Algorithms for nonlinear programming problems I

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Computational Aspects of Optimization

Algorithm classification

- **Order of derivatives[1]:** derivative-free, first order (gradient), second-order (Newton)
- **Feasibility of the constructed points**: interior and exterior point methods
- **Deterministic/randomized**
- **Local**/global

[1] If possible, deliver the derivatives.

Content

Unconstrained problems

Let $f : \mathbb{R}^n \to \mathbb{R}$, x^0 be a starting point, $d^k \in \mathbb{R}^n$ be a **descent direction**, and $\lambda \in \mathbb{R}$ be a **step length**.

Find a **descent direction** d^k, solve the **line search problem**

$$\lambda^k = \arg \min_{0 \le \lambda \le \lambda_{max}} f(x^k + \lambda d^k)$$

and set

$$x^{k+1} = x^k + \lambda^k d^k.$$

Iterate until a convergence criterion is not satisfied, e.g. $\left\| d^k \right\| < \varepsilon$ or $|f(x^k) - f(x^{k+1})| < \varepsilon$.

Review of line search methods

Bazaraa et al. (2006):

- Derivative-free: dichotomous search, golden section method, Fibonacci search
- Using derivatives: bisection search, Newton's method

Descent directions – Steepest descent

A vector d is called a descent direction of a function f at x if there exists a $\delta > 0$ such that

$$f(x + \lambda d) < f(x),\ \lambda \in (0, \delta).$$

Steepest descent d with $\|d\| = 1$ minimizes the limit

$$f'(x; d) := \lim_{\lambda \to 0_+} \frac{f(x + \lambda d) - f(x)}{\lambda} < 0.$$

If f is differentiable at x with a nonzero gradient, then

$$d = -\frac{\nabla f(x)}{\|\nabla f(x)\|}$$

leading to the gradient (Cauchy) method.

$$f'(x; d) = \nabla f(x)^T d.$$

Descent directions

If we set

$$h(\lambda) := f(x + \lambda d),$$

then

$$h'(0) = \nabla f(x)^T d.$$

h is decreasing $\Leftrightarrow$ f is decreasing in direction d.

Descent directions

Steepest descent – works well during the early steps, the **zigzagging** phenomenon often appears in later steps, see Bazaraa et al. (2006), Example 8.6.2

Descent directions – Newton direction

Approximation of f by a limited Taylor expansion around x^k

$$g(x) := f(x^k) + \nabla f(x^k)^T (x - x^k) + \frac{1}{2}(x - x^k)^T \nabla^2 f(x^k)(x - x^k)$$

Setting $\nabla_x g(x) = 0$, we obtain the **Newton direction**

$$d = -\left(\nabla^2 f(x^k)\right)^{-1} \nabla f(x^k).$$

If $\nabla^2 f(x^k) > 0$, then d is a descent direction[2].

[2] In general, $d = -A\nabla f(x^k)$ for $A > 0$ is a descent direction → **Quasi-Newton methods**.

Descent directions – Newton direction

Convergence of the algorithm: Bazaraa et al. (2006), Theorem 8.6.5 ($f \in C^2$, $\nabla f(\overline{x}) = 0$ and $\nabla^2 f(\overline{x}) > 0$ at a local minimum $\overline{x}$, starting point is sufficiently close.)

Descent directions – Example

$$\min_{x,y} (x-y)^4 + 2x^2 + y^2 - x + 2y$$

Partial derivatives

$$\begin{aligned} \frac{\partial f(x,y)}{\partial x} &= 4(x-y)^3 + 4x - 1 = 0, \\ \frac{\partial f(x,y)}{\partial y} &= -4(x-y)^3 + 2y + 2 = 0. \end{aligned} \tag{1}$$

Second-order partial derivatives

$$\begin{aligned} \frac{\partial^2 f(x,y)}{\partial x^2} &= 12(x-y)^2 + 4, \\ \frac{\partial^2 f(x,y)}{\partial x \partial y} &= -12(x-y)^2, \\ \frac{\partial^2 f(x,y)}{\partial y^2} &= 12(x-y)^2 + 2. \end{aligned} \tag{2}$$

Compare directions $d^{SD} = \nabla f(x)$ and $d^{Newton} = -\left(\nabla^2 f(x)\right)^{-1} \nabla f(x)$ ...

