Introduction to Optimization Introduction to Continuous Optimization II

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Dimo Brockhoff 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	С	Introduction to Continuous Optimization I [S118]
Fri, 13.11.2015	C	Introduction to Continuous Optimization II [from here onwards always: S205/S207]
Fri, 20.11.2015	С	Gradient-based Algorithms
Fri, 27.11.2015	С	End of Gradient-based Algorithms + Linear Programming Stochastic Optimization and Derivative Free Optimization I
Fri, 4.12.2015	С	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

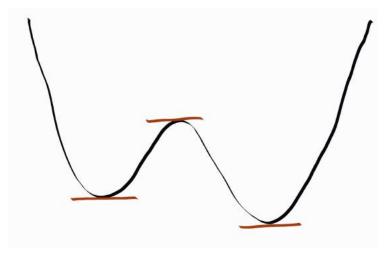
- CMA-ES (adaptive algorithms / Information Geometry)
- PhD thesis possible on this topic
 strongly related to ML, new promising research area, interesting open questions



Mathematical Characterization of Optima

Objective: Derive general characterization of optima

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



Final Goal:

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

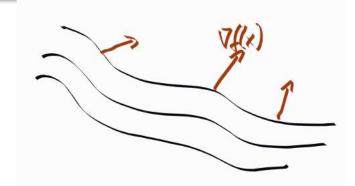
Exercise:

Let $L_c = \{x \in \mathbb{R}^n \mid f(x) = c\}$ be again a level set of a function f(x). Let $x_0 \in L_c \neq \emptyset$.

Compute the level sets for $f_1(x) = a^T x$ and $f_2(x) = ||x||^2$ and the gradient in a chosen point x_0 and observe that $\nabla f(x_0)$ is **orthogonal** to the level set in x_0 .

Again: if this seems too difficult, do it for two variables (and a concrete $a \in \mathbb{R}^2$ 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

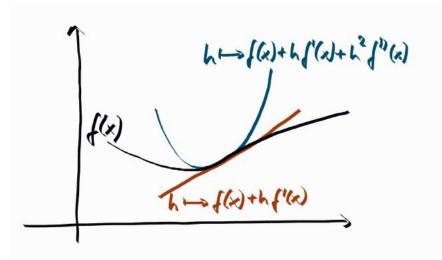
$$f(\mathbf{x} + \mathbf{h}) = f(\mathbf{x}) + (\nabla f(\mathbf{x}))^T \mathbf{h} + o(||\mathbf{h}||)$$

Reminder: Second Order Differentiability in 1D

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

Taylor Formula: Second Order Derivative

- If $f: \mathbb{R} \to \mathbb{R}$ is two times differentiable then $f(x+h) = f(x) + f'(x)h + f''(x)h^2 + o(||h||^2)$ i.e. for h small enough, $h \to f(x) + hf'(x) + h^2f''(x)$ approximates h + f(x+h)
- $h \to f(x) + hf'(x) + h^2f''(x)$ is a quadratic approximation (or order 2) of f in a neighborhood of x



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

Hessian Matrix

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

$$\nabla^{2}(f) = \begin{bmatrix} \frac{\partial^{2} f}{\partial x_{1}^{2}} & \frac{\partial^{2} f}{\partial x_{1} \partial x_{2}} & \dots & \frac{\partial^{2} f}{\partial x_{1} \partial x_{n}} \\ \frac{\partial^{2} f}{\partial x_{2} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{2}^{2}} & \dots & \frac{\partial^{2} f}{\partial x_{2} \partial x_{n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^{2} f}{\partial x_{n} \partial x_{1}} & \frac{\partial^{2} f}{\partial x_{n} \partial x_{2}} & \dots & \frac{\partial^{2} f}{\partial x_{n}^{2}} \end{bmatrix}$$

Exercise on Hessian Matrix

Exercise:

Let $f(x) = \frac{1}{2}x^T A x$, $x \in \mathbb{R}^n$, and $A \in \mathbb{R}^{n \times n}$ symmetric.

Compute the Hessian matrix of f.

