

An improved Levenberg–Marquardt method for nonsmooth equations with application to multi-stream heat exchangers

El Moudden M.¹, Benjelloun S.¹, Chkifa A.¹, Fawzi H.²

¹*Modeling, Simulation and Data Analysis (MSDA),*

Mohammed VI Polytechnic University, Benguerir, Morocco

²*Department of Applied Mathematics and Theoretical Physics (DAMTP),
University of Cambridge, United Kingdom*

(Received 3 January 2022; Accepted 15 May 2022)

Systems of nonsmooth equations are very useful in the study of nonlinear complementarity problems, variational inequality problems, bilevel programming problems, and arise in the mathematical modeling of many problems in chemical processing, mechanics and engineering. In this paper, we introduce a hybrid method for solving systems of nonsmooth equations, which combines the idea of Levenberg–Marquardt–type methods with bundle techniques, while avoiding the hypothesis of differentiability of the least squares merit function. Some numerical results comparing the proposed method with LP-Newton method indicate that the improved Levenberg–Marquardt algorithm works quite well in practice. As an application of the proposed algorithm, we consider the multi-stream heat exchanger network problem, where a heat exchange network must be designed to meet a specified exit temperature for a given set of streams.

Keywords: *systems of nonsmooth equations, Levenberg–Marquardt method, bundle techniques, multi-stream heat exchanger network, heat transfer.*

2010 MSC: 65K05

DOI: 10.23939/mmc2022.03.547

1. Introduction

Consider the following system of nonsmooth equations

$$F(x) = 0, \quad (1)$$

where $F: \mathbb{R}^n \rightarrow \mathbb{R}^m$ is supposed to be locally Lipschitz continuous (not necessarily smooth nor convex). There has been a growing interest in the study of nonsmooth equations, which arise from many applications, such as nonlinear complementary problems, variational inequality problems, bilevel programming problems, and arises for examples in process engineering, mechanics and equilibrium problems in economics (see, for example, [1, 2] and references therein).

As a result, solving a system of nonsmooth equations has become one of most active research directions in mathematical programming. There exist many methods for solving systems of nonsmooth equations, such as Newton–type methods [3, 4], Trust–region–type methods [5–7], Levenberg–Marquardt–type methods [8, 9]. However, there are some drawbacks in the first and second type of methods, as pointed out in [6, 10]. We are interested in Levenberg–Marquardt algorithms for solving nonsmooth equations, which are one of the most efficient methods, due to their superior numerical performances and theoretical results.

It is well known that the system of nonsmooth equations is equivalent to a least squares problem, whose minimizer is zero. In the case where the function F in the system (1) is nonsmooth but the least squares merit function $\|F(x)\|^2$ is continuously differentiable, the works mentioned above can be applied to solve this kind of nonsmooth system. However, in some cases such as solving semi-infinite programming or variational inequality, the mapping F involved in the system (1) has not this feature, hence the mentioned methods cannot be applied directly. To the best of our knowledge, there are few papers devoted to this situation [11, 12]. To overcome this difficulty, in this paper, we

propose a hybrid method for solving systems of nonsmooth equations, which combines the idea of Levenberg–Marquardt-type methods with bundle techniques. The basic idea of bundle techniques is to use the information from the previous iterations. Therefore, this information is gathered into a bundle providing an approximation for the subdifferential of the merit function.

One motivation to study systems of nonsmooth equations comes from the very important “multi-stream heat exchanger network” problems. Multistream heat exchanger is a heat-transfer equipment that allows multiple hot and cold streams to exchange heat simultaneously and is mainly used in energy intensive cryogenic processes, including air separation, natural gas processing, liquid hydrogen, petrochemicals and liquefied natural gas, etc; see, for example, [13–15].

The structure of the paper is as follows. In Section 2, we introduce the bundle Levenberg–Marquardt method for nonsmooth equations. Preliminary numerical results are reported in Section 3. An application to “multi-stream heat exchanger network” problems is given in Section 4. Finally, Section 5 concludes the paper and presents our perspectives.