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Algorithm convergence

Definition

Let $X \subseteq \mathbb{R}^p$, $Y \subseteq \mathbb{R}^q$ be nonempty closed sets. Let $F : X \to Y$ be a set-valued mapping. The map F is said to be **closed** at $x \in X$ if for any sequences $\{x^k\} \subset X$, and $\{y^k\}$ satisfying $x_k \to x$, $y^k \in F(x^k)$, $y^k \to y$ we have that $y \in F(x)$.
The map F is said to be closed on $Z \subseteq X$ if it is closed at each point in Z.

Algorithm convergence – Zangwill's theorem

Bazaraa et al. (2006), Theorem 7.2.3: Let

A1. $X \subseteq \mathbb{R}^p$ be a nonempty **closed** set,

A2. $\hat{X} \subseteq X$ be a **nonempty solution set**,

A3. $F : X \to X$ be a set-valued mapping **closed** over complement of $\hat{X}$,

A4. Given $x^1 \in X$ the sequence $\{x^k\}$ is generated iteratively as follows: If $x^k \in \hat{X}$, then STOP; otherwise, let $x^{k+1} \in F(x^k)$ and repeat,

A5. the sequence $x^1, x^2, \ldots$ be contained in a **compact** subset of X,

A6. there exist a **continuous function**[3] α such that $\alpha(y) < \alpha(x)$ if $x \notin \hat{X}$ and $y \in F(x)$.

Then either the algorithm stops in a finite number of steps with a point in $\hat{X}$ or it generates an infinite sequence $\{x^k\}$ such that all accumulation points belong to $\hat{X}$ and $\alpha(x^k) \to \alpha(x)$ for some $x \in \hat{X}$.

[3] descent function: $\alpha(x) = f(x)$ or $\alpha(x) = \|\nabla f(x)\|$

Algorithm convergence – Newton method

Let $\overline{x}$ be an optimal solution, set

$$\begin{aligned} F(x) &= x - \left(\nabla^2 f(x)\right)^{-1} \nabla f(x), \\ \alpha(x) &= \|x - \overline{x}\| . \end{aligned}$$

More details: Bazaraa et al. (2006), Theorem 8.6.5

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Method of Zoutendijk

Bazaraa et al. (2006), Section 10.1: $f : \mathbb{R}^n \to \mathbb{R}$, $g_j : \mathbb{R}^n \to \mathbb{R}$ **differentiable**

$$\min_x f(x) \text{ s.t. } g_j(x) \le 0,\ j = 1, \dots, m.$$

(Extension including equality constraints is possible.)

Method based on **improving feasible directions** (remember the "directional" optimality conditions).

Method of Zoutendijk

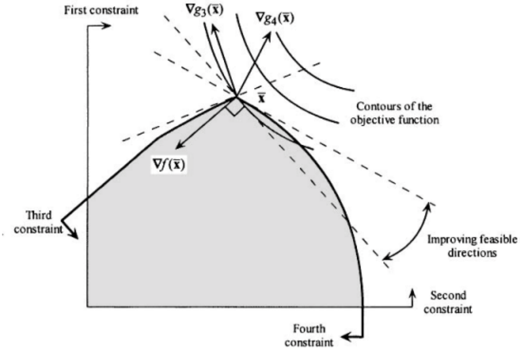
0. Start with a **feasible** x^1. For $k = 1, \dots (, K_{max})$ do
1. Set $J(x^k) = \{j : g_j(x^k) = 0\}$ and solve **linear programming problem for finding a direction**:

$$\begin{aligned} \min_{z,d} \; & z \\ \text{s.t. } & \nabla f(x^k)^T d \le z, \\ & \nabla g_j(x^k)^T d \le z, \; j \in J(x^k), \\ & -1 \le d_i \le 1, \; i = 1, \dots, n. \end{aligned}$$

Denote by $(z^k, d^k) \in \mathbb{R}^{1+n}$ the optimal solution.