If it is too complex, consider $f: \begin{cases} \mathbb{R}^2 \to \mathbb{R} \\ x \to \frac{1}{2} x^T A x \end{cases}$ with $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix}$

Second Order Differentiability in \mathbb{R}^n

Taylor Formula – Order Two

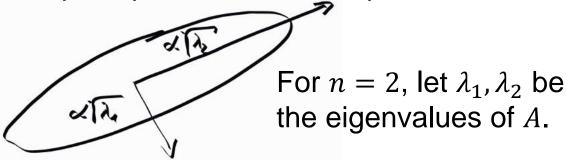
$$f(\mathbf{x} + \mathbf{h}) = f(\mathbf{x}) + (\nabla f(\mathbf{x}))^T \mathbf{h} + \frac{1}{2} \mathbf{h}^T (\nabla^2 f(\mathbf{x})) \mathbf{h} + o(||\mathbf{h}||^2)$$

Back to III-Conditioned Problems

We have seen that for a convex quadratic function

$$f(x) = \frac{1}{2}(x - x_0)^T A(x - x_0) + b \text{ of } x \in \mathbb{R}^n, A \in \mathbb{R}^{n \times n}, A \text{ SPD, } b \in \mathbb{R}^n$$
:

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.

Ill-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: $(H(x))^{-1} \cdot \nabla f(x)$

with $H(x) = \nabla^2 f(x)$ being the Hessian at x

Exercise:

Let again
$$f(x) = \frac{1}{2}x^T A x$$
, $x \in \mathbb{R}^2$, $A = \begin{pmatrix} 9 & 0 \\ 0 & 1 \end{pmatrix} \in \mathbb{R}^{2 \times 2}$.

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 $f: \mathbb{R} \to \mathbb{R}$

Assume *f* is differentiable

- x^* is a local optimum $\Rightarrow f'(x^*) = 0$ not a sufficient condition: consider $f(x) = x^3$
 - proof via Taylor formula: $f(x^* + h) = f(x^*) + f'(x^*)h + o(||h||)$
- points y such that f'(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 x^* is a local optimum of f, then $\nabla f(x^*) = 0$ proof via Taylor formula

Second Order Necessary and Sufficient Opt. Cond.

If *f* is twice continuously differentiable

• Necessary condition: if x^* is a local minimum, then $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive semi-definite

proof via Taylor formula at order 2

• Sufficient condition: if $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*)$ is positive definite, then x^* is a strict local minimum

Proof of Sufficient Condition:

Let $\lambda > 0$ be the smallest eigenvalue of $\nabla^2 f(x^*)$, using a second order Taylor expansion, we have for all h:

$$f(\mathbf{x}^* + \mathbf{h}) - f(\mathbf{x}^*) = \nabla f(\mathbf{x}^*)^T \mathbf{h} + \frac{1}{2} \mathbf{h}^T \nabla^2 f(\mathbf{x}^*) \mathbf{h} + o(||\mathbf{h}||^2)$$
$$> \frac{\lambda}{2} ||\mathbf{h}||^2 + o(||\mathbf{h}||^2) = \left(\frac{\lambda}{2} + \frac{o(||\mathbf{h}||^2)}{||\mathbf{h}||^2}\right) ||\mathbf{h}||^2$$

Convex Functions

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

$$f((1-t)x + ty) \le (1-t)f(x) + tf(y)$$

Theorem

If f is differentiable, then f is convex if and only if for all x, y

$$f(y) - f(x) \ge (\nabla f(x))^{T} (y - x)$$

if n = 1, the curve is on top of the tangent

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

Constrained Optimization

Equality Constraint

Objective:

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

Theorem:

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

$$\begin{cases} f(a) = \inf \{ f(x) \mid x \in \mathbb{R}^n, g(x) = 0 \} \\ g(a) = 0 \end{cases}$$

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

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

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

$$f(x,y) = y - x^2$$
 $g(x,y) = x^2 + y^2 - 1$

- 1) Plot the level sets of f, plot g = 0
- 2) Compute ∇f and ∇g
- 3) Find the solutions with $\nabla f + \lambda \nabla g = 0$

equation solving with 3 unknowns (x, y, λ)

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 $f: U \to \mathbb{R}$ and $g_k: U \to \mathbb{R}$ $(1 \le k \le p)$ are \mathcal{C}^1 .
- Let a be such that

$$\begin{cases} f(a) = \inf \{ f(x) \mid x \in \mathbb{R}^n, & g_k(x) = 0, \\ g_k(a) = 0 \text{ for all } 1 \le k \le p \end{cases}$$

• If $(\nabla g_k(a))_{1 \le k \le p}$ are linearly independent, then there exist p real constants $(\lambda_k)_{1 \le k \le p}$ such that

$$\nabla f(a) + \sum_{k=1}^{p} \lambda_k \nabla g_k(a) = 0$$

Lagrange multiplier

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

$$\mathcal{L}(x,\{\lambda_k\}) = f(x) + \sum_{k=1}^{p} \lambda_k g_k(x)$$

To find optimal solutions, we can solve the optimality system

Find
$$(x, \{\lambda_k\}) \in \mathbb{R}^n \times \mathbb{R}^p$$
 such that $\nabla f(x) + \sum_{k=1}^p \lambda_k \nabla g_k(x) = 0$

$$g_k(x) = 0 \text{ for all } 1 \le k \le p$$

$$\Leftrightarrow \begin{cases} \text{Find } (x, \{\lambda_k\}) \in \mathbb{R}^n \times \mathbb{R}^p \text{ such that } \nabla_x \mathcal{L}(x, \{\lambda_k\}) = 0 \\ \nabla_{\lambda_k} \mathcal{L}(x, \{\lambda_k\})(x) = 0 \text{ for all } 1 \le k \le p \end{cases}$$

