Nonsmooth Optimization: Bundle Methods

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Outline

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Nonsmooth Optimization and Application Areas

- In nonsmooth optimization (NSO) functions don't need to be differentiable
- The general problem is that we are minimizing functions that are typically not differentiable at their minimizers
- This type of problems arise in many fields of applications
  - Economics
  - Mechanics
  - Engineering
  - Computational chemistry and biology
  - Optimal control
  - Data mining

Cause of Nonsmoothness

- **Inherent**: Original phenomenon contains various discontinuities and irregularities.
- **Technological**: Caused by some extra technological constraints which may cause a nonsmooth dependence between variables and functions.
- **Methodological**: Some algorithms for constrained optimization may lead to a nonsmooth problem (for example, the exact penalty function method).
- **Numerical**: So called "stiff problems" which are analytically smooth but numerically unstable and behave like nonsmooth problems.

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Difficulties Caused by Nonsmoothness

The gradient does not exist at every point so we

- can't utilize the classical theory of optimization because it requires certain differentiability and strong regularity assumptions
- can't use smooth (gradient based) methods because they may lead failure in convergence, in optimality test or in gradient approximation
- have difficulties defining a descent direction

Nonsmooth Optimization Problem

General problem

Lets consider a nonsmooth optimization problem of the form

$$\begin{cases} \min & f(\boldsymbol{x}) \\ \text{s. t.} & \boldsymbol{x} \in X, \end{cases}$$

where

- Set $X \subseteq \mathbb{R}^n$ is a set of feasible solutions
- Objective function $f : \mathbb{R}^n \to \mathbb{R}$ is
  - not required to have continuous derivatives
  - supposed to be locally Lipschitz continuous on the set X

In the following the objective function f is assumed to be convex.

Convex Analysis

Definition 1

Let function $f : \mathbb{R}^n \to \mathbb{R}$ be convex. The *subdifferential* of f at $\boldsymbol{x} \in \mathbb{R}^n$ is a set

$$\partial f(\boldsymbol{x}) = \left\{\boldsymbol{\xi} \in \mathbb{R}^n \mid f(\boldsymbol{y}) \geq f(\boldsymbol{x}) + \boldsymbol{\xi}^T(\boldsymbol{y} - \boldsymbol{x}) \text{ for all } \boldsymbol{y} \in \mathbb{R}^n\right\}.$$

Each vector $\boldsymbol{\xi} \in \partial f(\boldsymbol{x})$ is called a *subgradient* of f at point $\boldsymbol{x}$.

The subdifferential $\partial f(\boldsymbol{x})$ is

- a nonempty, convex and compact set
- a generalization of a classical derivative because if $f : \mathbb{R}^n \to \mathbb{R}$ is convex and differentiable at $\boldsymbol{x} \in \mathbb{R}^n$, then $\partial f(\boldsymbol{x}) = \{\nabla f(\boldsymbol{x})\}$

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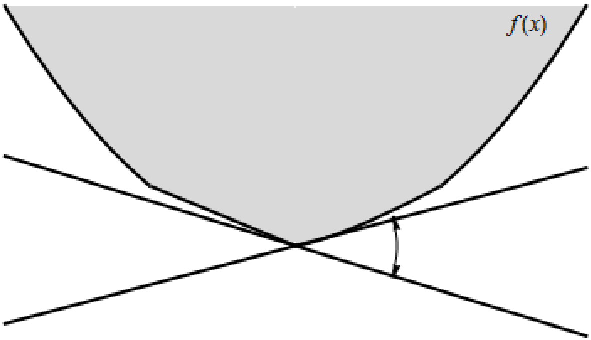
Convex Analysis



Subdifferential

Convex Analysis

Theorem 2

If $f : \mathbb{R}^n \to \mathbb{R}$ is convex then for all $\boldsymbol{y} \in \mathbb{R}^n$

$$f(\boldsymbol{y}) = \max\left\{ f(\boldsymbol{x}) + \boldsymbol{\xi}^T(\boldsymbol{y} - \boldsymbol{x}) \,|\, \boldsymbol{x} \in \mathbb{R}^n, \boldsymbol{\xi} \in \partial f(\boldsymbol{x}) \right\}.$$

Theorem 3

The direction $\boldsymbol{d} \in \mathbb{R}^n$ is a descent direction for a convex function $f : \mathbb{R}^n \to \mathbb{R}$ at $\boldsymbol{x} \in \mathbb{R}^n$ if

$$\boldsymbol{\xi}^T\boldsymbol{d} < 0 \text{ for all } \boldsymbol{\xi} \in \partial f(\boldsymbol{x}).$$

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Optimality Condition

For convex functions we have the following necessary and sufficient optimality condition:

Theorem 4

A convex function $f : \mathbb{R}^n \to \mathbb{R}$ attains its global minimum at point $\boldsymbol{x}$, if and only if

$$\mathbf{0} \in \partial f(\boldsymbol{x}).$$

Methods for Nonsmooth Optimization

The main problem: We usually don't know the whole subdifferential of the function but only one arbitrary subgradient at each point.