2. Bundle Levenberg–Marquardt method

As mentioned in the introduction, when the system (1) has a solution, it is equivalent to the following least squares problem, whose minimum is zero

$$\begin{aligned} \min \psi(x) &:= \frac{1}{2} \|F(x)\|^2, \\ \text{s.t. } x &\in \mathbb{R}^n. \end{aligned} \quad (2)$$

It is worth noting that, since $F(x)$ is nonsmooth, the problem (2) may still be nonsmooth. In this case, gradient-based methods cannot be applied directly. Throughout this paper, we assume that the merit function ψ is locally Lipschitz continuous but not necessarily smooth.

For a system of smooth equations, the Levenberg–Marquardt (LM) method is known to be an efficient solution method. For an arbitrary starting point $x_0 \in \mathbb{R}^n$, the LM method generates a sequence $\{x_k\}$ by setting x_{k+1} equal to the solution of the following subproblem

$$\begin{aligned} \min q_k(x), \\ \text{s.t. } x \in \mathbb{R}^n, \end{aligned}$$

with

$$\begin{aligned} q_k(x) &:= \frac{1}{2} \|F(x_k) + G_k(x - x_k)\|^2 + \frac{1}{2} \nu_k \|x - x_k\|^2 \\ &= \psi(x_k) + \langle \nabla \psi(x_k), x - x_k \rangle + \frac{1}{2} \langle (Q_k + \nu_k I)(x - x_k), x - x_k \rangle, \end{aligned}$$

where $\nabla \psi(x_k) = G_k^\top F(x_k)$, $Q_k = G_k^\top G_k$, G_k is the Jacobian matrix of F at x_k and ν_k is the Levenberg–Marquardt parameter. However, this approach cannot be applied in the nonsmooth case, as the gradient of the merit function does not exist in general. The objective of this paper is the construction of a nonsmooth Levenberg–Marquardt-type algorithm to solve the problem (1).

Let us consider the function $\varphi_k(x)$ defined by $\varphi_k(x) := \psi(x_k) + \langle \nabla \psi(x_k), x - x_k \rangle$. To deal with nonsmoothness of the merit function ψ , we may redefine the function $\varphi_k(x)$ as follows:

$$\begin{aligned} \varphi_k(x) &:= \psi(x_k) + \psi^\circ(x_k; x - x_k) \\ &= \max_{\xi \in \partial \psi(x_k)} \{ \psi(x_k) + \langle \xi, x - x_k \rangle \}. \end{aligned}$$

Actually, this can be impractical in the case where no explicit expression for the Clarke subdifferential $\partial \psi$ is known [16].

To overcome this disadvantage, we may use subgradients from previous iterations. These subgradients are collected into a bundle providing an approximation for the subdifferential of the merit function. In addition to the iteration points $x_k \in \mathbb{R}^n$, we assume that we have at our disposal some auxiliary points $y_i \in \mathbb{R}^n$ from past iterations and the corresponding subgradients $\xi_i \in \partial \psi(y_i)$, for $i \in \mathcal{I}^k$, where the index set \mathcal{I}^k is typically a nonempty subset of $\{0, 1, \dots, k\}$. The auxiliary point y_{k+1} is determined

by solving the following subproblem

$$\begin{aligned} \min q_k(y) &:= \varphi_k(y) + \frac{1}{2} \langle (Q_k + \nu_k I)(y - x_k), y - x_k \rangle, \\ \text{s.t. } y &\in \mathbb{R}^n. \end{aligned} \tag{3}$$

Here, $Q_k := G_k^\top G_k$, with G_k is an element of the Clarke generalized Jacobian of F at x_k [16], $\nu_k > 0$ is the Levenberg–Marquardt parameter and $\varphi_k(y)$ is defined by the following expression:

$$\varphi_k(y) = \max_{i \in \mathcal{I}^k} \left\{ \psi(x_k) + \langle \xi_i, y - x_k \rangle - \beta_i^k \right\}.$$