- If $z^k = 0$ then STOP (We have found a Fritz-John point).
- Else if $z^k < 0$ then continue with STEP 2.

Method of Zoutendijk



Bazaraa et al. (2006)

Method of Zoutendijk

2. Find **maximal possible step**

$$\lambda_{max} := \sup\{\lambda : \ g_j(x^k + \lambda d^k) \leq 0, j = 1, \dots, m\},$$

solve the **line search problem**

$$\lambda^k = \arg \min_{0 \leq \lambda \leq \lambda_{max}} f(x^k + \lambda d^k)$$

and set

$$x^{k+1} = x^k + \lambda^k d^k.$$

Continue with STEP 1.

Method of Zoutendijk

Where could be a problem? Direction as well as line search mappings need not to be closed...

Convergence: Bazaraa et al. (2006), part 10.2.

Method of Zoutendijk – example

Bazaraa et al. (2006), Example 10.1.8

$$\begin{aligned} \min\ & 2x_1^2 + 2x_2^2 - 2x_1x_2 - 4x_1 - 6x_2 \\ \text{s.t. }\ & x_1 + x_2 \le 5, \\ & 2x_1^2 - x_2 \le 0, \\ & -x_1 \le 0, \\ & -x_2 \le 0. \end{aligned} \tag{3}$$

$$\nabla f(x) = (4x_1 - 2x_2 - 4,\ 4x_2 - 2x_1 - 6)^T \tag{4}$$

Method of Zoutendijk – Example

Starting point $x^0 = (0, 0.75)^T$, $\nabla f(x^0) = (-5.5, -3)^T$, $J(x^0) = \{3\}$. The direction finding problem is then

$$\begin{aligned} & \min \ z \\ & \text{s.t.} \ -5.5 d_1 - 3 d_2 \leq z, \\ & \quad -d_1 \leq z, \\ & \quad -1 \leq d_1, d_2 \leq 1. \end{aligned} \tag{5}$$

with optimal solution $d^1 = (1, -1)$, $z^1 = -1$.

Method of Zoutendijk – Example

Then

$$x^0 + \lambda d^1 = (\lambda,\ 0.75 - \lambda)$$

and

$$f(x^0 + \lambda d^1) = 6\lambda^2 - 2.5\lambda - 3.375.$$

Maximize it over the set of feasible solutions M to obtain $\lambda_{max} = 0.4114$. Finally

$$\begin{aligned} &\min\ 6\lambda^2 - 2.5\lambda - 3.375 \\ &\text{s.t. } 0 \le \lambda \le \lambda_{max}. \end{aligned} \tag{6}$$

$\lambda^1 = 0.2083.$

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Cutting plane method

$f : \mathbb{R}^n \to \mathbb{R}$, $g_j : \mathbb{R}^n \to \mathbb{R}$

$$\min_x f(x) \text{ s.t. } g_j(x) \leq 0, \; j = 1, \dots, m.$$

Denote $M = \{x \in \mathbb{R} : \; g_j(x) \leq 0, \; j = 1, \dots, m\}$.

ASS. f is affine, g are convex and differentiable, M is compact.

Cutting plane method

0. Start with a polyhedral set M^0 such that $M \subset M^0$, e.g. a box $M^0 = [lb_1, ub_1] \times \cdots \times [lb_m, ub_m]$. For $k = 0, \ldots (, K_{max})$ do
1. Solve the **linear programming problem**

$$\min_x f(x) \text{ s.t. } x \in M^k,$$

and obtain $x^k \in M^k$. If $x^k \in M$, then STOP, we have found an optimal solution. Otherwise continue with STEP 2.

2. If $x^k \notin M$, then find $j^k = \arg\max_j g_j(x^k)$, construct a **cutting plane** and set

$$M^{k+1} = M^k \cap \left\{ x \in \mathbb{R} : \ g_{j^k}(x^k) + \nabla g_{j^k}(x^k)^T (x - x^k) \leq 0 \right\}.$$

Note that x^k violates the cut, and no $x \in M$ is cut off[4] (compare with the integer programming cuts). Return to STEP 1.

