

AN EFFICIENT MATRIX SOLVER FOR FINITE-ELEMENT ANALYSIS OF NON-NEWTONIAN FLUID FLOW PROBLEMS

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SUMMARY

When the Galerkin finite-element method with a nine-node isoparametric Lagrangian element is applied to solve non-Newtonian fluid flow problems, a considerable amount of computing time is required to solve the discretized non-linear system of equations by Newton's method. A method proposed by Broyden has been modified to compute the Jacobian matrix associated with Newton's method. This modified Broyden's method can be combined with the frontal method to efficiently solve the linearized finite-element equations during the iteration. Numerical results of a sample problem concerning the determination of the pressure-drop/flow-rate relationship for power-law fluids in rectangular ducts show that the application of this new method can reduce computing time substantially.

KEY WORDS Non-Newtonian Fluid Flow Nine-Node Lagrangian Element Broyden's Method Frontal Method

INTRODUCTION

The Galerkin finite-element method has been applied extensively for solving non-Newtonian fluid flow problems in recent years. Various types of elements have been used; simple triangular elements were preferred by several researchers,^{1–4} whereas others used eight-node serendipity elements⁵ or nine-node Lagrangian elements,^{6,7} to name just a few. It was reported⁸ that the nine-node Lagrangian element generates more accurate finite-element solutions of the Navier–Stokes equations than several other types of elements. A similar conclusion was reached for non-Newtonian fluid flow problems.⁷

Newton's method is a commonly used iterative scheme for the non-linear system of equations resulting from the finite-element discretization of non-Newtonian fluid flow problems. However, when the nine-node Lagrangian element is used, owing to the complexity of the constitutive equations of the non-Newtonian fluid models and the nature of the element, many numerical integrations are required in the evaluation of the Jacobian matrix during the iteration and, consequently, a considerable amount of computing time will be consumed.

Engelman *et al.*⁹ examined various quasi-Newton methods for finite-element solutions of Newtonian flow problems and concluded that a method proposed by Bryoden¹⁰ could be effectively used to save computer time. Engelman¹¹ later extended the analysis to non-Newtonian flow problems. Whereas the previous authors used a skyline solution approach, we found that Bryoden's method can be modified and then combined with the frontal method for non-Newtonian problems. This new approach can bypass the numerical integrations required for the updating of the Jacobian matrix, thereby saving computer time.

A sample problem will illustrate this approach. Comparisons of the numerical results and the CPU time required by the regular Newton's method with those of the new approach show that the new approach can reduce the computing time substantially.

The sample problem is the determination of the pressure-drop/flow-rate relationship for fully developed laminar flow of power-law fluids in rectangular ducts. This problem was previously solved by Wheeler and Wissler¹² using the finite-difference method and by others^{5,11,13} using the Galerkin finite-element method. The numerical solutions obtained here will be compared with the values given by Wheeler and Wissler.

FLOW MODEL OF THE SAMPLE PROBLEM

Consider the fully developed laminar flow of inelastic power-law fluids in a rectangular duct as shown in Figure 1. The flow is assumed to be unidirectional, and the equation of motion has the following form:^{12,13}

$$\frac{\partial}{\partial \bar{x}} \left(\bar{\eta} \frac{\partial \bar{w}}{\partial \bar{x}} \right) + \frac{\partial}{\partial \bar{y}} \left(\bar{\eta} \frac{\partial \bar{w}}{\partial \bar{y}} \right) = \frac{d\bar{p}}{d\bar{z}}, \quad \text{in } \bar{D}, \quad (1)$$

where

$$\bar{\eta} = \kappa \left[\left(\frac{\partial \bar{w}}{\partial \bar{x}} \right)^2 + \left(\frac{\partial \bar{w}}{\partial \bar{y}} \right)^2 \right]^{n-1/2}, \quad (2)$$

