed step-size $\sigma_{t}=$ $\frac{1}{L}$

Note: $A \leqslant B$ means $x^{T} A x \leq x^{T} B x$ for all $x$

$$
\begin{aligned}
x_{t+1}-x^{*}= & x_{t}-x^{*}-\sigma_{t} \nabla^{2} f\left(y_{t}\right)\left(x_{t}-x^{*}\right) \text { for some } y_{t} \in\left[x_{t}, x^{*}\right] \\
& x_{t+1}-x^{*}=\left(I_{d}-\frac{1}{L} \nabla^{2} f\left(y_{t}\right)\right)\left(x_{t}-x^{*}\right)
\end{aligned}
$$

$$
\text { Hence }\left\|x_{t+1}-x^{*}\right\|^{2} \leq\left\|\left\lvert\, I_{d}-\frac{1}{L} \nabla^{2} f\left(y_{t}\right)\right.\right\|\left\|^{2}\right\| x_{t}-x^{*} \|^{2}
$$

$$
\leq\left(1-\frac{\mu}{L}\right)^{2}\left\|x_{t}-x^{*}\right\|^{2}
$$

Linear convergence: $\left\|x_{t+1}-x^{*}\right\| \leq\left(1-\frac{\mu}{L}\right)\left\|x_{t}-x^{*}\right\|$
algorithm slower and slower with increasing condition number
Non-convex setting: convergence towards stationary point

## Newton Algorithm

## Newton Method

- descent direction: $-\left[\nabla^{2} f\left(x_{k}\right)\right]^{-1} \nabla f\left(x_{k}\right)$ [so-called Newton direction]
- The Newton direction:
- minimizes the best (locally) quadratic approximation of $f$ :

$$
\tilde{f}(x+\Delta x)=f(x)+\nabla f(x)^{T} \Delta x+\frac{1}{2}(\Delta x)^{T} \nabla^{2} f(x) \Delta \mathrm{x}
$$

- points towards the optimum on $f(x)=\left(x-x^{*}\right)^{T} A\left(x-x^{*}\right)$
- however, Hessian matrix is expensive to compute in general and its inversion is also not easy
quadratic convergence

$$
\text { (i.e. } \lim _{k \rightarrow \infty} \frac{\left|x_{k+1}-x^{*}\right|}{\left|x_{k}-x^{*}\right|^{2}}=\mu>0 \text { ) }
$$

## Remark: Affine Invariance

Affine Invariance: same behavior on $f(x)$ and $f(A x+b)$ for $A \in$ GLn(R)

- Newton method is affine invariant see http://users.ece.utexas.edu/~cmcaram/EE381V_2012F/ Lecture_6_Scribe_Notes.final.pdf
- same convergence rate on all convex-quadratic functions
- Gradient method not affine invariant


## Quasi-Newton Method: BFGS

$x_{t+1}=x_{t}-\sigma_{t} H_{t} \nabla f\left(x_{t}\right)$ where $H_{t}$ is an approximation of the inverse Hessian

## Key idea of Quasi Newton:

successive iterates $x_{t}, x_{t+1}$ and gradients $\nabla f\left(x_{t}\right), \nabla f\left(x_{t+1}\right)$ yield second order information

$$
\begin{gathered}
q_{t} \approx \nabla^{2} f\left(x_{t+1}\right) p_{t} \\
\text { where } p_{t}=x_{t+1}-x_{t} \text { and } q_{t}=\nabla f\left(x_{t+1}\right)-\nabla f\left(x_{t}\right)
\end{gathered}
$$

Most popular implementation of this idea: Broyden-Fletcher-Goldfarb-Shanno (BFGS)

- default in MATLAB's fminunc and python's scipy.optimize.minimize


## Conclusions

I hope it became clear...
...what are gradient and Hessian
...what are sufficient and necessary conditions for optimality
...what is the difference between gradient and Newton direction
...and that adapting the step size in descent algorithms is crucial.