The term β_i^k is the displacement related to the auxiliary point y_i defined as follows:

$$\beta_i^k = \max \left\{ 0, \psi(x_k) - \psi(y_i) + \langle \xi_i, y_i - x_k \rangle, \gamma \|y_i - x_k\|^2 \right\},$$

with $\gamma > 0$ is a parameter to be selected in the algorithm. It is worth observing that the problem (3) is still nonsmooth. However, with an additional variable $\alpha \in \mathbb{R}$, the problem can equivalently be written as

$$\begin{aligned} \min \alpha &+ \frac{1}{2} \langle (Q_k + \nu_k I)(y - x_k), y - x_k \rangle, \\ \text{s.t. } \psi(x_k) - \beta_i^k + \langle \xi_i, y - x_k \rangle &\leq \alpha, \quad i \in \mathcal{I}^k. \end{aligned} \tag{4}$$

In the above subproblem, we choose the LM parameter as follows:

$$\nu_k := \mu \|F(x_k)\|^\delta, \quad \text{where } \delta \in [1, 2], \quad \mu > 0.$$

After the new auxiliary point y_{k+1} is determined, we have to decide whether it should be accepted as the new iterate x_{k+1} or not. For a fixed parameter $0 \leq \eta \leq 1$, the decision is as follows: if

$$\psi(x_k) - \psi(y_{k+1}) \geq \eta (\psi(x_k) - q_k(y_{k+1})), \tag{5}$$

then y_{k+1} is accepted to become x_{k+1} . A step satisfying condition (5) is called a *serious step*. On the other hand, if condition (5) is not satisfied, then y_{k+1} is rejected and such a step is called a *null step*. In that case, we compute a new subgradient ξ_{k+1} of the merit function ψ at y_{k+1} , and add it to the bundle in order to improve our working model.

The iteration is terminated if

$$\psi(x_k) - q_k(y_{k+1}) \leq \varepsilon, \tag{6}$$

where $\varepsilon > 0$ is a final accuracy tolerance supplied by the user.

We describe the complete algorithm of the proposed bundle Levenberg–Marquardt method as follows.

Algorithm 1 Bundle Levenberg–Marquardt method

Step 0. Choose a starting point x_0 , a final accuracy tolerance $\varepsilon > 0$ and parameters η, μ, δ such that $\eta \in (0, 1)$, $\mu > 0$, $\delta \in [1, 2]$. Set $y_0 = x_0$, $\xi_0 \in \partial\psi(y_0)$, $\beta_0^0 = 0$, $\mathcal{I}^0 = \{0\}$ and $k := 0$.

Step 1. If $\|F(x_k)\| = 0$, then stop. Otherwise, go to the step 2.

Step 2. Set $\nu_k = \mu \|F(x_k)\|^\delta$ and find a new auxiliary y_{k+1} by solving the following subproblem

$$\begin{aligned} \min \alpha &+ \frac{1}{2} \langle (G_k^\top G_k + \nu_k I)(y - x_k), y - x_k \rangle \\ \text{s.t. } \psi(x_k) - \beta_i^k + \langle \xi_i, y - x_k \rangle &\leq \alpha, \quad i \in \mathcal{I}^k, \end{aligned}$$

where $G_k \in \partial F(x_k)$ and ν_k is the Levenberg–Marquardt parameter.

Step 3. If $\psi(x_k) - q_k(y_{k+1}) \leq \varepsilon$, then stop. Otherwise, go to Step 4.