and κ, n are material constants. The no-slip boundary condition requires

$$\bar{w} = 0. \quad \text{on } \partial \bar{D}. \quad (3)$$

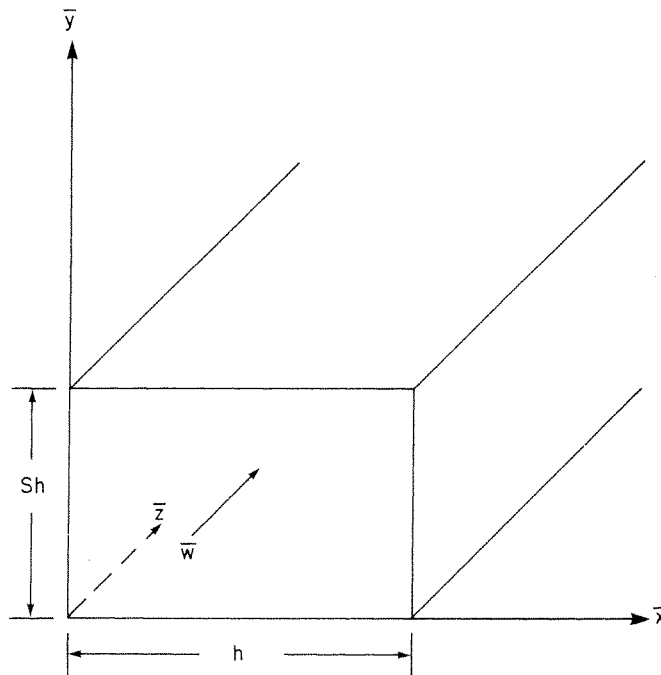


Figure 1. Flow geometry

The dimensionless variables are defined as

$$x = \bar{x}/h, \quad y = \bar{y}/(Sh), \quad w = \frac{\bar{w}}{h} \left(\frac{\kappa}{h} \right)^{1/n} \left(-\frac{d\bar{p}}{d\bar{z}} \right)^{-1/n}. \quad (4)$$

Introducing (4) into (1), we obtain

$$\frac{\partial}{\partial x} \left(\eta \frac{\partial w}{\partial x} \right) + \frac{1}{S^2} \frac{\partial}{\partial y} \left(\eta \frac{\partial w}{\partial y} \right) = -1, \quad \text{in } D, \quad (5)$$

where

$$\eta = \left[\left(\frac{\partial w}{\partial x} \right)^2 + \frac{1}{S^2} \left(\frac{\partial w}{\partial y} \right)^2 \right]^{n-1/2}, \quad (6)$$

with boundary condition

$$w = 0, \quad \text{on } \partial D. \quad (7)$$

Note that our non-dimensionalization is different from that of References 5 and 11; the pressure gradient does not appear explicitly in (5)–(7).

The volumetric flow rate Q is defined as

$$Q \equiv \int_{\bar{b}} \int \bar{w} d\bar{x} d\bar{y}. \quad (8)$$

Substituting (4) into (8), we obtain

$$Q = \lambda(n) \frac{Sh^{3+(1/n)} \left(-\frac{d\bar{p}}{d\bar{z}} \right)^{1/n}}{(\kappa)^{1/n}}, \quad (9)$$

where the shape factor $\lambda(n)$ is given as

$$\lambda(n) \equiv \int_D \int w dx dy. \quad (10)$$

Equation (9) expresses the pressure-drop/flow-rate relationship for power-law fluids in rectangular ducts. The Galerkin finite-element method is applied to solve (5)–(7) for w . After w is determined, a numerical integration is performed to obtain $\lambda(n)$. The values of $\lambda(n)$ obtained will be compared with those given by Wheeler and Wissler.

