New Approach for Secant Update Generalized Version of PSB

N. Boutet, R. Haelterman, and J. Degroote

***Abstract*—Working with Quasi-Newton methods in optimization leads to one important challenge, being to find an estimate of the Hessian matrix as close as possible to the real matrix. While multisecant methods are regularly used to solve root finding problems, they have been little explored in optimization because the symmetry property of the Hessian matrix estimation is generally not compatible with the multisecant property. In this paper, we propose a solution to apply multisecant methods to optimization problems. Starting from the Powell-Symmetric-Broyden (PSB) update formula and adding pieces of information from the previous steps of the optimization path, we want to develop a new update formula for the estimate of the Hessian. A multisecant version of PSB is, however, generally mathematically impossible to build. For that reason, we provide a formula that satisfies the symmetry and is as close as possible to satisfy the multisecant condition and vice versa for a second formula. Subsequently, we add enforcement of the last secant equation to the symmetric formula and present a comparison between the different methods.**

***Index Terms*—Non-linear, optimization, quasi-Newton formulas, multisecant equations, symmetric gradient.**

I. INTRODUCTION

Solving high-dimensional or complex problems is now a common situation in engineering. Thanks to the combination of the increasingly available computational power and the development of specific solver tools, numerical methods make it possible to solve problems that are increasingly complex and heavier. In most industrial applications, the computation can simply be considered as a black box solving a problem based on given input variables.

When such a black box is available, optimization is a logical further step. Indeed a new question quickly arises: which value should be given to the variables in order to optimize some objective function?

For root finding problems, one important strategy in recent research and applications, in particular in interaction problems, is the use of multisecant methods [1]-[4]. However, this strategy has been very little explored in the context of optimization where symmetrical methods (BFGS in the lead) are the most used. The fact that the combination of symmetrical and multisecant properties is generally impossible is probably the cause of the weak exploration of this solution [5]-[9]. In our new approach, we impose the symmetry of the new estimate of the Hessian matrix and minimize the non-satisfaction of the multiple sequential equations, in order to get as close as possible to the multisecant property.

In this paper, we are solving problems expressed as the root finding problem

$$\nabla g(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{0}$$

where $g: D_F \subset \mathbb{R}^n \to \mathbb{R}$ g:DF⊂ℝn→ℝ is the objective function of the optimization problem

$$\min_{\boldsymbol{x}} g(\boldsymbol{x})$$minxg(x)

We assume the problems we want to solve have the following characteristics.

1) The objective function value $g(\boldsymbol{x})$ can be calculated with some code.
2) The analytic form of $g(\boldsymbol{x})$ is unknown, the Hessian is not available. Therefore, Newton's method cannot be used.
3) It is possible to estimate the gradient of the problem $\nabla g(\boldsymbol{x})$, for instance with methods like adjoint state [1], [10].
4) The evaluation of $g(\boldsymbol{x})$ and $\nabla g(\boldsymbol{x})$ is computationally costly, because of the size or the complexity of the root finding problem. We therefore use the required number of evaluations (or 'function calls') as a measure of the performance.

II. QUASI-NEWTON LEAST CHANGE

As it is not possible to use the exact Jacobian of the gradient vector $\boldsymbol{f}(\boldsymbol{x})$, due to the characteristic 2), we use Quasi-Newton methods.

To estimate the Jacobian matrix, one can define different suitable properties. In most cases, it is not sufficient to define one unique estimate for the Jacobian by imposing those properties. We add the Least Change principle: the new estimate of the Jacobian is the matrix that has the desired properties and that is the closest to the previous estimate in a given norm.

The choice of the estimate of the Jacobian matrix can thus be summarized as:

$$\begin{aligned} \arg\min_{B_{i+1}} \quad & \tfrac{1}{2}\|B_i - B_{i+1}\|_F^2 \\ \textit{such that} \quad & \text{some properties} \end{aligned}$$

where "some properties" lists the properties we want to be

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N. Boutet and R. Haelterman are with Royal Military Academy, Brussels, and University Ghent, Belgium (e-mail: Nicolas.boutet@ugent.be).
J. Degroote is with University of Ghent, Belgium.