[4] From convexity $g_{j^k}(x^k) + \nabla g_{j^k}(x^k)^T (x - x^k) \leq g_{j^k}(x) \leq 0$.

Cutting plane method – Example

$$\min_x \; -x_1 - x_2$$
$$\text{s.t. } x_1^2 + x_2^2 - 1 \le 0,$$
$$x_1, x_2 \ge 0.$$

Set $M = \{(x_1, x_2) : \; x_1^2 + x_2^2 - 1 \le 0, x_1, x_2 \ge 0\}$, $\nabla g(x)^T = (2x_1, 2x_2)$.

Cutting plane method – Example

0. Set $M^0 = [0,1]^2$.
1. Solve $\min_x -x_1 - x_2$ s.t. $x \in M^0$ with optimal solution $x^0 = (1,1)^T$.
2. Since $x^0 \notin M$, construct the cut

$$g(x^0) + \nabla g(x^0)^T (x - x^0) \le 0,$$

and set

$$M^1 = M^0 \cap \{(x_1, x_2) :\ x_1 + x_2 \le 3/2\}.$$

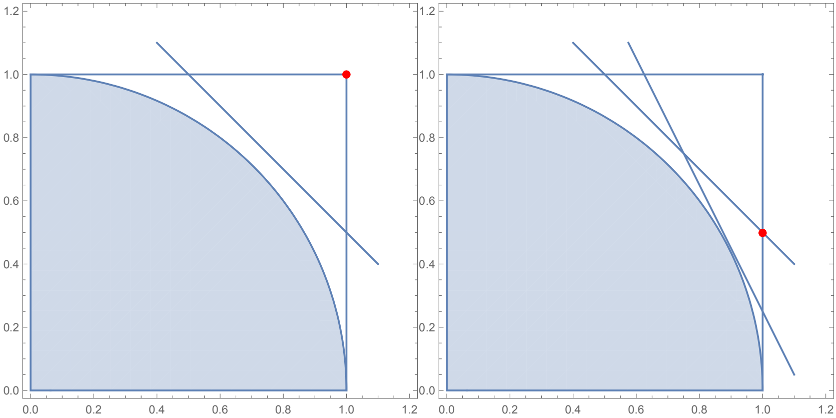
Continue with STEP 1.

Cutting plane method – Example

$x^1 = (1, 0.5)^T$, $x^1 \notin M$,

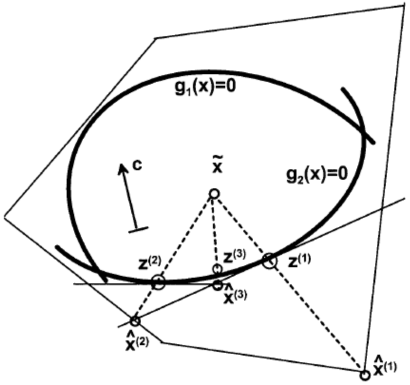
$$M^2 = M^1 \cap \{(x_1, x_2) : \; 2x_1 + x_2 \leq 9/4\}.$$

Cutting plane method



Cutting plane method

Algorithm with projection ...



Kall and Mayer (2005).

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Penalty method

Perfect penalty (rather theoretical)

$$PP(x) = \begin{cases} 0 & \text{if } g(x) \leq 0, h(x) = 0, \\ \infty & \text{otherwise.} \end{cases}$$

Compare with the Lagrangian duality (sup over multipliers).

The following problem is equivalent to the original constrained one.

$$\min_x f(x) + PP(x).$$

Penalty method

$L_{p,q}-$ **penalty function**, $p,q \in \{1,2,\dots\}$:

$$PF_N(x) = N \cdot \left(\sum_{j=1}^{m} [g_j(x)]_+^p + \sum_{i=1}^{l} |h_i(x)|^q \right),$$

where $N > 0$ is the penalty parameter, $[\cdot]_+ = \max\{\cdot, 0\}$.