FINITE-ELEMENT SOLUTION

Because the nine-node isoparametric element is used, w , x and y can be approximated in each element as

$$\begin{bmatrix} w \\ x \\ y \end{bmatrix} = \sum_{i=1}^9 \begin{bmatrix} w_i \\ x_i \\ y_i \end{bmatrix} \phi_i, \quad (11)$$

where the interpolation function ϕ can be found in several textbooks.^{14–16}

Applying the Galerkin process to (5), we obtain, after performing an integration by parts,

$$f_m(w) = K_{mi} w_i - A_m = 0, \quad m, i = 1, 2, \dots, 9, \quad (12)$$

where

$$K_{mi} = \int_e \int \eta \beta_{mi} dx dy, \quad (13)$$

$$A_m = \int_e \int \phi_m dx dy, \quad (14)$$

and

$$\beta_{mi} = \frac{\partial \phi_m}{\partial x} \frac{\partial \phi_i}{\partial x} + \frac{1}{S^2} \frac{\partial \phi_m}{\partial y} \frac{\partial \phi_i}{\partial y}. \quad (15)$$

e is the area of the element. Define

$$\mathbf{F}^T(\mathbf{w}) \equiv [f_1, f_2, \dots, f_9], \quad (16)$$

$$\mathbf{w}^T \equiv [w_1, w_2, \dots, w_9]. \quad (17)$$

Applying Newton's method to (16), we have

$$\mathbf{J}^v(\mathbf{w}^{v+1} - \mathbf{w}^v) = -\mathbf{F}(\mathbf{w}^v), \quad (18)$$

where v stands for the number of the iteration. The elements of the Jacobian matrix \mathbf{J} are defined as follows:

$$(\mathbf{J})_{mj} = \left(\frac{\partial f_m}{\partial w_j} \right), \quad m, j = 1, 2, \dots, 9, \quad (19)$$

and

$$\frac{\partial f_m}{\partial w_j} = K_{mj} + \sum_{i=1}^9 \frac{\partial K_{mi}}{\partial w_j} w_i, \quad (20)$$

where

$$\frac{\partial K_{mi}}{\partial w_j} = \int_e \int \frac{\partial \eta}{\partial w_j} \beta_{mi} dx dy. \quad (21)$$

To solve the linear system of equations (18) efficiently, we can apply the frontal method. The frontal method was first developed by Irons¹⁷ for symmetric coefficient matrices and later extended by Hood¹⁸ for unsymmetric coefficient matrices for the solution of the linear system of equations arising in the finite-element method.

This method can be considered as carrying out the Gaussian elimination in a discrete manner. The method starts by loading each of the element stiffness matrices to a working matrix consecutively until the number of the fully summed unknowns exceeds a preset value, then the Gaussian elimination will proceed. The eliminated coefficients will be stored for back substitution. The elimination process will stop when the number of the fully summed unknowns falls below the preset value, and the loading will resume. The process will repeat until all the coefficients have been eliminated and the solution is obtained by a back-substitution procedure.

The stiffness matrix of the element corresponds to \mathbf{J} in (18) for this flow problem. To evaluate the elements of \mathbf{J} , we need to perform the integrations in (20). The integrations can be transformed to a local co-ordinate system, and a 3×3 Gaussian quadrature is used to approximate the integrations. Owing to the complexity of (20), which results from the non-linear fluid model and the use of the Lagrangian element, many numerical integrations are necessary for the construction of \mathbf{J} . Therefore, a considerable amount of computer time will be consumed.

BROYDEN'S METHOD

Broyden proposed a class of methods that are modifications to Newton's method designed to reduce the computing time in the evaluation of the Jacobian matrix. The method we chose to use is explained briefly here.

Consider a set of non-linear algebraic equations

$$\hat{f}_j(\hat{x}_1, \hat{x}_2, \dots, \hat{x}_N) = 0, \quad j = 1, 2, \dots, N, \quad (22)$$

or

$$\hat{\mathbf{F}}(\hat{\mathbf{X}}) = \mathbf{0}. \quad (23)$$

Suppose $\hat{\mathbf{X}}^v$ is the v th approximation to the solution of (23), and $\hat{\mathbf{F}}^v$ is written for $\hat{\mathbf{F}}(\hat{\mathbf{X}}^v)$, then Newton's method is defined by

$$\hat{\mathbf{X}}^{v+1} \equiv \hat{\mathbf{X}}^v - (\hat{\mathbf{J}}^v)^{-1} \hat{\mathbf{F}}^v, \quad (24)$$

where $\hat{\mathbf{J}}^v$ is the Jacobian matrix $[\partial \hat{f}_j / \partial \hat{x}_i]$ evaluated at $\hat{\mathbf{X}}^v$. Broyden's method proceeds as follows:

1. Select an initial estimate solution $\hat{\mathbf{X}}^0$ and an initial Jacobian matrix $\hat{\mathbf{J}}^0$.
2. Compute $\hat{\mathbf{F}}^0 = \hat{\mathbf{F}}(\hat{\mathbf{X}}^0)$.
3. Solve for $\hat{\mathbf{X}}^1$, where $\hat{\mathbf{X}}^1 = \hat{\mathbf{X}}^0 - (\hat{\mathbf{J}}^0)^{-1} \hat{\mathbf{F}}^0$.
4. Compute $\hat{\mathbf{F}}^1$. Test $\hat{\mathbf{F}}^1$ for convergence, if not, then
5. Compute $\hat{\mathbf{q}} = \hat{\mathbf{X}}^1 - \hat{\mathbf{X}}^0$, $\hat{\mathbf{Y}} = \hat{\mathbf{F}}^1 - \hat{\mathbf{F}}^0$.
6. Compute $\hat{\mathbf{J}}^1 = \hat{\mathbf{J}}^0 + \frac{(\hat{\mathbf{Y}} - \zeta \hat{\mathbf{J}}^0 \hat{\mathbf{q}}) \hat{\mathbf{q}}^T}{\zeta \hat{\mathbf{q}}^T \hat{\mathbf{q}}}$,

where ζ is an acceleration parameter. For convenience, we take $\zeta = 1$.

7. Replace $\hat{\mathbf{X}}^0$ by $\hat{\mathbf{X}}^1$, $\hat{\mathbf{J}}^0$ by $\hat{\mathbf{J}}^1$, and repeat from (2).

We found that this method, like the frontal method, can also be carried out in a discrete manner. A simple proof is given in the Appendix. Therefore, this method can be combined with the frontal method to bypass the large number of numerical integrations in (20).

However, when we update $\hat{\mathbf{J}}^v$ with Broyden's method, the sparseness of the Jacobian matrix is destroyed. From step (6) above, we observe that after applying Broyden's method, the element \hat{J}_{ij} that previously has the value zero will now be

$$\hat{J}_{ij}^{v+1} = \frac{\hat{f}_i^{v+1}(\hat{x}_j^{v+1} - \hat{x}_j^v)}{\sum_{l=1}^N (\hat{x}_l^{v+1} - \hat{x}_l^v)^2}. \quad (25)$$

To retain the original sparse pattern of the Jacobian matrix for Newton's method, we force this term to be zero, and the error produced by neglecting the contribution of (25) is

$$\frac{\hat{f}_i^{v+1}(\hat{x}_i^{v+1} - \hat{x}_j^v)(\hat{x}_j^{v+2} - \hat{x}_j^{v+1})}{\sum_{l=1}^N (\hat{x}_l^{v+1} - \hat{x}_l^v)^2}.$$

Generally, this error will decrease as v increases. Therefore unless a close initial guess is available, it is better to start the iteration process with one or two Newton's iterations, then to continue the iteration by the new method. We found that this approach can generate convergent solutions for our test problems satisfactorily.

After one or two Newton's iterations, \mathbf{J} in (18) is updated as follows:

$$\mathbf{J}^{v+1} = \mathbf{J}^v + \frac{(\mathbf{Y} - \mathbf{J}^v \mathbf{q}) \mathbf{q}^T}{\mathbf{q}^T \mathbf{q}}, \quad (26)$$

where

$$\mathbf{Y} = \mathbf{F}(\mathbf{w}^{v+1}) - \mathbf{F}(\mathbf{w}^v), \quad (27)$$

$$\mathbf{q} = \mathbf{w}^{v+1} - \mathbf{w}^v. \quad (28)$$

The evaluation of \mathbf{J} using (26) is simple and straightforward and requires much less computational effort than using (20).