Different methods to solve a nonsmooth optimization problem

- Bundle Methods
- Derivative Free Methods
- Subgradient Methods
- Gradient Sampling Methods
- Hybrid Methods
- Special Methods

About Standard Bundle Method

- We consider an unconstrained convex nonsmooth problem

$$\begin{cases} \min & f(\boldsymbol{x}) \\ \text{s. t.} & \boldsymbol{x} \in \mathbb{R}^n \end{cases}$$

- Assumption: At every point $\boldsymbol{x} \in \mathbb{R}^n$ we can evaluate the value $f(\boldsymbol{x})$ and one arbitrary $\boldsymbol{\xi} \in \partial f(\boldsymbol{x})$
- Converges to the global minimum of f (if it exists)

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The main idea:

- Approximate the subdifferential of the objective function with a *bundle*
- Bundle consists of subgradients from previous iterations
- Subgradient information is used to construct a piecewise linear approximation to the objective function
- This approximation is used to determine a descent direction
- If approximation is not adequate then we add more information to the bundle

Bundle

- At iteration k in the current iteration point $\boldsymbol{x}_k$ our *bundle* is

$$\mathcal{B}_k = \{(\boldsymbol{y}_j, f(\boldsymbol{y}_j), \boldsymbol{\xi}_j) \mid j \in J_k\}.$$

  where
  - $\boldsymbol{y}_j \in \mathbb{R}^n$ is a trial point
  - $\boldsymbol{\xi}_j \in \partial f(\boldsymbol{y}_j)$ is a subgradient
  - J_k is a nonempty subset of $\{1, 2, \ldots, k\}$

- By using the bundle we can construct a *cutting plane model* which is a piecewise linear approximation of function f

Cutting Plane Model

- The cutting plane model is

$$\hat{f}_k(\boldsymbol{x}) = \max_{j \in J_k} \left\{ f(\boldsymbol{y}_j) + \boldsymbol{\xi}_j^T (\boldsymbol{x} - \boldsymbol{y}_j) \right\} \quad \text{for all } \boldsymbol{x} \in \mathbb{R}^n.$$

- It is a convex function and $\hat{f}_k(\boldsymbol{x}) \leq f(\boldsymbol{x})$.
- This approximation can be written in equivalent form

$$\hat{f}_k(\boldsymbol{x}) = \max_{j \in J_k} \left\{ f(\boldsymbol{x}_k) + \boldsymbol{\xi}_j^T (\boldsymbol{x} - \boldsymbol{x}_k) - \alpha_j^k \right\}$$

with the *linearization error*

$$\alpha_j^k = f(\boldsymbol{x}_k) - f(\boldsymbol{y}_j) - \boldsymbol{\xi}_j^T (\boldsymbol{x}_k - \boldsymbol{y}_j) \geq 0 \quad \text{for all } j \in J_k.$$

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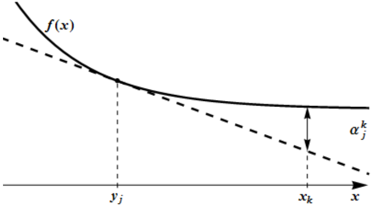
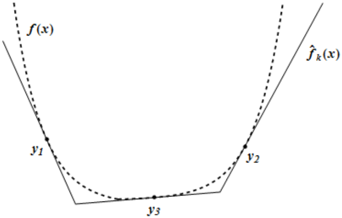
Cutting Plane Model



Linearization error



Cutting plane model

Algorithm: Direction Finding Problem

To determine the search direction $\boldsymbol{d}_k$ we need to solve

$$\min_{\boldsymbol{d}\in\mathbb{R}^n} \left\{ \hat{f}_k(\boldsymbol{x}_k + \boldsymbol{d}) + \frac{1}{2}\boldsymbol{d}^T \boldsymbol{M}_k \boldsymbol{d} \right\}$$

where

- $\boldsymbol{M}_k$ is a positive definite and symmetric $n \times n$ matrix.
- $\frac{1}{2}\boldsymbol{d}^T \boldsymbol{M}_k \boldsymbol{d}$ is a stabilizing term which
  - guarantees existence of the unique solution $\boldsymbol{d}_k$
  - keeps approximation local enough

