Algorithms for nonlinear programming problems II

Martin Branda

Charles University
Faculty of Mathematics and Physics
Department of Probability and Mathematical Statistics

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.

Barrier method

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

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

(Extension including equality constraints is straightforward.)

Assumption

$$\{x : \ g(x) < 0\} \neq \emptyset.$$

Barrier method

Barrier functions: continuous with the following properties

$$B(y) \ge 0, y < 0,\ \lim_{y \to 0_-} B(y) = \infty.$$

Examples

$$\frac{-1}{y},\ -\log \min\{1, -y\}.$$

Maybe the most popular barrier function:

$$B(y) = -\log -y$$

Set

$$\tilde{B}(x) = \sum_{j=1}^m B\big(g_j(x)\big),$$

and solve

$$\min f(x) + \mu \tilde{B}(x), \tag{1}$$

where $\mu > 0$ is a parameter.

Interior point methods

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

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

(Extension including equality constraints is straightforward.)

New slack decision variables $s \in \mathbb{R}^m$

$$\begin{aligned} &\min_{x,s}\ f(x) \\ &\text{s.t. } g_j(x) + s_j = 0,\ j = 1, \dots, m, \\ &\quad s_j \ge 0. \end{aligned} \tag{2}$$

Interior point methods

Barrier problem

$$\begin{aligned} &\min_{x,s}\ f(x) - \mu \sum_{j=1}^{m} \log s_j \\ &\text{s.t. } g(x) + s = 0. \end{aligned} \tag{3}$$

The barrier term prevents the components of s from becoming too close to zero.

Lagrangian function

$$L(x, s, z) = f(x) - \mu \sum_{j=1}^{m} \log s_j - \sum_{j=1}^{m} z_j (g_j(x) + s_j).$$

Interior point methods

KKT conditions for barrier problem (matrix notation)

$$\begin{aligned} \nabla f(x) - \nabla g^T(x) z &= 0, \\ -\mu S^{-1} e - z &= 0, \\ g(x) + s &= 0, \end{aligned}$$

$S = \text{diag}\{s_1, \dots, s_m\}$, $Z = \text{diag}\{z_1, \dots, z_m\}$, $\nabla g(x)$ is the Jacobian matrix (components of function in rows?)

Multiply the second equality by S

$$\begin{aligned} \nabla f(x) - \nabla g^T(x) z &= 0, \\ -SZe &= \mu e, \\ g(x) + s &= 0, \end{aligned}$$

= Nonlinear system of equalities $\to$ Newton's method

Newton's method

$$\nabla f(x + v) = \nabla f(x) + \nabla^2 f(x) v = 0$$

with the solution (under $\nabla^2 f(x) \succ 0$)

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

Interior point methods

Use Newton's method to obtain a step $(\Delta x, \Delta s, \Delta z)$

$$\begin{pmatrix} H(x,z) & 0 & -\nabla g^T \\ 0 & -Z & -S \\ \nabla g & I & 0 \end{pmatrix} \begin{pmatrix} \Delta x \\ \Delta s \\ \Delta z \end{pmatrix} = \begin{pmatrix} -\nabla f(x) + \nabla g^T(x) z \\ SZe + \mu e \\ -g(x) - s \end{pmatrix}$$

$H(x,z) = \nabla^2 f(x) - \sum_{j=1}^m z_j \nabla^2 g_j(x)$, $\nabla^2 f$ denotes the Hessian matrix.

Interior point methods

Stopping criterion:

$$E = \max \left\{ \left\| \nabla f(x) - \nabla g^T(x) z \right\|, \|SZe + \mu e\|, \|g(x) + s\| \right\} \le \varepsilon,$$

$\varepsilon > 0$ small.

Interior point methods

ALGORITHM:

0. Choose x^0 and $s^0 > 0$, and compute initial values for the multipliers $z^0 > 0$. Select an initial barrier parameter $\mu^0 > 0$ and parameter $\sigma \in (0,1)$, set $k = 1$.
1. Repeat until a stopping criterion for the nonlinear program is satisfied:
   - Solve the nonlinear system of equalities using Newton's method and obtain (x^k, s^k, z^k).
   - Decrease barrier parameter $\mu^{k+1} = \sigma \mu^k$, set $k = k + 1$.