Because the values of the stiffness matrix and the right-hand-side vector in the previous iteration are used in the updating of the Jacobian matrix as shown in (26), additional space is required to store these values. The vector used for storing the values has the length (total number of elements) \times (number of variables per element) \times (number of variables per element + 1).

NUMERICAL RESULTS

We used two grids for our computation. The domain of integration reduces to a unit square after non-dimensionalization. Grid 1 which consists of 16 equal square elements is shown in Figure 2 and grid 2 consists of 36 equal square elements. There are 81 and 169 nodes in grids 1 and 2, respectively.

We selected two cases for comparison. Case I corresponds to a square duct, and case II corresponds to a rectangular duct with $S = 0.5$.

All the computations were performed on a CDC Cyber 170 computer with single-precision arithmetic. The power-law index n was fixed to be 0.75, the tolerance of convergence was chosen to

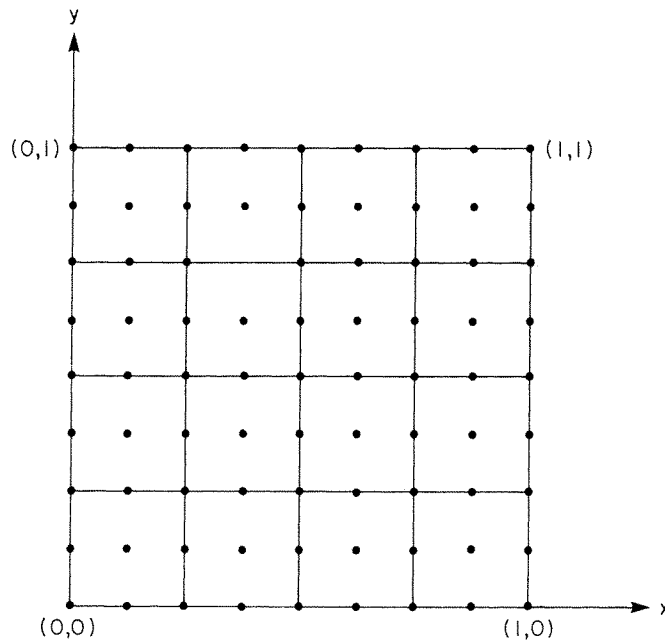


Figure 2. Grid 1

Table I. Numerical results of case I

Case	Grid 1	Grid 2	NT*	BR	TI	CPU time, s	$\lambda \times 10$	$\frac{\bar{\lambda} - \lambda}{\bar{\lambda}} \times 100\%$
I-1	×		5	0	5	340.52	0.20994	0.16
I-2	×		2	4	6	159.38	0.20996	0.15
I-3	×		1	10	11	117.90	0.20994	0.15
I-4		×	5	0	5	776.11	0.21024	0.015
I-5		×	2	4	6	351.06	0.21023	0.019
I-6		×	1			no convergence after 20 iterations.		

*NT: Newton's iteration, BR: Broyden's iteration, TI: total number of iterations, $\bar{\lambda}$: value of λ in Reference 12.

Table II. Numerical results of case II

Case	Grid 1	Grid 2	NT	BR	TI	CPU time, s	$\lambda \times 100$	$\frac{\bar{\lambda} - \lambda}{\bar{\lambda}} \times 100\%$
II-1	×		5	0	5	351.73	0.74697	0.20
II-2	×		2	5	7	164.48	0.74089	0.62
II-3		×	6	0	6	926.41	0.74539	0.016
II-4		×	2	6	8	373.82	0.74634	0.11

be 10^{-4} , and the initial guess for w was 0.1 for all cases. $\mathbf{q}^T \mathbf{q}$ in (26) was replaced by 1.0 when its value was less than 10^{-5} .

Because the 9×9 stiffness matrix \mathbf{J} is symmetric, we needed to evaluate only 45 elements of \mathbf{J} .

The values of λ given by Wheeler and Wissler were used for comparison; they reported that the errors for these values are < 0.1 per cent.

