Introduction to Optimization

Introduction to Continuous Optimization III / Gradient-Based Algorithms

November 20, 2015

École Centrale Paris, Châtenay-Malabry, France

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	C	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	**C**	**Gradient-based Algorithms [+ finishing the intro]**
Fri, 27.11.2015	C	~~End of Gradient-based Algorithms + Linear Programming~~ *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

Remark on Last Lecture

Question: Is the Hessian matrix always symmetric?

Answer: No, but f having continuous second order partial derivatives is a sufficient condition for the Hessian to be symmetric ("Schwarz' theorem").

Remark on Last Lecture II

Question: How do we prove in general that the gradient is orthogonal to the level sets?

Answer:

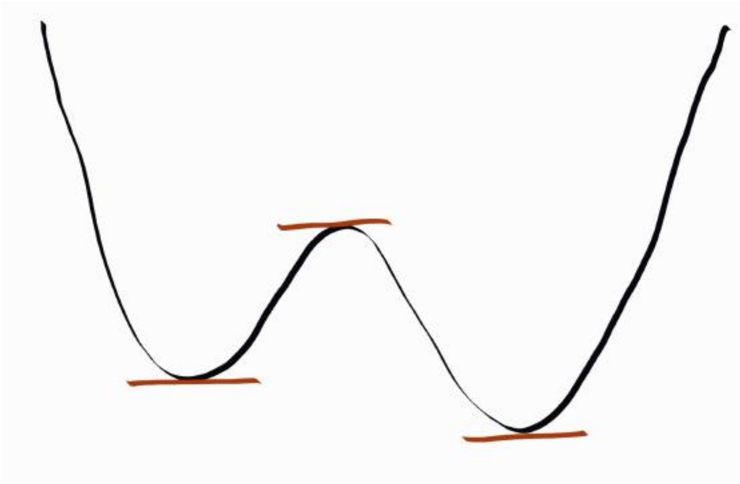
- similar to what we did for two variables
- take any curve within the level set, parametrized by $t \longmapsto c(t)$
- clear: $f(c(t)) = c$ for all t
- derivative wrt to t: $\frac{d}{dt} f\big(c(t)\big) = 0$
- but also $\frac{d}{dt} f(c(t)) = \nabla(f(c(t))\ \frac{d}{dt} c(t)$
  [via chain rule, $\frac{d}{dt} c(t)$ is a vector, tangent to the curve in t]

Mathematical Tools to Characterize Optima

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

Optimality Conditions for Unconstrained Problems

Optimality Conditions: First Order Necessary Cond.

For 1-dimensional optimization problems $\boldsymbol{f}: \mathbb{R} \to \mathbb{R}$

Assume f is differentiable

- $\boldsymbol{x}^*$ is a local optimum $\Longrightarrow f'(\boldsymbol{x}^*) = 0$

  not a sufficient condition: consider $f(\boldsymbol{x}) = \boldsymbol{x}^3$

  proof via Taylor formula: $f(\boldsymbol{x}^* + \boldsymbol{h}) = f(\boldsymbol{x}^*) + f'(\boldsymbol{x}^*)\boldsymbol{h} + o(||\boldsymbol{h}||)$

- points $\boldsymbol{y}$ such that $f'(\boldsymbol{y}) = 0$ are called critical or stationary points

Generalization to $\boldsymbol{n}$-dimensional functions

If $f: U \subset \mathbb{R}^n \longmapsto \mathbb{R}$ is differentiable

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

  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 $\nabla f(\boldsymbol{x}^*) = 0$ and $\nabla^2 f(\boldsymbol{x}^*)$ is positive semi-definite

proof via Taylor formula at order 2

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

Proof of Sufficient Condition:

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

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

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 $\boldsymbol{x}, \boldsymbol{y} \in U$ and for all $t \in [0,1]$

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

Theorem

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

$$f(\boldsymbol{y}) - f(\boldsymbol{x}) \geq \big(\nabla f(x)\big)^T(\boldsymbol{y} - \boldsymbol{x})$$

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 $\nabla^2 f(\boldsymbol{x})$ is positive semi-definite for all $\boldsymbol{x}$.

Examples of Convex Functions:

- $f(\boldsymbol{x}) = a^T\boldsymbol{x} + b$
- $f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x} + a^T\boldsymbol{x} + b$, A symmetric positive definite
- the negative of the entropy function (i.e. $f(\boldsymbol{x}) = \sum_{i=1}^{n} \boldsymbol{x}_i \ln(\boldsymbol{x}_i)$ for positive $\boldsymbol{x}$)

Exercise:

Let $f: U \to \mathbb{R}$ be a convex and differentiable function on a convex open U.
Show that if $\nabla f(\boldsymbol{x}^*) = 0$, then $\boldsymbol{x}^*$ is a global minimum of f

Why convexity? local minima are also global under convexity assumption.