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fulfilled.

Overviews of Quasi-Newton Least Change methods and of the properties that can be used are available in [11]-[13]. We list some of them.

1) In optimization, the matrix B_{i+1} is a symmetric matrix (called Hessian matrix). This property can be written as $B_{i+1} = B_{i+1}^T$.
2) Another interesting property, used in the well-known Broyden's good method [14]-[15], consists in using the information available from the previous step on the optimization path by choosing the estimate such that $B_{i+1}\boldsymbol{s}_i = \boldsymbol{y}_i$ *where* $\boldsymbol{s}_i = \boldsymbol{x}_i - \boldsymbol{x}_{i-1}$ *and* $\boldsymbol{y}_i = \boldsymbol{f}(\boldsymbol{x}_i) - \boldsymbol{f}(\boldsymbol{x}_{i-1})$. This is called Secant Update.
3) Using multiple previous points on the optimization path, the previous property can be generalized to multiple secant equations $B_{i+1}\mathbf{s}_k = \mathbf{y}_k$ for $k = 1 \dots m \leq n$. Grouping the vectors into a matrix, this can be reformulated as $B_{i+1}S_i = Y_i$. We call the methods using this generalisation multisecant methods [1], [2], [16]-[17].

One can of course combine some of those properties. The Powell-Symmetric-Broyden (PSB) method, for instance, uses the combination of the Least Change principle, the symmetry and the Secant Update property [18], [19].

Our objective is to improve PSB by combining the least change and multisecant properties with the symmetry, which would lead to a generalized PSB (gPSB).

$$\begin{aligned} \arg\min_{B_{i+1}} \quad & \tfrac{1}{2}\|B_i - B_{i+1}\|_F^2 \\ \textit{such that} \quad & B_{i+1} = B_{i+1}^T \\ & B_{i+1}S_i = Y_i \end{aligned} \tag{2.1}$$

Unfortunately, it has already been proved by Schnabel that the system (2.1) can only be solved if $Y_i^T S_i$ is symmetric, which is a very restrictive condition [20].

Our strategy in order to tackle the impossibility of the construction of a gPSB update formula is to develop a multisecant version of PSB as close as possible of being symmetric and a symmetric version as close as possible of satisfying the multisecant condition.

III. Generalized PSB

In order to combine the different characteristics that we want to give to the new update formula, we will use a method called the alternating projections. It is the successive projection P_i of a point x on different subspaces (K_i). Each projection maps x to the point $P_i x \in K_i$, the closest to x. If we note ${}_jB$, the j-th projection of B on K_i and we project alternatively on K_1 and K_2, the alternating projections lead to the following sequence of matrices.

$${}_0B \rightarrow {}_1B_{K_1} \rightarrow {}_1B_{K_2} \rightarrow {}_2B_{K_1} \rightarrow {}_2B_{K_2} \rightarrow \cdots$$

We start with a generalisation of Broyden's update formula [14]-[15]. Broyden's update formula is a Secant Update formula. The generalisation we use is a multisecant version of the same formula. It projects a matrix ${}_jB$ on a matrix ${}_{j+1}B$ such that to ${}_{j+1}BS_i = Y_i$.

$${}_{j+1}B = {}_jB + (Y_i - {}_jBS_i)(S_i^T S_i)^{-1} S_i^T \tag{3.1}$$

As the previous formula is not symmetric, we combine it with a projection that creates a symmetric matrix. This is given by the formula (3.2).

$${}_j\bar{B} = \tfrac{1}{2}({}_jB + {}_jB^T) \tag{3.2}$$

Taking ${}_0B$ symmetric, alternating formula (3.1) and (3.2) and taking the limit of the sequence leads to the following two expressions.