The numerical results for case I are shown in Table I. It is clear that using the nine-node Lagrangian isoparametric element can generate numerical solutions of high accuracy, even on a relatively coarse grid. Using the new method can save at least 50 per cent of CPU time, although starting with only one Newton's iteration can save more, as expected.

Table II shows the numerical results for case II. Similarly, the numerical solutions are quite accurate, and the new method can also save more than 50 per cent of CPU time.

We could not obtain convergent solutions after 20 iterations if we started with only one Newton's iteration for case I-6 and all cases in Table II.

DISCUSSION AND CONCLUSION

The Galerkin finite-element method has become a powerful tool to analyse non-Newtonian fluid flow problems, and the nine-node Lagrangian isoparametric element has been identified to be superior to several other types of elements for generating numerical solutions of high accuracy. However, owing to the complexity of the constitutive equations of the fluid models and the nature of the Lagrangian element, much computing time is needed in the evaluation of the Jacobian matrix for Newton's method. We propose a new method to reduce the computing time, which is a modification of Broyden's method and can be combined with the frontal method to efficiently solve the linear system of equations resulting from the application of Newton's method to the discretized finite-element equations.

One numerical example has been given to illustrate this new method. Computational results show that at least 50 per cent of CPU time can be saved relative to the regular Newton's method. Based on the numerical results, it is advisable to start with two Newton's iterations, then proceed with the new iterative scheme developed here.

The objective of this paper is to convey the idea that the combination of Broyden's method with the frontal method provides a useful means to save CPU time, and it is easy to implement this new approach. The substantial savings of computer time for the test problem are due to the fact that the numbers of unknowns are relatively small. As the number of unknowns increases, the cost of the *LU* decomposition starts to dominate the cost of the numerical integrations. Typical savings resulting from the bypassing of numerical integrations for large problems, as one of the reviewers pointed out, would be around 10 per cent in solution time per iteration.

If simple triangular elements are used for non-Newtonian fluid flow problems, the new method cannot save much computing time because there is no numerical integration involved. Crochet and Bezy¹⁹ reported that using a modified Newton's method did not save much computing time for their finite-element flow study.

It is our hope that this paper will initiate some numerical experiments for problems with large numbers of unknowns.

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NOTATIONS

- A_m = integration, equation (14)
- \bar{D} = domain of integration
- $\partial\bar{D}$ = boundary of \bar{D}
- D = domain of integration, dimensionless
- ∂D = boundary of D
- e = area of an element
- \mathbf{F} = vector, equation (16)
- $\hat{\mathbf{F}}$ = vector, equation (23)
- f_m = function, equation (12)
- \hat{f} = function, equation (22)
- h = length of the longer side of a rectangle
- \mathbf{J} = Jacobian matrix
- K_{mi} = integration, equation (13)
- n = power-law index
- \bar{p} = fluid pressure
- Q = volumetric flow rate
- \mathbf{q} = vector, equation (28)
- $\hat{\mathbf{q}}$ = vector appearing in Broyden's method
- S = aspect ratio
- \bar{w} = axial velocity component
- w = axial velocity component, dimensionless
- \mathbf{w} = vector, equation (17)
- $\hat{\mathbf{x}}$ = unknown vector, equation (23)

- $\bar{x}, \bar{y}, \bar{z}$ = Cartesian co-ordinates
 \hat{x} = unknown variable, equation (22)
 x, y = lateral Cartesian co-ordinates, dimensionless
 \mathbf{Y} = vector, equation (27)
 $\hat{\mathbf{Y}}$ = vector appearing in Broyden's method

Greek letters

- β_{mi} = function, equation (15)
 $\bar{\eta}$ = apparent viscosity, equation (2)
 η = apparent viscosity, dimensionless, equation (6)
 κ = material constant of power-law model
 λ = shape factor, equation (10)
 ν = number of iterations
 ϕ = interpolation function
 ζ = acceleration parameter in Broyden's method

