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Study on the GMRES (m) Method of Krylov Subspace and Its Application

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Abstract

The Krylov subspace GMRES (m) method is the programming arithmetic based on the projection method. Now, it has become into the excellent arithmetic to solve the linear problem with large scale, and it also can be applied in the nonlinear programming problems. In this article, we translate the nonlinear optimization problems into the non-smooth equations to solve them. We put forward the iterative method of Newton-GMRES to solve the non-smooth equations, and for large-sized problem, this method is especially applied. And the samples also prove the validity of this method.

Keywords: Non-smooth Equations, Newton-GMRES method

It is the important task to solve the large-sized nonlinear programming problem in the computation mathematics and the scientific engineering computation. The Krylov subspace method is used more in recent twenty years, and it is a sort of iterative method based on the projection method which is applied extensively. The common subspace arithmetic includes FOM, IOM, GMERS and conjugate gradient method and Lanczos, CG, B iGGSTAB aiming at the symmetric array, and some excellent arithmetic have entered into the tool box of MATLAB. In this article, we apply the Krylov subspace GMRES arithmetic in the typical Newton's method, and obtain the Newton-GMRES method which has very important function to solve large-sized nonlinear programming problems.

Many nonlinear programming problems such as nonlinear optimal problems and nonlinear variational inequalities can be translated into non-smooth equations to solve. Therefore, the non-smooth equation offers a general frame to solve these problems in fact. The solutions of the non-smooth equation are extensively noticed, and one new research hotspot in the nonlinear programming domain forms (Hrker et al. 1990, IP et al, 1992, Pang et al, 1990, 1993, Qi et al, 1993a, 1993b).

For the solution of the nonlinear equation,

$$p(x)=0 \qquad (1.1)$$

here, *F:* R_n - R_n is a nonlinear mapping. When *F* is continual and differentiable, one usual method to solve the equations (1.1) is the Newton's method (Ortega et al, 1970).

$$x_{k+1}=x_k-F'(x_k)^{-1}F(x^k) \qquad (1.2)$$

Many effective methods to solve the equations are related with the Newton's methods such as Quasi-Newton Methods and so on.

Suppose that *F* is not a smooth map, but a local map, so $F'(x)$ may not exist, so we can not use the equation (1.2) to solve the non-smooth equations (1.1). If $\partial F(x_k)$ is the generalized Jacobi of $F(x)$ on x_k , i.e. $\partial F(x_k)Co\left\{\lim\limits_{\substack{x_i\to x\\ x_i\in D_F}} F'(x_i)\right\}$, we can use the generalized Jacobi of $F(x)$ to replace *F* (Qi, et al, 1993b), and it can offer a sort of generalized Newton Method to solve the non-smooth equations.

$$x_{k+1}=x_k+V_k^{\ -1}(x_k) \qquad (1.3)$$

Where, $V_k\in\partial F(x_k)$. It proves the local super-linear convergence of the generalized Newton Method when $F(x)$ is half-smooth.

In actual application, when we use the equation (1.3) to solve the non-smooth problem, V_k is very difficult to be estimated especially for large-sized problems. In addition, it is the problem how to effectively solve $V_k d_k + F(x^k) = 0$ to deserve us to deeply study.

For the GMRES arithmetic and other Krylov subspace iterative methods to solve the linear equations, we only need the product of the matrix V_k and the vector *u*, and needn't directly compute the matrix of V_k. Therefore, under the non-smooth condition, we can use $F'(x_k, u) \approx \frac{F(x_k + \delta_u) - F(x_k)}{\delta}$ to approximately replace $V_k d_k$. Combining with the arithmetic (1.3), we can obtain a sort of nested algorithm to solve the equation (1.1). The algorithm can not only overcome the difficulty to compute V_k, but also effectively solve the equation (1.1).

Many scholars considered the Krylov subspace iterative method of nonlinear equations (Peter et al, 1987), we they only limited the problem in the smooth condition. In this article, we consider the non-smooth condition, which is the generalization for the smooth condition. Because the generalized Jacobi is difficult to be estimate, so this Newton-GMRES arithmetic is very applicable.

1. Nonlinear Newton-GMRES method

Now, we offer a sort of Newton-GMRES iterative arithmetic to solve non-smooth equations.

Step 1. Supposed that $\varepsilon > 0$, $\{\varepsilon_k\}$ $\varepsilon_k > 0$ $\varepsilon_k \to 0$.

Select initial approximate $x_0 \in R^n$, $k = 0$.