$$\begin{aligned} {}_\infty B &= {}_0B - {}_0BS_iS_i^+ - (S_i^+)^T S_i^T {}_0B + Y_iS_i^+ + (S_i^+)^T Y_i^T \\ &\quad + (S_i^+)^T S_i^T {}_0BS_iS_i^+ - (S_i^+)^T Y_i^T S_i S_i^+ \end{aligned} \tag{3.3}$$

$$\begin{aligned} {}_\infty \bar{B} &= {}_0B - {}_0BS_iS_i^+ - (S_i^+)^T S_i^T {}_0B + Y_iS_i^+ + (S_i^+)^T Y_i^T \\ &\quad + (S_i^+)^T S_i^T {}_0BS_iS_i^+ - \tfrac{(S_i^+)^T Y_i^T S_i S_i^+}{2} - \tfrac{(S_i^+)^T S_i^T Y_i S_i^+}{2} \end{aligned} \tag{3.4}$$

In the previous formulas, we used the Moore-Penrose pseudo-inverse $S^+S = I$ where $S^+ = (S^TS)^{-1}S^T$. Based on characteristic 4) in Section I, we consider that the cost of the needed inversion is negligible compared to the calculation of the function value and gradient value.

Formula (3.2) is symmetric and, because of its construction with alternating projection, it is as close as possible to the set of multisecant matrices. From this equation, we can then build a Quasi-Newton update formula which we call this formula gPSB Sym (3.5). Expressed formally, it gives:

Let $B_i \in \mathbb{R}^{n\times n}$, B_i *symmetric,* Y_i *and* $S_i \in \mathbb{R}^{n\times m}$, *with* $m \leq n$ *and* S_i *full-rank. Let* $K_{Sym \triangleright MS}$ *be the set of matrices* B *such that:*

- B *is symmetric*
- B *is the closest to the set* $K_{MS} = \{A \in \mathbb{R}^{n\times n}: AS_i = Y_i\}$

Then, $B_{i+1} \in K_{Sym \triangleright MS}$ *such that* $\|B_{i+1} - B_i\|_F$ *is minimal is given by*

$$\begin{aligned} B_{i+1} &= B_i - B_iS_iS_i^+ - (S_i^+)^T S_i^T B_i + Y_iS_i^+ + (S_i^+)^T Y_i^T \\ &\quad + (S_i^+)^T S_i^T B_iS_iS_i^+ - \tfrac{(S_i^+)^T Y_i^T S_i S_i^+}{2} - \tfrac{(S_i^+)^T S_i^T Y_i S_i^+}{2} \end{aligned} \tag{3.5}$$

On the other hand, equation (3.3) fulfils the multisecant condition ${}_\infty BS_i = Y_i$. By its construction, it is as close as possible to the set of symmetric matrices. From this equation, we can then build a second Quasi-Newton update formula which we call gPSB MS (3.6). Formally:

Let $B_i \in \mathbb{R}^{n\times n}$, B_i *symmetric,* Y_i *and* $S_i \in \mathbb{R}^{n\times m}$, *with* $m \leq n$ *and* S_i *full-rank. Let* $K_{MS \triangleright Sym}$ *be the set of matrices* B *such that:*

- $BS_i = Y_i$
- B *is the closest to the set* $K_{Sym} = \{A \in \mathbb{R}^{n\times n}: A = A^T\}$

Then, $B_{i+1} \in K_{MS \triangleright Sym}$ *such that* $\|B_{i+1} - B_i\|_F$ *is minimal is given by:*

TABLE I: OVERVIEW OF THE FORMULAS

Formula	Secant Update	Multi Secant	Sym	Ref
PSB	YES	NO	YES	[12]-[13]
gPSB	YES	YES	YES	UC** [14]
gPSB Sym	NO	ACAP*	YES	(3.5)
gPSB MS	YES	YES	ACAP*	(3.6)
SUgPSB	YES	YES	YES	(4.4)