Step 4. If

$$\psi(x_k) - \psi(y_{k+1}) \geq \eta (\psi(x_k) - q_k(y_{k+1}))$$

set $x_{k+1} = y_{k+1}$, and $\mathcal{I}_{k+1} = \mathcal{I}^k \cup \{k + 1\}$, where $\mathcal{I}^k \subseteq \mathcal{I}^k$ (serious step). Otherwise, set $x_{k+1} = x_k$ and $\mathcal{I}_{k+1} = \mathcal{I}^k \cup \{k + 1\}$ (null step).

Step 5. Compute $\xi_{k+1} \in \partial\psi(y_{k+1})$ and β_j^{k+1} for $j \in \mathcal{I}_{k+1}$, and set $k = k + 1$. Go to Step 1.

Remark 1. Note that, since the merit function ψ is assumed to be locally Lipschitz continuous in this paper, then a arbitrary subgradient ξ of the merit function at point x is calculated as $\xi = G^\top F(x)$ for all $G \in \partial F(x)$, by using the standard calculus rules [16].

3. Numerical results

In this section, we present some numerical results in order to confirm the effectiveness of the proposed algorithm. We tested Algorithm 1 on some systems of non-smooth equations collected from the literature, and compared it with the LP-Newton presented in [17]. All implementations were done in MATLAB R2016a. The parameters used were as follows:

$$\eta = 10^{-4}, \quad \varepsilon = 10^{-10}, \quad \mu = 0.1 \quad \text{and} \quad \delta = 2.$$

The subproblem to compute the auxiliary point y_{k+1} requires minimizing a quadratic cost function subject to linear constraints. In order to solve this subproblem efficiently, the Matlab function `fmincon` was used.

In our experiments, we considered the following seven problems (P1–P7), where P1, P2 and P3 are taken from [18], P4, P5 and P6 are taken from [19], and Problem P7 is taken from [20]. Problem P7 is scalable in the sense that it can be defined with different numbers of variables n .

P1. Let $F(x) = (F_1(x), F_2(x))^\top$, where

$$\begin{aligned} F_1(x) &= |x_1| + (x_2 - 1)^2 - 1, \\ F_2(x) &= (x_1 - 1)^2 + |x_2| - 1. \end{aligned}$$

P2. Let $F(x) = (F_1(x), F_2(x))^\top$, where

$$\begin{aligned} F_1(x) &= (x_2 - x_1) \ln[(x_2 - x_1)^2 + 1] + x_2 - x_1, \\ F_2(x) &= \begin{cases} -\exp(-x_1 - x_2) + 1 & \text{for } x_2 \geq 0, \\ \frac{1 - \exp(-x_1)}{1 - x_2} & \text{for } x_2 \leq 0. \end{cases} \end{aligned}$$

P3. Let $F(x) = (F_1(x), F_2(x))^\top$, where

$$\begin{aligned} F_1(x) &= \min\{x_1, 2x_1 + x_2^2 - 6\}, \\ F_2(x) &= \min\{x_2, -x_1^2 + 4x_1 + 0.5x_2 - 3\}. \end{aligned}$$

P4. Let $F(x) = (F_1(x), F_2(x), F_3(x))^\top$, where

$$\begin{aligned} F_1(x) &= \min\{x_1, x_1 - 2\}, \\ F_2(x) &= \min\{x_2, x_2 - x_3 + x_2^3 + 3\}, \\ F_3(x) &= \min\{x_3, x_2 + x_3 + 2x_3^3 - 3\}. \end{aligned}$$

P5. Let $F(x) = \max\{x, Mx + q\}$, where

$$M = \begin{pmatrix} 1 & 2 & 2 & \dots & 2 \\ & 1 & 2 & \dots & 2 \\ & & 1 & \dots & 2 \\ & & & \ddots & \vdots \\ & & & & 2 \end{pmatrix} \quad \text{and} \quad q = \begin{pmatrix} -1 \\ -1 \\ -1 \\ \vdots \\ -1 \end{pmatrix}.$$