Inequality Constraints: Definitions

Let
$$\mathcal{U} = \{x \in \mathbb{R}^n \mid g_k(x) = 0 \text{ (for } k \in E), \ g_k(x) \le 0 \text{ (for } k \in I)\}.$$

Definition:

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

Definition:

Let $a \in \mathcal{U}$, 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 $f: U \to \mathbb{R}, g_k: U \to \mathbb{R}$, all \mathcal{C}^1 Furthermore, let $a \in U$ satisfy

$$\begin{cases} f(a) = \inf(f(x) \mid x \in \mathbb{R}^n, g_k(x) = 0 \text{ (for } k \in E), g_k(x) \leq 0 \text{ (for } k \in I) \\ g_k(a) = 0 \text{ (for } k \in E) \\ g_k(a) \leq 0 \text{ (for } k \in I) \end{cases} \text{ also works again for } a \text{ being a local minimum}$$

Let I_a^0 be the set of constraints that are active in a. Assume that $(\nabla g_k(a))_{k \in E \cup I_a^0}$ are linearly independent.

Then there exist $(\lambda_k)_{1 \le k \le p}$ that satisfy

$$\begin{cases} \nabla f(a) + \sum_{k=1}^{p} \lambda_k \nabla g_k(a) = 0 \\ g_k(a) = 0 \text{ (for } k \in E) \\ g_k(a) \le 0 \text{ (for } k \in I) \\ \lambda_k \ge 0 \text{ (for } k \in I_a^0) \\ \lambda_k g_k(a) = 0 \text{ (for } k \in E \cup I) \end{cases}$$

Inequality Constraint: Karush-Kuhn-Tucker Theorem

Theorem (Karush-Kuhn-Tucker, KKT):

Let U be an open set of (E, || ||) and $f: U \to \mathbb{R}$, $g_k: U \to \mathbb{R}$, all \mathcal{C}^1 Furthermore, let $a \in U$ satisfy

$$\begin{cases} f(a) = \inf(f(x) \mid x \in \mathbb{R}^n, g_k(x) = 0 \text{ (for } k \in E), g_k(x) \leq 0 \text{ (for } k \in I) \\ g_k(a) = 0 \text{ (for } k \in E) \\ g_k(a) \leq 0 \text{ (for } k \in I) \end{cases}$$

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 $(\lambda_k)_{1 \le k \le p}$ that satisfy

$$\begin{cases} \nabla f(a) + \sum_{k=1}^{p} \lambda_k \nabla g_k(a) = 0 \\ g_k(a) = 0 \text{ (for } k \in E) \\ g_k(a) \le 0 \text{ (for } k \in I) \\ \lambda_k \ge 0 \text{ (for } k \in I_a^0) \\ \lambda_k g_k(a) = 0 \text{ (for } k \in E \cup I) \end{cases}$$

either active constraint or $\lambda_k = 0$

Descent Methods

Descent Methods

General principle

- choose an initial point x_0 , set t = 1
- while not happy
 - choose a descent direction $d_t \neq 0$
 - line search:
 - choose a step size $\sigma_t > 0$
 - set $x_{t+1} = x_t + \sigma_t d_t$
 - set t = t + 1

Remaining questions

- how to choose d_t ?
- how to choose σ_t ?

Gradient Descent

Rationale: $d_t = -\nabla f(x_t)$ is a descent direction indeed for f differentiable

$$f(x - \sigma \nabla f(x)) = f(x) - \sigma ||\nabla f(x)||^2 + o(\sigma ||\nabla f(x)||)$$

 $< f(x)$ for σ small enough

Step-size

- optimal step-size: $\sigma_t = \underset{\sigma}{\operatorname{argmin}} f(\mathbf{x}_t \sigma \nabla f(\mathbf{x}_t))$
- Line Search: total or partial optimization w.r.t. σ 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

see next slide and exercise

Stopping criteria:

norm of gradient smaller than ϵ

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 σ and reduces it until f is reduced enough
- what is enough?
 - assuming a linear f e.g. $m_k(x) = f(x_k) + \nabla f(x_k)^T (x x_k)$
 - expected decrease if step of σ_k is done in direction \boldsymbol{d} : $\sigma_k \nabla f(x_k)^T \boldsymbol{d}$
 - actual decrease: $f(x_k) f(x_k + \sigma_k d)$
 - stop if actual decrease is at least constant times expected decrease (constant typically chosen in [0, 1])