Interior point methods

Convergence of the method (Nocedal and Wright 2006, Theorem 19.1): continuously differentiable f, g_j, LICQ at any limit point, then the limits are stationary points of the original problem

Interior point method – Example

$$\min_{x} \ (x_1-2)^4+(x_1-2x_2)^2 \quad \text{s.t. } x_1^2-x_2\le 0. \tag{4}$$

$$\min_{x,s} \ (x_1-2)^4+(x_1-2x_2)^2 \quad \text{s.t. } x_1^2-x_2+s=0,\ s\ge 0. \tag{5}$$

$$\min_{x,s} \ (x_1-2)^4+(x_1-2x_2)^2-\mu\log s \quad \text{s.t. } x_1^2-x_2+s=0. \tag{6}$$

Interior point method – Example

Lagrange function

$$L(x_1,x_2,s,z)=(x_1-2)^4+(x_1-2x_2)^2-\mu\log s-z(x_1^2-x_2+s).$$

Optimality conditions together with feasibility

$$\begin{aligned}\frac{\partial L}{\partial x_1}&=4(x_1-2)^3+2(x_1-2x_2)-2zx_1=0,\\ \frac{\partial L}{\partial x_2}&=-4(x_1-2x_2)+z=0,\\ \frac{\partial L}{\partial s}&=-\frac{\mu}{s}-z=0,\\ \frac{\partial L}{\partial z}&=x_1^2-x_2+s=0.\end{aligned} \tag{7}$$

We have obtained 4 equations with 4 variables ...

Interior point method – Example

Slight modification

$$4(x_1-2)^3+2(x_1-2x_2)-2zx_1 = 0, \tag{8}$$
$$-4(x_1-2x_2)+z = 0, \tag{9}$$
$$-sz-\mu = 0, \tag{10}$$
$$x_1^2-x_2+s = 0. \tag{11}$$

Necessary derivatives

$$H(x_1,x_2,z) = \begin{pmatrix} 12(x_1-2)^2+2-2z & -4\\ -4 & 8\end{pmatrix} \tag{12}$$

$$\nabla g(x) = \begin{pmatrix} 2x_1\\ -1\end{pmatrix} \tag{13}$$

Interior point method – Example

System of linear equations for Newton's step

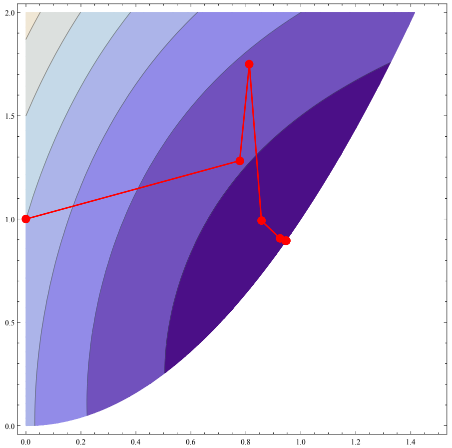
$$\begin{pmatrix} 12(x_1-2)^2+2-2z & -4 & 0 & -2x_1\\ -4 & 8 & 0 & 1\\ 0 & 0 & -z & -s\\ 2x_1 & -1 & 1 & 0\end{pmatrix}\begin{pmatrix}\Delta x_1\\ \Delta x_2\\ \Delta s\\ \Delta z\end{pmatrix} = \begin{pmatrix} -4(x_1-2)^3-2(x_1-2x_2)+2zx_1\\ 4(x_1-2x_2)-z\\ sz+\mu\\ -x_1^2+x_2-s\end{pmatrix}$$

Interior point method – Example

Starting point $x^0 = (0,1)$, $z^0 = 1$, $s^0 = 1$, $\mu > 0$, then the step ...

$$\begin{pmatrix} 48 & -4 & 0 & 0 \\ -4 & 8 & 0 & 1 \\ 0 & 0 & -1 & -1 \\ 0 & -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} \Delta x_1 \\ \Delta x_2 \\ \Delta s \\ \Delta z \end{pmatrix} = \begin{pmatrix} 36 \\ -9 \\ 1+\mu \\ 0 \end{pmatrix}$$