P6. Let $F(x) = (F_1(x), F_2(x), F_3(x), F_4(x))^\top$, where

$$\begin{aligned} F_1(x) &= \min\{x_1, 3x_1^2 + 2x_1x_2 + 2x_2^2 + x_3 + 3x_4 - 6\}, \\ F_2(x) &= \min\{x_2, 2x_1^2 + x_1 + x_2^2 + 10x_3 + 2x_4 - 2\}, \\ F_3(x) &= \min\{x_3, 3x_1^2 + x_1x_2 + 2x_2^2 + 2x_3 + 9x_4 - 9\}, \\ F_4(x) &= \min\{x_4, x_1^2 + 2x_2^2 + 2x_3 + 3x_4^3 - 3\}. \end{aligned}$$

P7. Let $F(x) = (F_1(x), \dots, F_n(x))^T$, where

$$F_i(x) = x_i - \sin |x_i|, \quad i = 1, \dots, n.$$

The numerical results for considered algorithms are listed in Table 1. With regard to this table, n indicates the dimension of the test-problem, “iter” and “time” represent the number of iterations and the elapsed CPU time in seconds, respectively.

Table 1. Number of iterations, CPU time in seconds and norm of the residual at the stopping point for Algorithm 1 and the LP-Newton method.

Problem	n	Algorithm 1			LP-Newton method		
		iter	time	$\ F(x_k)\ $	iter	time	$\ F(x_k)\ $
1	2	8	0.39	2.22e-16	10	1.16	1.02e-11
2	2	3	0.27	6.21e-14	7	1.09	8.37e-11
3	3	9	0.43	1.19e-16	10	1.19	4.44e-15
4	2	7	0.40	5.74e-12	9	1.16	2.57e-11
5	8	4	0.30	2.88e-15	16	1.23	8.05e-12
6	4	9	0.32	3.66e-13	12	1.19	4.53e-11
7	10	5	0.29	9.97e-12	7	1.17	2.63e-11
7	50	5	0.31	4.39e-12	7	1.18	2.63e-11
7	100	5	0.31	4.98e-12	7	1.21	2.63e-11
7	200	5	0.36	8.61e-12	7	1.20	2.63e-11
7	500	5	0.53	3.11e-16	7	1.41	2.63e-11

As seen in Table 1, the number of iterations and the CPU time of Algorithm 1 is less than that of the LP-Newton method. This further confirms that the efficiency and robustness of our proposed algorithm.

4. Nonsmooth multistream heat exchanger model

The nonsmooth multistream heat exchanger (MHEX) model developed by Watson et al. [21] is a natural generalization of the classical two-stream countercurrent heat exchanger model. A schematic representation of its combined configuration is shown in Fig.1, in which n_H hot streams exchange heat with n_C cold streams. Here, each hot stream $i \in \{1, \dots, n_H\}$ has a constant molar heat capacity flowrate $mCp_{H,i}$, enters at temperature $T_{H,i}^{IN}$, and exits at temperature $T_{H,i}^{OUT}$ (with $T_{H,i}^{IN} \geq T_{H,i}^{OUT}$). Similarly, each cold stream $j \in \{1, \dots, n_C\}$ has a constant molar heat capacity flowrate $mCp_{C,j}$, enters at temperature $T_{C,j}^{IN}$, and exits at temperature $T_{C,j}^{OUT}$ (with $T_{C,j}^{IN} \leq T_{C,j}^{OUT}$).

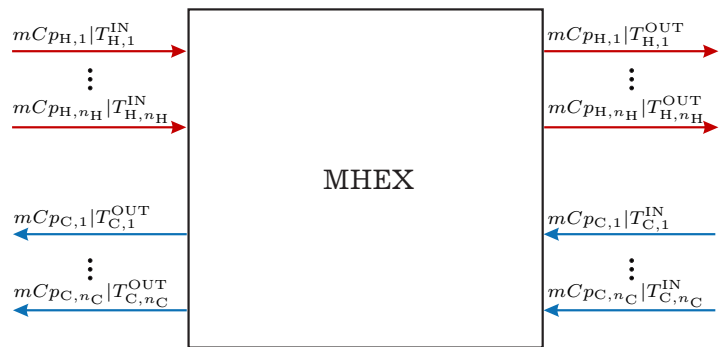


Fig. 1. A multistream heat exchanger with n_H hot streams and n_C cold streams.