Constrained Optimization

Objective:

Generalize the necessary condition of $\nabla f(x) = 0$ at the optima of 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 $f: U \to \mathbb{R}$, $g: U \to \mathbb{R}$ in $\mathcal{C}^1$.

Let $a \in E$ satisfy

$$\begin{cases} f(a) = \inf \{f(x) \mid x \in U, g(x) = 0\} \\ g(a) = 0 \end{cases}$$

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

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

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

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

Exercise:

Consider the problem

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

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

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

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

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

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

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

Inequality Constraints: Definitions

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

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

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

also works again for a being a local minimum

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

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

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

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

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

also works again for a being a local minimum

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

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

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

either active constraint or $\lambda_k = 0$

Descent Methods

Descent Methods

General principle

1. choose an initial point $\boldsymbol{x}_0$, 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 σ_t?

Gradient Descent

Rationale: $\boldsymbol{d}_t = -\nabla f(\boldsymbol{x}_t)$ is a descent direction

indeed for f differentiable

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

Step-size

- optimal step-size: $\sigma_t = \underset{\sigma}{\operatorname{argmin}} f(\boldsymbol{x}_t - \sigma\nabla f(\boldsymbol{x}_t))$
- **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

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 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: $f(x_k) - f(x_k + \sigma_k \boldsymbol{d})$
  - stop if actual decrease is at least constant times expected decrease (constant typically chosen in [0, 1])

The Armijo-Goldstein Rule

The Actual Algorithm:

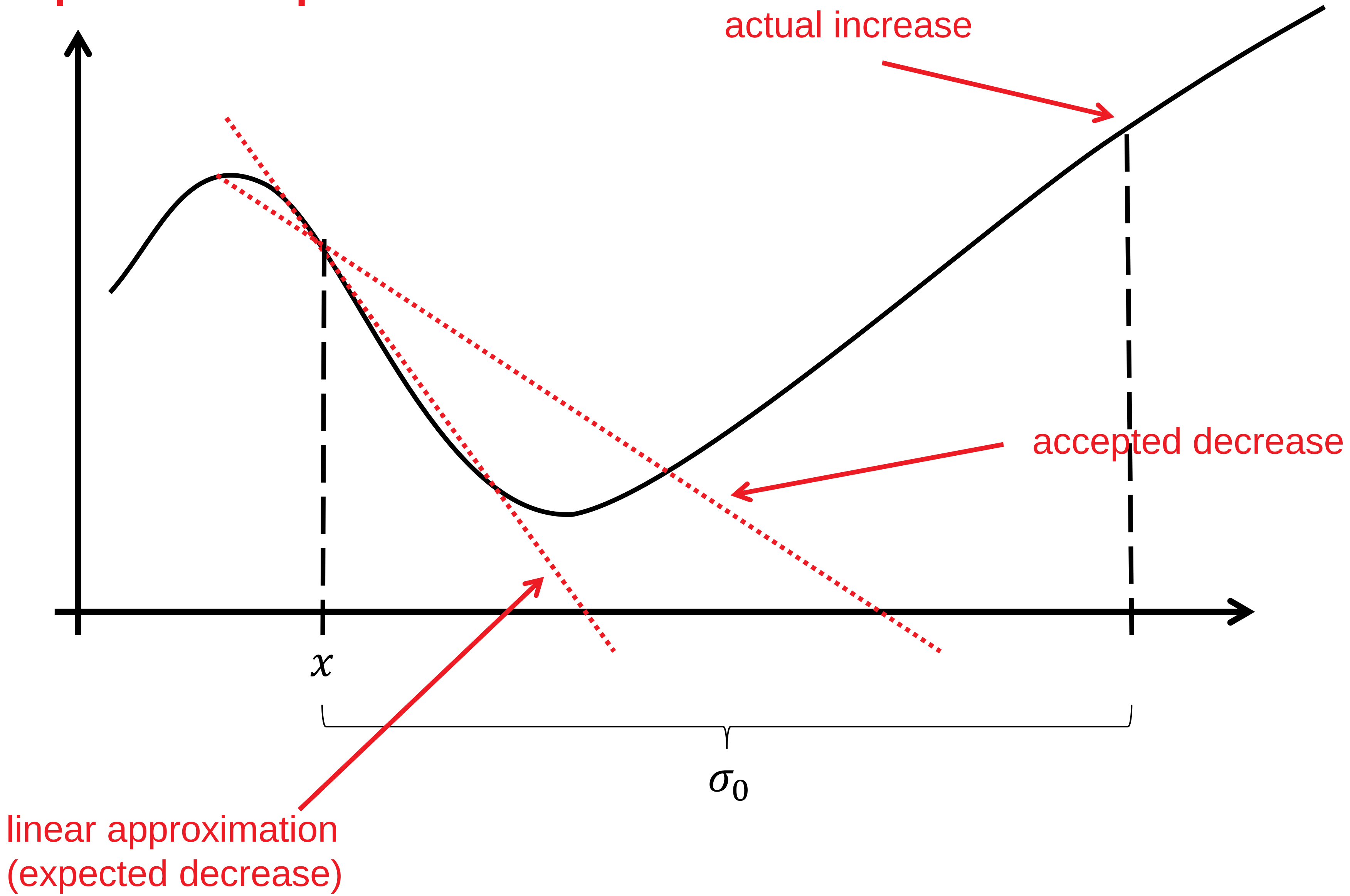
Input: descent direction $\mathbf{d}$, point $\mathbf{x}$, objective function $f(\mathbf{x})$ and its gradient $\nabla f(\mathbf{x})$, parameters $\sigma_0 = 10$, $\theta \in [0,1]$ and $\beta \in (0,1)$
Output: step-size σ