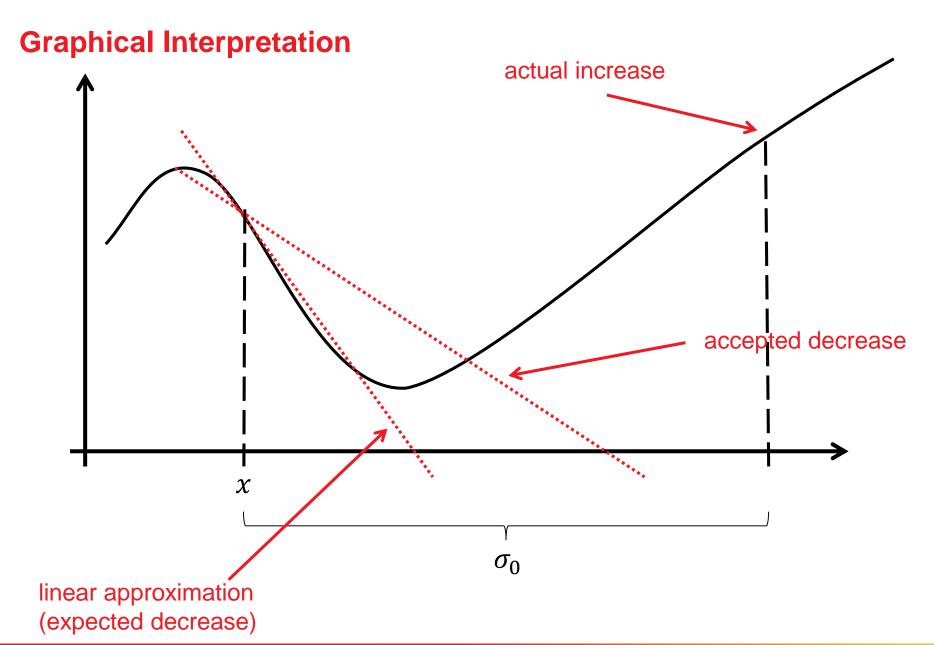
The Actual Algorithm:

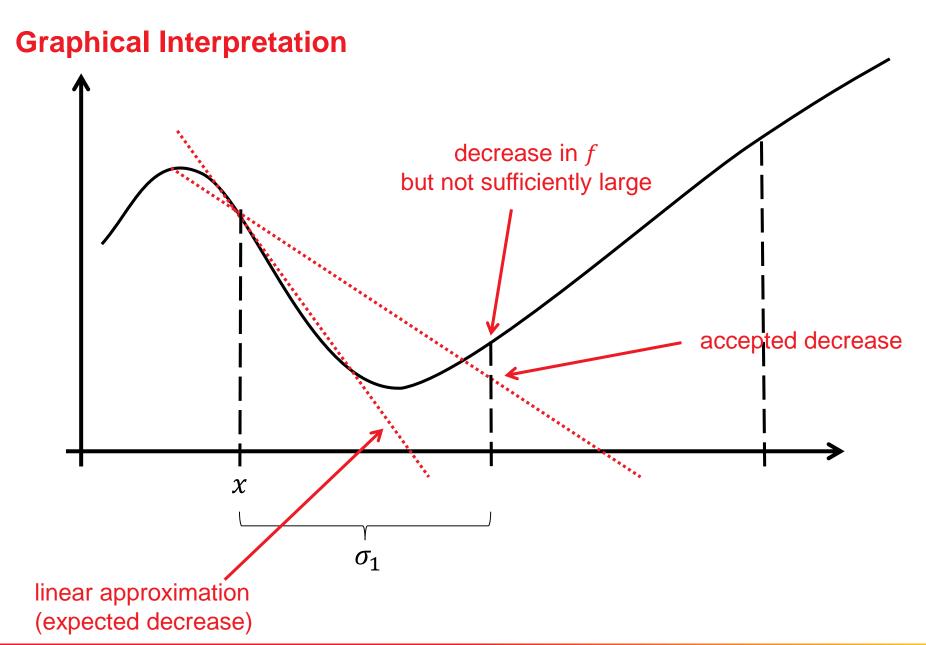
Input: descent direction **d**, point **x**, objective function $f(\mathbf{x})$ and its gradient $\nabla f(\mathbf{x})$, parameters $\sigma_0 = 10$, $\theta \in [0, 1]$ and $\beta \in (0, 1)$