*ACAP= As close as possible

**UC= Under condition $Y_i^T S_i$ is symmetric

$$\begin{aligned} B_{i+1} &= B_i - B_i S_i S_i^+ - (S_i^+)^T S_i^T B_i + Y_i S_i^+ + (S_i^+)^T Y_i^T \\ &+ (S_i^+)^T S_i^T B_i S_i S_i^+ - (S_i^+)^T Y_i^T S_i S_i^+ \qquad (3.6) \end{aligned}$$

The two formulas being different, it confirms the conclusion of Schnabel [20]. We can also easily check that (3.5) and (3.6) are identical if and only if $Y_i^T S_i = S_i^T Y_i$, which is the symmetry condition we mentioned at the end of Section II.

IV. SECANT UPDATE GENERALIZED PSB

Compared to PSB, the gPSB Sym update formula (3.5) has one drawback. Indeed, while PSB is a Secant Update formula, gPSB Sym is not. So, if we want to maximize the amount of information from the previous steps when building the estimate of the Hessian matrix, we should add the Secant update property to (3.5).

Therefore, we apply the alternating projections again. The first projection we use, is a generalisation of PSB for a non-symmetrical start. In fact, we simply apply the formula (3.2) on the previous matrix ${}_jB$ before applying the PSB update formula. The projection is given by:

$$ {}_{j+1}B = {}_j\bar{B} + \frac{\bar{\mathbf{w}}_i \mathbf{s}_i^T}{\mathbf{s}_i^T \mathbf{s}_i} + \frac{\mathbf{s}_i \bar{\mathbf{w}}_i^T}{\mathbf{s}_i^T \mathbf{s}_i} - \frac{\bar{\mathbf{w}}_i^T \mathbf{s}_i}{(\mathbf{s}_i^T \mathbf{s}_i)^2} \mathbf{s}_i \mathbf{s}_i^T \qquad (4.1)$$

where $\bar{\mathbf{w}}_i = \mathbf{y}_i - {}_j\bar{B}\mathbf{s}_i$.

For the second projection, we use the equation (3.3). This projection is better than (3.1) because apart from the multisecant properties the expression is already as close as possible to a symmetric matrix.

Writing ${}_0\bar{B} = \frac{{}_0B + {}_0B^T}{2}$, the limit of the new sequence leads to the following two expressions.

$$\begin{aligned} {}_\infty B &= {}_0\bar{B} - {}_0\bar{B} S_i S_i^+ - (S_i^+)^T S_i^T {}_0\bar{B} + Y_i S_i^+ + (S_i^+)^T Y_i^T \\ &+ (S_i^+)^T S_i^T {}_0\bar{B} S_i S_i^+ - (S_i^+)^T Y_i^T S_i S_i^+ \qquad (4.2) \end{aligned}$$

$$\begin{aligned} {}_\infty\bar{B} &= {}_0\bar{B} - {}_0\bar{B} S_i S_i^+ - (S_i^+)^T S_i^T {}_0\bar{B} + Y_i S_i^+ + (S_i^+)^T Y_i^T \\ &+ (S_i^+)^T S_i^T {}_0\bar{B} S_i S_i^+ - \frac{(S_i^+)^T S_i^T Y_i S_i^+}{2} - \frac{(S_i^+)^T Y_i^T S_i S_i^+}{2} \\ &+ \frac{(S_i^+)^T S_i^T \mathbf{y}_i \mathbf{s}_i^T}{2\mathbf{s}_i^T \mathbf{s}_i} + \frac{\mathbf{s}_i \mathbf{y}_i^T S_i S_i^+}{2\mathbf{s}_i^T \mathbf{s}_i} - \frac{(S_i^+)^T Y_i^T \mathbf{s}_i \mathbf{s}_i^T}{2\mathbf{s}_i^T \mathbf{s}_i} - \frac{\mathbf{s}_i \mathbf{s}_i^T Y_i S_i^+}{2\mathbf{s}_i^T \mathbf{s}_i} \end{aligned} \qquad (4.3)$$

In the same way as we have defined a pair of formulas for gPSB, we can now define a pair of formulas of SUgPSB.