More general penalty using $\Phi(y) = 0$ for $y \leq 0$ and $\Phi(y) > 0$ for $y > 0$ and $\Psi(y) = 0$ for $y = 0$ and $\Psi(y) > 0$ for $y \neq 0$.

Penalty method

Algorithm:

0. Set $\varepsilon > 0$, $N^1 > 0$, $\beta > 1$. For $k = 1, \ldots (, K_{max})$ do:
1. Solve
$$\min_x f(x) + PF_{N^k}(x).$$
and obtain x^k
2. IF $PF_{N^k}(x^k) < \varepsilon$, then STOP. ELSE set $N^{k+1} = N^k \cdot \beta$ and continue with STEP 1.

Exterior point method.

Penalty method

Convergence of the method: Bazaraa et al. (2006), Theorem 9.2.2 (continuous f, g_j, h_i, $x_k \in X \cap U$ compact).

Penalty functions – Example

Consider

$$\begin{aligned} \min\ & x_1^2 + x_2^2 \\ \text{s.t.}\ & x_1 + x_2 = 2. \end{aligned}$$

with optimal solution $\hat{x}_1 = \hat{x}_2 = 1$. Penalty function problem

$$\min x_1^2 + x_2^2 + N(x_1 + x_2 - 2)^2.$$

Using optimality conditions

$$\hat{x}_1^N = \hat{x}_2^N = \frac{2N}{2N+1}.$$

Penalty method

Remarks

- **Sequential Unconstrained Minimization** (SUMT): optimal solution x^k is used as a starting point in the next iteration[5] to solve the penalty problem with N_{k+1}.
- **Exact penalty**: Instead of $N \to \infty$ it is sufficient to converge $N \to \overline{N} < \infty$ (numerically more stable).

[5] "warm starting"

Content

Augmented Lagrangian Method

Nocedal and Wright (2006), Section 17.3: $f : \mathbb{R}^n \to \mathbb{R}$, $h_i : \mathbb{R}^n \to \mathbb{R}$ **differentiable**

$$\min_x \ f(x)$$
$$\text{s.t. } h_i(x) = 0, \ i = 1, \dots, l.$$

(Extension including inequality constraints is possible.)

$$L(x, v) = f(x) - \sum_{i=1}^{l} v_i h_i(x).$$

Augmented Lagrangian Method

Augmented Lagrangian function – combination of the **Lagrangian function** with the **quadratic penalty term**

$$L_A(x, \lambda, \mu) = f(x) - \sum_{i=1}^{l} \lambda_i h_i(x) + \frac{\mu}{2} \sum_{i=1}^{l} (h_i(x))^2 .$$

$$\begin{aligned} \nabla_x L_A(x, \lambda, \mu) &= \nabla_x f(x) - \sum_{i=1}^{l} \lambda_i \nabla_x h_i(x) + \mu \sum_{i=1}^{l} h_i(x) \nabla_x h_i(x) \\ &= \nabla_x f(x) - \sum_{i=1}^{l} \left(\lambda_i - \mu h_i(x)\right) \nabla_x h_i(x). \end{aligned}$$

We have that $v_i \approx \lambda_i - \mu h_i(x)$.

Augmented Lagrangian Method

0. Set initial $\mu^1 > 0$, $\beta > 1$ and λ^1. Select a tolerance $\varepsilon > 0$. For $k = 1, \dots (, K_{max})$ do:
1. Solve unconstrained problem
$$\min_x L_A(x, \lambda^k, \mu^k)$$
and obtain x^k. If $\left\| \nabla_x L_A(x^k, \lambda^k, \mu^k) \right\| \leq \varepsilon$, STOP. Otherwise continue with STEP 2.
2. Update the Lagrange multipliers $\lambda_i^{k+1} = \lambda_i^k - \mu^k h_i(x^k)$ and the penalty parameter $\mu^{k+1} = \beta \mu^k$. Go to STEP 1.

Augmented Lagrangian Method

Convergence of the algorithm: Nocedal and Wright (2006), Theorem 17.5 (LICQ, SOSC).

Literature

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