Interior point method – Example



Interior point method for LP

Nocedal and Wright (2006), Chapter 14: $A \in \mathbb{R}^{m \times n}$ full row rank

$$\begin{aligned} &(P) \quad \min c^T x, \ \text{s.t.}\ Ax = b,\ x \geq 0, \\ &(D) \quad \max b^T \lambda, \ \text{s.t.}\ A^T\lambda + s = c,\ s \geq 0. \end{aligned} \tag{14}$$

Lagrangean function

$$L(x,\lambda,s) = c^T x - \lambda^T (Ax - b) - s^T x.$$

KKT optimality conditions

$$\begin{aligned} &A^T\lambda + s = c, \\ &Ax = b, \\ &s^T x = 0, \\ &x \geq 0,\ s \geq 0. \end{aligned} \tag{15}$$

Interior point method for LP

Define the mapping

$$F(x,\lambda,s) = \begin{bmatrix} A^T\lambda + s - c \\ Ax - b \\ XSe \end{bmatrix} = 0, \tag{16}$$

under $x \geq 0,\ s \geq 0$, where $S = \text{diag}\{s_1,\dots,s_n\}$, $X = \text{diag}\{x_1,\dots,x_n\}$.
To obtain a step, solve

$$\mathcal{J}(x,\lambda,s) \begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta s \end{bmatrix} = -F(x,\lambda,s), \tag{17}$$

under $x \geq 0,\ s \geq 0$ leading to

$$\begin{bmatrix} 0 & A^T & I \\ A & 0 & 0 \\ S & 0 & X \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta s \end{bmatrix} = \begin{bmatrix} -A^T\lambda - s + c \\ -Ax + b \\ -XSe \end{bmatrix}. \tag{18}$$

Interior point method for LP

$$\begin{aligned} \min\ & c^T x - \mu \sum_{j=1}^{n} \log x_j \\ \text{s.t. } & Ax = b. \end{aligned} \tag{19}$$

KKT conditions ...

Sequential Quadratic Programming

Nocedal and Wright (2006): Let $f, h_i : \mathbb{R}^n \to \mathbb{R}$ be smooth functions,

$$\begin{aligned} \min_x\ & f(x) \\ \text{s.t. } & h_i(x) = 0,\ i = 1, \ldots, l. \end{aligned} \tag{20}$$

Lagrange function

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

and KKT optimality conditions

$$\begin{aligned} \nabla_x L(x, v) &= \nabla_x f(x) + A(x)^T v = 0, \\ h(x) &= 0, \end{aligned} \tag{21}$$

where $h(x)^T = (h_1(x), \ldots, h_l(x))$ and
$A(x)^T = [\nabla h_1(x), \nabla h_2(x), \ldots, \nabla h_l(x)]$ denotes the Jacobian matrix.

Sequential Quadratic Programming

We have system of $n + l$ equations in the $n + l$ unknowns x and v:

$$\nabla L(x, v) = \begin{bmatrix} \nabla_x f(x) + A(x)^T v \\ h(x) \end{bmatrix} = 0. \tag{22}$$

ASS. (LICQ) Jacobian matrix $A(x)$ has full row rank.
The Jacobian is given by

$$\nabla^2 L(x, v) = \begin{bmatrix} \nabla^2_{xx} L(x, v) & A(x)^T \\ A(x) & 0 \end{bmatrix}. \tag{23}$$

We can use the **Newton algorithm** ..

Sequential Quadratic Programming

Setting $f_k = f(x^k)$, $\nabla^2_{xx} L_k = \nabla^2_{xx} L(x^k, v^k)$, $A_k = A(x^k)$, $h_k = h(x^k)$, we obtain the Newton step by solving the system

$$\begin{bmatrix} \nabla^2_{xx} L_k & A_k^T \\ A_k & 0 \end{bmatrix} \begin{bmatrix} p_x \\ p_v \end{bmatrix} = \begin{bmatrix} -\nabla f_k - A_k^T v_k \\ -h_k \end{bmatrix} \tag{24}$$

Then we set $x^{k+1} = x^k + p_x$ and $v^{k+1} = v^k + p_v$.