Equation (4.3) gives a symmetric expression. Noting that $S_i S_i^+ \boldsymbol{s}_i = \boldsymbol{s}_i$ and $Y_i S_i^+ \boldsymbol{s}_i = \boldsymbol{y}_i$, we can easily check that it satisfies the Secant Update equation ${}_\infty B \mathbf{s}_i = \mathbf{y}_i$. Thanks to the way we construct it, we also know it is as close as possible to satisfy multiple secant equations. We can thus build a Secant Update version of generalized PSB Sym (SUgPSB Sym):

Let $B_i \in \mathbb{R}^{n\times n}$, $\bar{B}_i = \frac{B_i + B_i^T}{2}$, Y_i and $S_i \in \mathbb{R}^{n\times m}$ with $m \le n$, $\boldsymbol{s}_i$ the last column of S_i, $\boldsymbol{y}_i$ the last column of Y_i and S_i full-rank. Let $K_{SymSUcMS}$ be the set of matrices B such that:

- *B is symmetric*
- *$B\boldsymbol{s}_i = \boldsymbol{y}_i$*
- *B is the closest to the set $K_{MS} = \{A \in \mathbb{R}^{n\times n}: AS_i = Y_i\}$*

Then, $B_{i+1} \in K_{SymSUcMS}$, such that $\|B_{i+1} - B_i\|_F$ is minimal, is given by:

$$\begin{aligned} \bar{B}_{i+1} &= \bar{B}_i - \bar{B}_i S_i S_i^+ - (S_i^+)^T S_i^T \bar{B}_i + Y_i S_i^+ + (S_i^+)^T Y_i^T \\ &+ (S_i^+)^T S_i^T \bar{B}_i S_i S_i^+ - \frac{(S_i^+)^T S_i^T Y_i S_i^+}{2} - \frac{(S_i^+)^T Y_i^T S_i S_i^+}{2} \\ &+ \frac{(S_i^+)^T S_i^T \mathbf{y}_i \mathbf{s}_i^T}{2\mathbf{s}_i^T \mathbf{s}_i} + \frac{\mathbf{s}_i \mathbf{y}_i^T S_i S_i^+}{2\mathbf{s}_i^T \mathbf{s}_i} - \frac{(S_i^+)^T Y_i^T \mathbf{s}_i \mathbf{s}_i^T}{2\mathbf{s}_i^T \mathbf{s}_i} - \frac{\mathbf{s}_i \mathbf{s}_i^T Y_i S_i^+}{2\mathbf{s}_i^T \mathbf{s}_i} \end{aligned} \qquad (4.4)$$

We see that (4.2) is identical to (3.3). This is quite logical as gPSB MS already satisfies the Secant Update property. So, the update formula SUgPSB MS is the same as gPSB MS (3.3).

One can easily verify that SUgPSB Sym (4.4) and SUgPSB MS (3.3) are equal if and only if $S_i Y_i^T = Y_i S_i^T$. This is the same result as for gPSB Sym and gPSB MS.

Based on the two previous remarks, since SUgPSB MS does not bring any improvement compared to SUgPSB, we will use the acronym SUgPSB to refer to SUgPSB Sym.

In order to help the reader to compare the properties of the different formulas exposed in this article, we provide a summary in Table I.

V. NUMERICAL EXPERIMENTS

To test the robustness of the algorithms we make use of a set of 146 unconstrained problems of the type "sum of squares" from the CUTEst collection [21]. Where it was possible to choose, we took the highest dimension from the standard available values in CUTEst. We used four different standard starting points. Testing the performance of the algorithms for different starting points helps to test the robustness by multiplying the number of test cases.

We have implemented PSB, gPSB Sym (3.5), gPSB MS (3.6), SUgPSB (4.4) and BFGS.

The algorithms are written in Matlab and the scripts have been run on a HPC cluster. An optional line search of the type MINPACK [22] is included within the algorithm. A QR filtering [23] makes it possible to avoid ill-conditioning, which arises when constituent vectors (secant equations) of the matrices S_i and Y_i become (nearly) linearly dependent.