Step 2. Supposed that $q_0 = \left(F\left(x_k + \sigma_0{}^{(k)} d_0\right) - F(x_k)\right) / \sigma_0{}^{(k)}$, and $d^{(0)}$ is one approximate solution of the linear equations (1.4). $r^{(0)} = -F(x_k) - q_0$, $\beta^{(0)} = \left\|r^{(0)}\right\|$, $u_1 = r^{(0)} / \beta^{(0)}$, $j = 0$.

Step 3. $j = j + 1$

$$q_{j+1} = \left(F\left(x_k + \sigma_j{}^{(k)} u_j\right) - F(x_k)\right) / \sigma_j{}^{(k)}$$

$$W_{j+1} = q_{j+1} - \sum_{i=1} h_{ij} ui$$

$$h_{ij} = (q_{j+1}, u_i) \quad i = 1, \cdots, j$$

$$h_{j+1,j} = \left\|W_{j+1}\right\|$$

$$u_{j+1} = w_{j+1} / h_{j+1,j}$$

Define the Hessenberg matrix $(j+1) \times j$, h_j, and its nonzero unit is h_{ij}.

To solve the minimization problem,

$$\min_{y \in R} \left\|\beta^{(0)} e_1 - \overline{H}_j y\right\| \qquad (2.1)$$

Where, $e_1 = (1, 0, \cdots, 0)^T$ is the unit vector with *j+1* dimensions. Note y_j is one solution of the equation (2.1).

$$d^{(j)} = d^{(o)} + u_j y_j \quad u_j = \lfloor u_1, u_2 \cdots u_j \rfloor$$

Compute the residual

$$\rho_j = \left\|r^{(j)}\right\| = \left\|F(x_k) + \left(F\left(x_k + \sigma_j{}^{(k)} d^{(j)} - F(x_k)\right) / \sigma_j{}^{(k)}\right)\right\|$$

Step 4. If $\rho_j \le \varepsilon_k$ or $j = n$, so next, or else turn to Step 3.

Step 5. Supposed that $x_{k+1} = x_k + d^{(j)}$,

If $\left\|F(x_{k+1}) \le \varepsilon\right\|$, then end, or else, turn to Step 2.

Generally, in the computation of value, we take $d_0 = (0, \cdots, 0)^T$,

$$V_{(x)} u = \left(F(x + \sigma_u) - F(x)\right) / \sigma \qquad (2.2)$$

$$\sigma = \sqrt{\varepsilon} \frac{\|x\|}{\|u\|} \qquad (2.3)$$

ε is a value close to the precision of the machine. In the flowing value computation, we take $\varepsilon = 10^{-8}$.

2. Examples

Many actual problems can be translated into non-smooth equations to solve. For the problem of nonlinear complementarity problem, seek $x \in R_n$ to make

$x \geq 0$, $H(x) \geq 0$, $x^T H(x) = 0$ (2.4)

and prove the problem is equivalent to the nonlinear equations

$F(x) = \min(x, H(x)) = 0$ (2.5).

Example: Seek $x \geq 0$, $H(x) \geq 0$, $x^T H(x) = 0$,

where, $H(x) = c(x) + A(x) + b$

$$c(x) = (c_1(x_1), c_2(x_2), \cdots c_n(x_n))$$

$$c_i(x_i) = 10\arctan(x_i) \qquad i = 1,2,\cdots n$$

$$M = \begin{bmatrix} 2.5 & -1 & & & & \\ -1 & 2.5 & -1 & & & \\ & -1 & 2.5 & -1 & & \\ & & \cdots & & & \\ & & & -1 & 2.5 & -1 \\ & & & & -1 & 2.5 \end{bmatrix}$$

$$b = \left(-\frac{n}{2}, -\frac{n}{2} + 1, \cdots - \frac{n}{2} + n - 1 \right)^T$$

This question is equivalent to the solution of the following equations.

$F(x) = \min(x, H(x)) = 0$

The appointed stop standard is $\|F(x)\| \leq 10^{-6}$. For the problems with different sizes, its iterative steps are in Table 1, where x_0 is the appointed initial value, and D_n is the dimension number of the question.

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Table 1. The steps of iteration method of different scale problem

x_0	$(1,\cdots 1)$	$(1,0,\cdots 1,0)$	$(1,0\cdots 0,1)$	$(1,1,0\cdots 0,1,1)$	$(1,0\cdots 0110\cdots 01)$
$D_n = 50$	*15*	*11*	*9*	*9*	*9*
$D_n = 100$	*8*	*9*	*8*	*8*	*8*
$D_n = 200$	*7*	*9*	*10*	*8*	*10*
$D_n = 500$	*8*	*10*	*9*	*9*	*8*