Sequential Quadratic Programming

ASS. (SOSC) For all $d \in \{\tilde{d} \neq 0 : \; A(x)\tilde{d} = 0\}$, it holds

$$d^T \nabla^2_{xx} L(x, v) d > 0.$$

Sequential Quadratic Programming

Important alternative way to see the Newton iterations: Consider the **quadratic program**

$$\begin{aligned} \min_p \; & f_k + p^T \nabla f_k + \frac{1}{2} p^T \nabla^2_{xx} L_k p \\ \text{s.t. } & h_k + A_k p = 0. \end{aligned} \tag{25}$$

KKT optimality conditions

$$\begin{aligned} \nabla^2_{xx} L_k p + \nabla f_k + A_k^T \tilde{v} &= 0 \\ h_k + A_k p &= 0, \end{aligned} \tag{26}$$

$$\begin{bmatrix} \nabla^2_{xx} L_k & A_k^T \\ A_k & 0 \end{bmatrix} \begin{bmatrix} p_x \\ p_{\tilde{v}} \end{bmatrix} = \begin{bmatrix} -\nabla f_k \\ -h_k \end{bmatrix} \tag{27}$$

which is the same as the Newton system if we add $A_k^T v_k$ to the first equation. Then we set $x^{k+1} = x^k + p_x$ and $v^{k+1} = p_{\tilde{v}}$.

Sequential Quadratic Programming

Algorithm: Start with an initial solution (x^0, v^0) and iterate until a convergence criterion is met:

1. Evaluate $f_k = f(x^k)$, $h_k = h(x^k)$, $A_k = A(x^k)$, $\nabla^2_{xx} L_k = \nabla^2_{xx} L(x^k, v^k)$.
2. Solve the Newton equations OR the quadratic problem to obtain new (x^{k+1}, v^{k+1}).

If possible, deliver explicit formulas for first and second order derivatives.

Sequential Quadratic Programming

$f, g_j, h_i : \mathbb{R}^n \to \mathbb{R}$ are smooth. We use a **quadratic approximation** of the objective function and linearize the constraints, $p \in \mathbb{R}^p$

$$\begin{aligned} \min_p \; & f(x^k) + p^T \nabla_x f(x^k) + \frac{1}{2} p^T \nabla^2_{xx} L(x^k, u^k, v^k) p \\ \text{s.t. } & g_j(x^k) + p^T \nabla_x g_j(x^k) \le 0, \; j = 1, \dots, m, \\ & h_i(x^k) + p^T \nabla_x h_i(x^k) = 0, \; i = 1, \dots, l. \end{aligned} \tag{28}$$

Use an algorithm for quadratic programming to solve the problem and set $x^{k+1} = x^k + p_k$, where u^{k+1}, v^{k+1} are Lagrange multipliers of the quadratic problem which are used to compute new $\nabla^2_{xx} L$.

Convergence: Nocedal and Wright (2006), Theorem 18.1

Conjugate gradient method

Nocedal and Wright (2006), Chapter 5: Consider (unconstrained) quadratic programming problem

$$\min \frac{1}{2} x^T A x - b^T x.$$

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric positive definite matrix. We say that vectors $p^1, \dots p^n$ are conjugate with respect to A if

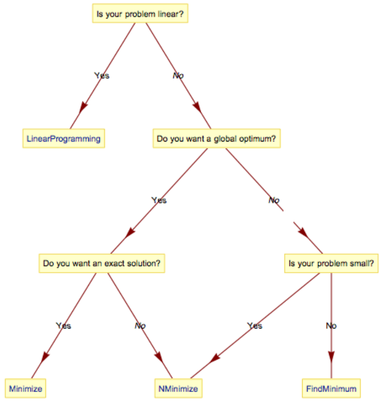
$$(p^i)^T A p^j = 0 \text{ for all } i \neq j.$$

If we set $x^{k+1} = x^k + \alpha^k p^k$, where

$$\begin{aligned} r^k &= A x^k - b, \\ \alpha^k &= -\frac{(r^k)^T p^k}{(p^k)^T A p^k}, \end{aligned} \tag{29}$$

then x^{n+1} is an optimal solution.

Mathematica – Solver Decision Tree



Literature

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