Subscripts

- l, i, j, m = dummy indices

APPENDIX: UPDATING THE JACOBIAN MATRIX BY BROYDEN'S METHOD IN A DISCRETE MANNER

Consider the linear system of equations

$$\mathbf{A}^{(n)} \mathbf{x}^{(n)} = \mathbf{y}^{(n)}. \quad (29)$$

Let $\mathbf{A}^{(n)}$ be the sum of two submatrices, i.e.

$$\mathbf{A}^{(n)} = \mathbf{A}_1^{(n)} + \mathbf{A}_2^{(n)} \quad (30)$$

and

$$\mathbf{A}_1^{(n)} \mathbf{x}^{(n)} = \mathbf{y}_1^{(n)}, \quad (31)$$

$$\mathbf{A}_2^{(n)} \mathbf{x}^{(n)} = \mathbf{y}_2^{(n)}, \quad (32)$$

where

$$\mathbf{y}^{(n)} = \mathbf{y}_1^{(n)} + \mathbf{y}_2^{(n)}. \quad (33)$$

Applying Broyden's method to update the matrices in (29), (31) and (32), we obtain

$$\mathbf{A}^{(n+1)} = \mathbf{A}^{(n)} + \frac{(\bar{\mathbf{y}} - \mathbf{A}^{(n)} \bar{\mathbf{x}}) \bar{\mathbf{x}}^T}{\bar{\mathbf{x}}^T \bar{\mathbf{x}}}, \quad (34)$$

$$\mathbf{A}_1^{(n+1)} = \mathbf{A}_1^{(n)} + \frac{(\bar{\mathbf{y}}_1 - \mathbf{A}_1^{(n)} \bar{\mathbf{x}}) \bar{\mathbf{x}}^T}{\bar{\mathbf{x}}^T \bar{\mathbf{x}}}, \quad (35)$$

$$\mathbf{A}_2^{(n+1)} = \mathbf{A}_2^{(n)} + \frac{(\bar{\mathbf{y}}_2 - \mathbf{A}_2^{(n)} \bar{\mathbf{x}}) \bar{\mathbf{x}}^T}{\bar{\mathbf{x}}^T \bar{\mathbf{x}}}, \quad (36)$$

where

$$\begin{aligned}
 \bar{\mathbf{y}} &= \mathbf{y}^{(n+1)} - \mathbf{y}^{(n)}, & \bar{\mathbf{x}} &= \mathbf{x}^{(n+1)} - \mathbf{x}^{(n)}, \\
 \bar{\mathbf{y}}_1 &= \mathbf{y}_1^{(n+1)} - \mathbf{y}_1^{(n)}, & \bar{\mathbf{y}}_2 &= \mathbf{y}_2^{(n+1)} - \mathbf{y}_2^{(n)}, \\
 \bar{\mathbf{y}} &= \bar{\mathbf{y}}_1 + \bar{\mathbf{y}}_2.
 \end{aligned} \quad (37)$$

Adding (35) and (36), we obtain

$$\mathbf{A}_1^{(n+1)} + \mathbf{A}_2^{(n+1)} = (\mathbf{A}_1^{(n)} + \mathbf{A}_2^{(n)}) + \frac{[(\bar{\mathbf{y}}_1 + \bar{\mathbf{y}}_2) - (\mathbf{A}_1^{(n)} + \mathbf{A}_2^{(n)})\bar{\mathbf{x}}]\bar{\mathbf{x}}^T}{\bar{\mathbf{x}}^T\bar{\mathbf{x}}} \quad (38a)$$

$$= \mathbf{A}^{(n)} + \frac{(\bar{\mathbf{y}} - \mathbf{A}^{(n)}\bar{\mathbf{x}})\bar{\mathbf{x}}^T}{\bar{\mathbf{x}}^T\bar{\mathbf{x}}} \quad (38b)$$

$$= \mathbf{A}^{(n+1)}. \quad (38c)$$

Therefore $\mathbf{A}^{(n)}$ can be updated by Broyden's method in a discrete manner, i.e. each of its submatrices can be updated separately, and $\mathbf{A}^{(n+1)}$ is obtained by adding the updated submatrices.

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