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

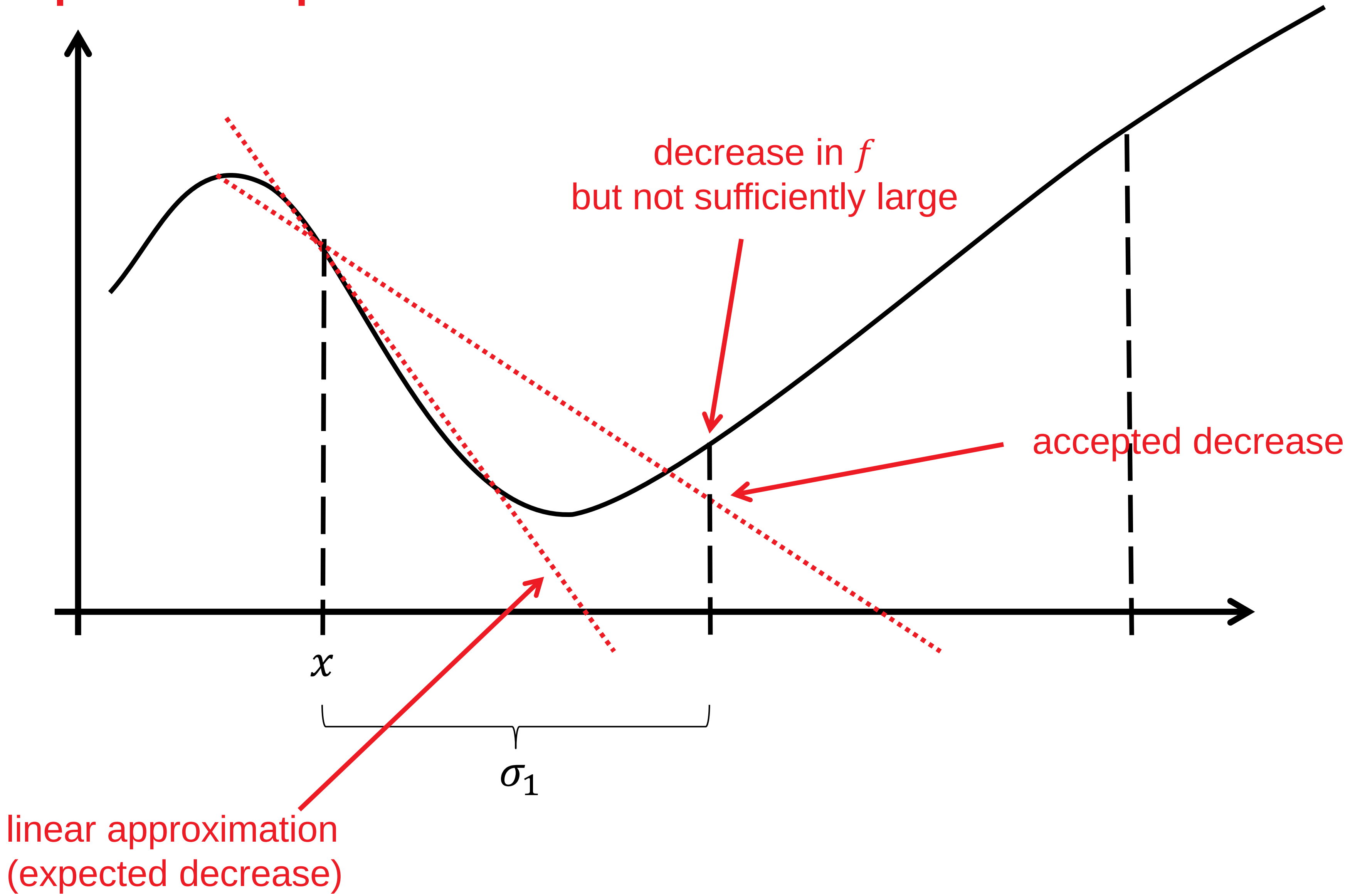
Armijo, in his original publication chose $\beta = \theta = 0.5$.