The formulation of the nonsmooth MHEX model is given by Eqs. (7) and (8), which represent the energy balance and the second law requirement that heat flows from hot to cold, respectively.

$$Q_H + \sum_{i=1}^{n_H} mCp_{H,i} (T_{H,i}^{IN} - T_{H,i}^{OUT}) - Q_C - \sum_{j=1}^{n_C} mCp_{C,j} (T_{C,j}^{OUT} - T_{C,j}^{IN}) = 0, \tag{7}$$

$$\min_{p \in P} \{EBP_C^p - EBP_H^p\} = -Q_C, \tag{8}$$

where P is the index set of pinch point candidates, Q_H is the heat load of the heating utilities, Q_C is the heat load of the cooling utilities, and $EBP_{H/C}^p$ are the enthalpies of extended hot/cold composite

curves for pinch point candidate p , evaluated from the following expressions:

$$EBP_H^p := \sum_{i=1}^{n_H} mCp_{H,i} \left[\max \{0, T^p - T_{H,i}^{OUT}\} - \max \{0, T^p - T_{H,i}^{IN}\} - \max \{0, T_H^{MIN} - T^p\} + \max \{0, T^p - T_H^{MAX}\} \right], \quad \forall p \in P,$$

$$EBP_C^p := \sum_{j=1}^{n_C} mCp_{C,j} \left[\max \{0, (T^p - \Delta T_{MIN}) - T_{C,j}^{IN}\} - \max \{0, (T^p - \Delta T_{MIN}) - T_{C,j}^{OUT}\} + \max \{0, (T^p - \Delta T_{MIN}) - T_C^{MAX}\} - \max \{0, T_C^{MIN} - (T^p - \Delta T_{MIN})\} \right], \quad \forall p \in P,$$

where ΔT_{MIN} is the minimum approach temperature and $T_{H/C}^{MAX}$ and $T_{H/C}^{MIN}$ are the maximum and minimum temperatures of the hot/cold streams in the heat exchanger, respectively. All pinch point candidates with temperatures T^p are defined by their hot stream temperature:

$$T^p := \begin{cases} T_{H,i}^{IN}, & \forall p = i \in \{1, \dots, n_H\}, \\ T_{H,j}^{IN} + \Delta T_{MIN}, & \forall p = j \in \{1, \dots, n_C\}. \end{cases}$$

Note that Eq. (7) is clearly differentiable and Eq. (8) includes the max function which is nondifferentiable. The resulting system is thus a nonsmooth system.

Case study. Consider the process data in Table 2 for two hot streams and two cold streams in a MHEX. The minimum approach temperature ΔT_{MIN} is specified as 10 °C. We consider the special case of a MHEX where external utilities are not present ($Q_H = 0$ and $Q_C = 0$). We use Algorithm 1 to solve the system consisting of Eqs. (7) and (8) with the unknown temperatures $x^1 := T_{H,1}^{OUT}$ and $x^2 := T_{C,2}^{OUT}$. From the starting point $x_0 = (80, 230)$. Algorithm 1 converges to the solution $x_{opt} = (120, 205)$ after 6 iterations, while the LP-Newton method converges to the same solution after 66 iterations. The hot and cold composite curves at the solution x_{opt} are depicted in Fig. 2.

Table 2. Data of process streams.