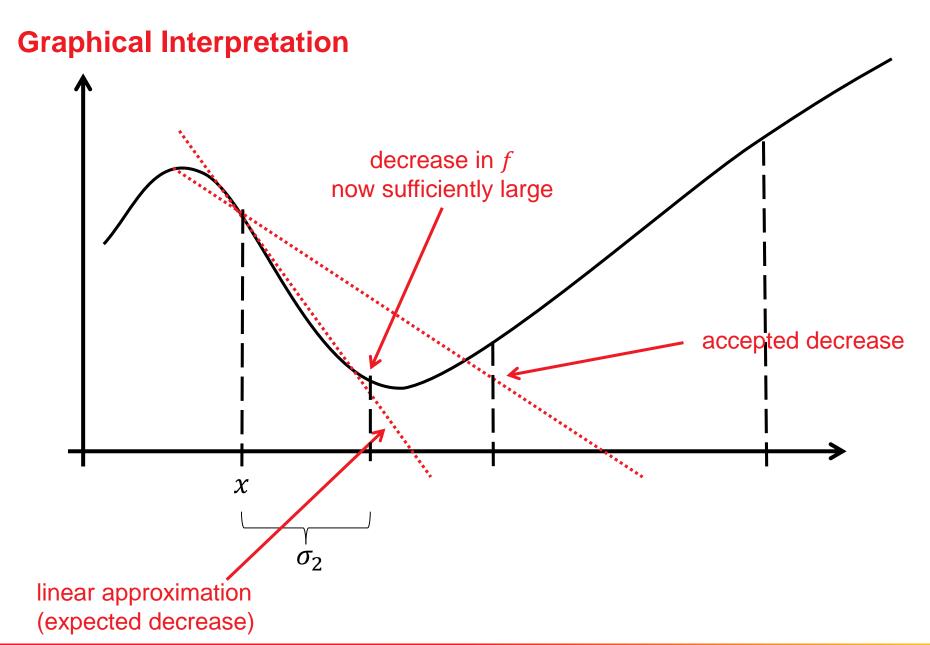
Output: step-size σ

Initialize σ : $\sigma \leftarrow \sigma_0$ 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.







Gradient Descent: Simple Theoretical Analysis

Assume f is twice continuously differentiable, convex and that $\mu I_d \leq \nabla^2 f(x) \leq L I_d$ with $\mu > 0$ holds, assume a fixed step-size $\sigma_t = \frac{1}{I}$

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

$$x_{t+1} - x^* = x_t - x^* - \sigma_t \nabla^2 f(y_t) (x_t - x^*) \text{ for some } y_t \in [x_t, x^*]$$

$$x_{t+1} - x^* = \left(I_d - \frac{1}{L} \nabla^2 f(y_t)\right) (x_t - x^*)$$
Hence $||x_{t+1} - x^*||^2 \le |||I_d - \frac{1}{L} \nabla^2 f(y_t)|||^2 ||x_t - x^*||^2$

$$\le \left(1 - \frac{\mu}{L}\right)^2 ||x_t - x^*||^2$$

Linear convergence:
$$||x_{t+1} - x^*|| \le (1 - \frac{\mu}{L})||x_t - x^*||$$

algorithm slower and slower with increasing condition number

Non-convex setting: convergence towards stationary point

Newton Algorithm

Newton Method

- descent direction: $-[\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$ [so-called Newton direction]
- The Newton direction:
 - minimizes the best (locally) quadratic approximation of f: $\tilde{f}(x + \Delta x) = f(x) + \nabla f(x)^T \Delta x + \frac{1}{2} (\Delta x)^T \nabla^2 f(x) \Delta x$
 - points towards the optimum on $f(x) = (x x^*)^T A(x x^*)$
- however, Hessian matrix is expensive to compute in general and its inversion is also not easy

quadratic convergence

(i.e.
$$\lim_{k\to\infty} \frac{|x_{k+1}-x^*|}{|x_k-x^*|^2} = \mu > 0$$
)

Remark: Affine Invariance

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

Newton method is affine invariant

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

Quasi-Newton Method: BFGS

 $x_{t+1} = x_t - \sigma_t H_t \nabla f(x_t)$ where H_t is an approximation of the inverse Hessian

Key idea of Quasi Newton:

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

$$q_t \approx \nabla^2 f(x_{t+1}) p_t$$
 where $p_t = x_{t+1} - x_t$ and $q_t = \nabla f(x_{t+1}) - \nabla f(x_t)$

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.