The initial approximation for the Hessian is $B_0 = I$. The iteration is terminated when $||\nabla g(\mathbf{x}_i)||_2 \le \gamma$ or after n_g gradient function calls. To limit the number of multisecant equations, we used $m = 2,4,8,16$.

Thanks to characteristic 4) in Secton I, the efficiency is compared on Performance Profiles based on the number of gradient function calls [24]-[25]. We apply the fixed-cost approach mentioned in [24] with a 1% tolerance as the solutions of the problems are not known in advance.

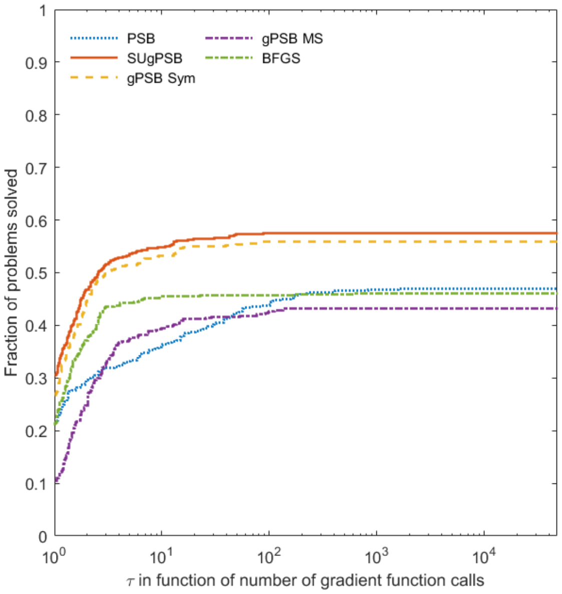

Fig. 1. Performance Profiles for m=16, $\gamma = 10^{-6}$, $n_g = 5 \times 10^5$.

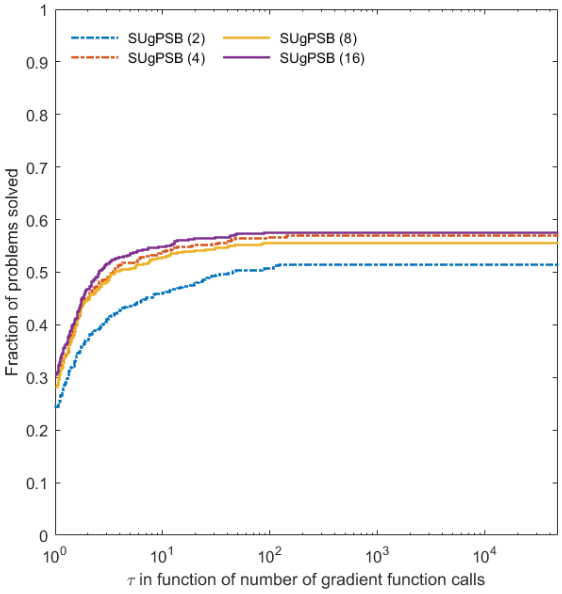

Fig. 2. Performance profiles for $\gamma = 10^{-6}$, $n_g = 5 \times 10^5$. Value of m is given into brackets in the legend.

The results of the algorithm using the different update formulas are given in Fig. 1. For a value τ, the graph gives the fraction of tested problems solved by the given algorithm in less than $\tau \times n_{min}$ gradient function calls where n_{min} is the number of needed gradient function calls for the most efficient tested algorithm on this problem. If the curve is higher, the algorithm solves more problems. If the curve is more on the left side, the algorithm solves the problems more quickly.

First of all, we observe an important difference between gPSB Sym and gPSB MS. The symmetrical version of the formula performs a lot better than the multisecant one. In our applications, the symmetric property seems to be more important than the multisecant property.