Stream Name	$T_{H/C}^{IN}$ (°C)	$T_{H/C}^{OUT}$ (°C)	$mCp_{H/C}$ (MW °C ⁻¹)
H1	250	40	0.15
H2	200	x^1	0.25
C1	20	180	0.20
C2	140	x^2	0.30

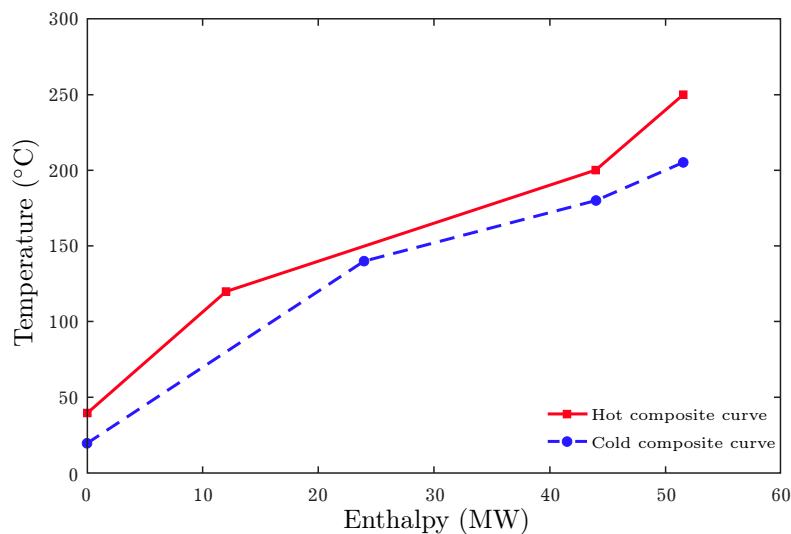


Fig. 2. The hot and cold composite curves at the solution.

5. Concluding remarks

This paper discusses the solution of systems of nonsmooth equations. First, we have proposed a hybrid method for solving nonsmooth equations, which combines the idea of Levenberg–Marquardt-type method with bundle techniques, while avoiding the hypothesis of differentiability of the least squares merit function. Second, some numerical results are given indicating a good behavior of the proposed algorithm compared to the LP-Newton method. Finally, we have applied the proposed method to solve the nonsmooth multi-stream heat exchange model, guaranteeing the feasibility of heat exchange.

There are several important issues worth studying in the future research, the first is to prove the convergence rate of the proposed algorithm, and the second is to extend the algorithm for solving systems of constrained equations. Also, applying the algorithm to simultaneous multiple resources integration in process systems engineering is an interesting work. These points are subject to ongoing research and will be addressed in a forthcoming paper.

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Удосконалений метод Левенберга–Марквардта для негладких рівнянь із застосуванням до багатопотокових теплообмінників

Ель Мудден М.¹, Бенджеллон С.¹, Чкіфа А.¹, Фаузі Х.²

¹ *Моделювання, симуляція та аналіз даних (МСАД),*

Політехнічний університет Мохаммеда VI, Бенгеріп, Марокко

² *Кафедра прикладної математики та теоретичної фізики (КПМТФ),*

Кембриджський університет, Великобританія

Системи негладких рівнянь дуже корисні для вивчення нелінійних задач доповнюваності, варіаційних нерівностей, задач дворівневого програмування та виникають під час математичного моделювання багатьох задач хімічної обробки, механіки та техніки. У цій роботі вводимо гібридний метод розв'язування систем негладких рівнянь, який поєднує ідею методів типу Левенберга–Марквардта з методами розшарування, уникаючи при цьому гіпотези про диференційовність оціночної функції найменших квадратів. Деякі чисельні результати порівняння запропонованого методу з ЛП-методом Ньютона свідчать про те, що вдосконалений алгоритм Левенберга–Марквардта досить добре працює на практиці. Як застосування запропонованого алгоритму розглянуто задачу мережі багатопотокових теплообмінників, де теплообмінна мережа повинна бути спроектована так, щоб відповідати заданій температурі на виході для заданого набору потоків.

Ключові слова: *системи негладких рівнянь, метод Левенберга–Марквардта, методи розшарування, багатопотокова теплообмінна мережа, теплообмін.*