The search direction $\boldsymbol{d}_k$ is also a descent direction to the original objective

Algorithm: Quadratic Direction Finding Problem

$$\min_{\boldsymbol{d}\in\mathbb{R}^n} \left\{ \max_{j\in J_k} \left\{ f(\boldsymbol{x}_k) + \boldsymbol{\xi}_j^T \boldsymbol{d} - \alpha_j^k \right\} + \frac{1}{2} \boldsymbol{d}^T \boldsymbol{M}_k \boldsymbol{d} \right\} \tag{1}$$

- The problem (1) can be rewritten as a *smooth quadratic direction finding problem*

$$\begin{cases} \min & v + \frac{1}{2} \boldsymbol{d}^T \boldsymbol{M}_k \boldsymbol{d} \\ \text{s. t.} & \boldsymbol{\xi}_j^T \boldsymbol{d} - \alpha_j^k \le v \quad \forall j \in J_k, \\ & v \in \mathbb{R},\ \boldsymbol{d} \in \mathbb{R}^n \end{cases} \tag{2}$$

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Algorithm: Search Direction and Stopping Condition

- The solution $(v_k, \boldsymbol{d}_k)$ of (2) can also be calculated from the dual problem
- The next iteration candidate is $\boldsymbol{y}_{k+1} = \boldsymbol{x}_k + \boldsymbol{d}_k$
- Value

$$v_k = \hat{f}_k(\boldsymbol{y}_{k+1}) - f(\boldsymbol{x}_k)$$

  is the predicted descent of f at $\boldsymbol{y}_{k+1}$
- If $v_k = 0$ then the current point $\boldsymbol{x}_k$ is the global minimum
- It is convenient to stop algorithm when $-v_k \leq \varepsilon$ where $\varepsilon > 0$ is a final accuracy tolerance

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Algorithm: Serious and Null Step

- Now we perform either a serious step or a null step
- A *serious step*

  $$\boldsymbol{x}_{k+1} = \boldsymbol{y}_{k+1}$$

  is performed if

  $$f(\boldsymbol{y}_{k+1}) - f(\boldsymbol{x}_k) \leq m v_k$$

  where $m \in (0, 1/2)$ is a line search parameter.
- Otherwise we make a *null step*

  $$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k$$

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Algorithm: Updating the Bundle

- In both steps we improve the approximation by adding

$$(\boldsymbol{y}_{k+1}, f(\boldsymbol{y}_{k+1}), \boldsymbol{\xi}_{k+1})$$

  into the bundle where $\boldsymbol{\xi}_{k+1} \in \partial f(\boldsymbol{y}_{k+1})$
- Easiest way to do this is to set $J_{k+1} = J_k \cup \{k+1\}$
  - stores all subgradients
  - causes difficulties with storage and computation
- By using *the subgradient aggregation strategy* we can keep the size of the bundle bounded

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Nonconvex Bundle Methods

- Objective function is only supposed to be locally Lipschitz continuous
- Cannot guarantee even local optimality of a solution without some convexity assumption
- Not as efficient methods as convex bundle methods
- Best nonconvex bundle methods are generalizations of convex bundle methods with suitable modifications
- Not developed from the nonconvex perspective

Difference of two Convex functions

Definition 5

A function $f : \mathbb{R}^n \to \mathbb{R}$ is called a *DC function* if it can be written in the form

$$f(\boldsymbol{x}) = f_1(\boldsymbol{x}) - f_2(\boldsymbol{x})$$

where f_1 and f_2 are convex functions on $\mathbb{R}^n$.

- If a DC function f is nonsmooth then at least one of the functions f_1 and f_2 is nonsmooth
- For DC functions it is still possible to utilize convex analysis and convex optimization theory to some extent
- Many problems of nonconvex optimization can be described by using DC functions

Future Work

Only a few efficient nonconvex nonsmooth optimization methods exist so my goal is

- Develop a local bundle method for unconstrained nonconvex nonsmooth problems where the objective is a DC function
- Add good features of gradient sampling methods to possibly get a better method
- Extend the method to constrained case
- Modify the local method so that we get a global solution both in unconstrained and constrained case

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Thank you for your attention!