Next, we observe that the two symmetric formulas being as close as possible to satisfy multiple secant equations, gPSB Sym (3.5) and SUgPSB (4.4), outperform the classical non-multisecant formulas (PSB and BFGS). The addition of pieces of information coming from extra secant equations seems to make the difference with PSB.

Finally, to a lesser degree, adding the secant update property to transform gPSB Sym into SUgPSB slightly improves the performance. Our tests also show that the choice of m has a bigger influence on the performance of gPSB Sym than on SUgPSB. This tends to indicate that the Secant Update property contributes to the stability of the method.

Fig. 2 shows the Performance Profiles of SUgPSB for increasing values of m. We clearly see that an increasing value of m improves the performance of the algorithm. So adding more secant equations helps to define a better estimate of the Hessian.

The rate of improvement is however decreasing with the value of m. The contribution of extra secant equations (so older secant equation on the optimization path) is less important. Moreover, depending on the problem, we found out that sooner or later adding extra secant equations begins to degrade the efficiency of the algorithm.

This is a consequence of the construction of SUgPSB. The formula is as close as possible to satisfy multiple secant equations at once. Additional older secant equations have the same importance as the most recent one, because we minimize $\|B_{i+1}S_i - Y_i\|_F$ which encompasses every secant equation at once. Adding too old equations corresponds to introducing obsolete information, that will offset and eventually outweigh useful information. By adding too many secant equations, we finally degrade the quality of the estimate of the Hessian.

As a further improvement we could try to implement some kind of forgetting mechanism in order to mitigate the impact of secant equations that are too old.

VI. Conclusion

Our objective was to improve the PSB Quasi-Newton update formula by adding information from the former secant equations from the optimization path (multisecant property). As it is impossible to impose both symmetry and multisecant at the same time in general, we have enforced one of them and tried to be as closed as possible to the other one. This leads to gPSB Sym and gPSB MS.

In a second phase, we added the Secant Update property to gPSB Sym, which was missing in the previous approach, in order to create the SUgPSB formula that can be seen as a generalisation of PSB being as close as possible to satisfy multiple secant equations.

Finally, SUgPSB, used with a limited number of secant equations, clearly outperforms the existing PSB formula, the two versions of the gPSB we also developed, and even BFGS as shown by the numerical experiments.

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Nicolas Boutet obtained a MScEng degree at the Royal Military Academy, Brussels, Belgium in 2007. In 2017, he also obtained a second MScEng in applied mathematics at UCLouvain, Louvain-la-Neuve, Belgium. He is currently working on a Ph.D. thesis about Quasi-Newton optimization, in collaboration between the Royal Military School and the University of Ghent, Belgium.

He works as an ERP specialist for material, operations and maintenance management for the Directorate General Material Resources of Belgian Defense.

Rob Haelterman obtained MScEng degree from the Royal Military Academy in 1998. He graduated for the course in Fluid Dynamics at the von Karman Institute for Fluid Dynamics, Belgium, in 2005. In 2009, he obtained a Ph.D. at Royal Military Academy and University of Ghent, Belgium. His research concerns numerical methods for interaction problems, unmanned vehicles, extended reality and hyperspectral imaging.

He is currently military professor, the head of the Chair of Theoretical Mathematics and the head of the Extended Reality Lab at the Royal Military Academy, Belgium. He teaches, among other things, algebra and numerical analysis.

Joris Degroote obtained a MScEng degree and a Ph.D. in electromechanical engineering at University of Ghent, Belgium, respectively in 2006 and 2010. His research is focused on numerical simulation of fluid-structure interaction (FSI) using computational fluid dynamics and computational solid mechanics, with focus on the fluid mechanics. He develops quasi-Newton algorithms for partitioned simulation of FSI and apply them in various fields.

He is since 2020 full professor at the Department of Electromechanical Systems and Metal Engineering of University of Ghent, where he has been associate professor since 2013. He teaches, among other things, fluid mechanics and numerical optimisation. He also teaches fluid-structure intercation for Industrial applications at von Karman Institute for fluid dynamics, Belgium.