Choosing $\theta = 0$ means the algorithm accepts any decrease.

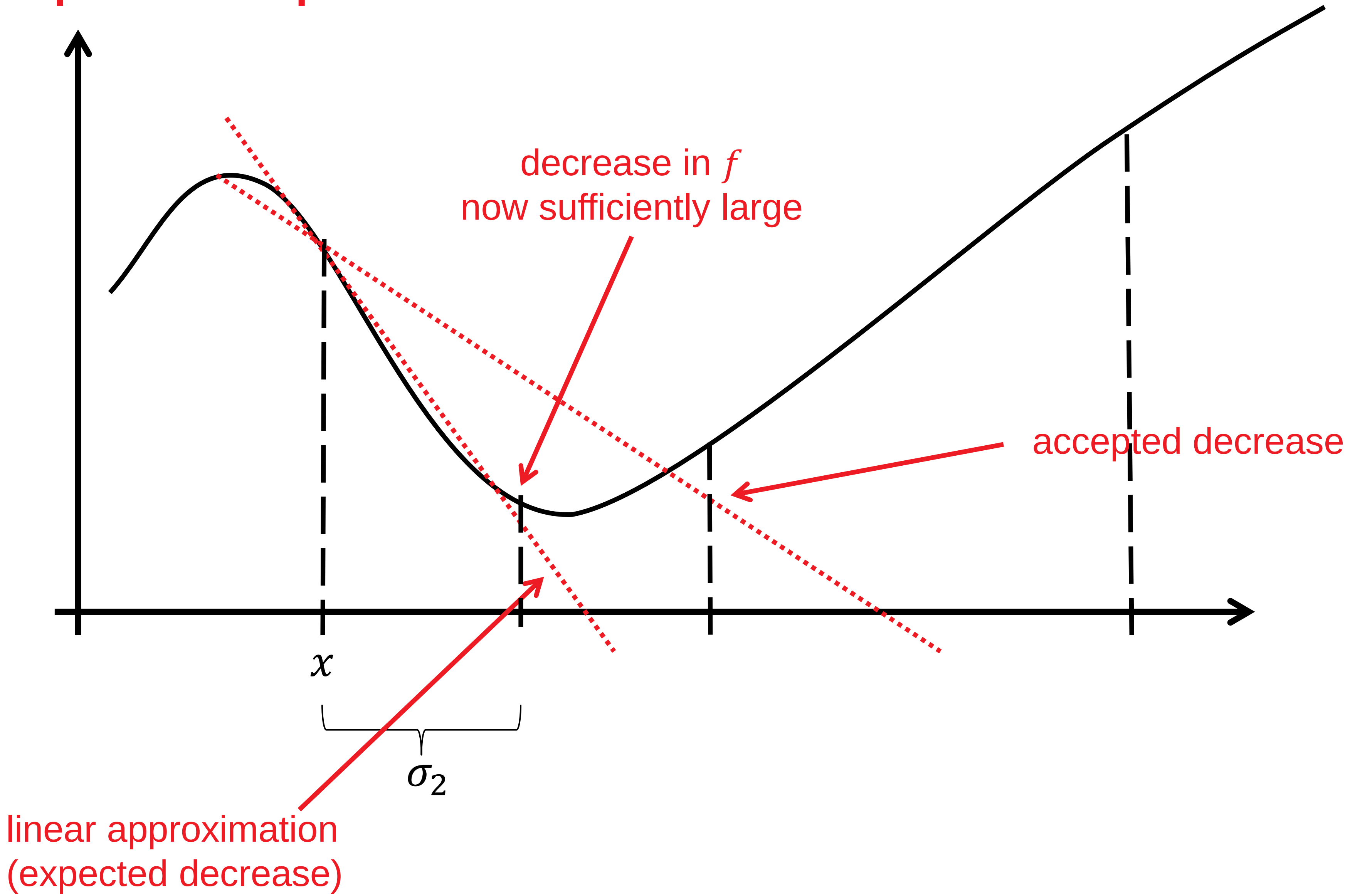
Graphical Interpretation



Graphical Interpretation



Graphical Interpretation



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: $A \preccurlyeq B$ 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 $||x_{t+1} - x^*||^2 \leq |||I_d - \frac{1}{L}\nabla^2 f(y_t)|||^2 \; ||x_t - x^*||^2$

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

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

algorithm slower and slower with increasing condition number

Non-convex setting: convergence towards stationary point

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

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

Remark: Affine Invariance

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

- 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

$x_{t+1} = x_t - \sigma_t H_t \nabla f(x_t)$ 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.