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ON THE STRUCTURE OF VARIABLE METRIC UPDATES

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Abstract: The key idea of the material presented in the paper is that all commonly used variable metric updates consist of the projection part that nullifies vector parallel to differences of the derivatives of the minimized function and the second one (the same for all known formulae) ensuring verification of the quasi-Newton condition at each step of the method.

In the paper a new class of updates ensuring inheritance of the conjugacy property (when applied to a strictly convex QP problem with exact directional minimization) is introduced. Its properties are analysed and some preliminary computational results on some test problems suggested by Moré [4] are reported.

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1. Introduction

The current paper is a continuation of the research inspirated by the numerical experience with the problem of determining stresses in RC ring sections with openings (see Lechman and Stachurski [3] and Stachurski and Lechman [6]). The least squares approach and application of the BFGS quasi-Newton update in most cases has failed. Funally the BFGS and Hooke+Jeeves methods have been used to locate the starting point to the Brozden secant method for solving

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sets of nonlinear equations directly.

In Stachurski [7] a new update using an ortohogonal projection has been proposed. However the resulting updating formula is not fully satisfactory. It preserves symmetry and strict positive definiteness of the approximating matrix. However it seems to be impossible to prove inheritance of the conjugacy property of the previous search directions. In the current paper we propose another affine projection matrix. This leads to a new class of variable metric updates, totally different from the existing ones.

2. Analysis of the Projection Part of the Variable Metric Updates

In what follows we shall use the following notation

— $\boldsymbol{s}_k = \boldsymbol{x}^{k+1} - \boldsymbol{x}^k$ – change in $\boldsymbol{x}$ during the k-th iteration;

— $\boldsymbol{r}_k = \nabla f\left(\boldsymbol{x}^{k+1}\right) - \nabla f\left(\boldsymbol{x}^k\right)$ – change in the derivatives values during the k-th iteration.

It has been proved in Stachurski [7] that the BFGS updating formula

$$\begin{aligned} \boldsymbol{H}^{k+1}_{BFGS} &= \boldsymbol{H}^k + \left(1 + \frac{\boldsymbol{r}_k^T \boldsymbol{H}^k \boldsymbol{r}_k}{\boldsymbol{r}_k^T \boldsymbol{s}_k}\right) \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k} \\ &\quad - \frac{\boldsymbol{s}_k \boldsymbol{r}_k^T \boldsymbol{H}^k + \boldsymbol{H}^k \boldsymbol{r}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k} \end{aligned} \tag{1}$$

may be equivalently expressed as follows

$$\boldsymbol{H}^{k+1} = \left(\boldsymbol{P}^k\right)^T \boldsymbol{H}^k \boldsymbol{P}^k + \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k}, \quad \text{where} \quad \boldsymbol{P}^k = \boldsymbol{I} - \frac{\boldsymbol{r}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k}. \tag{2}$$

Similarly for the DFP update

$$\boldsymbol{H}^{k+1}_{DFP} = \boldsymbol{H}^k - \frac{\boldsymbol{H}^k \boldsymbol{r}_k \boldsymbol{r}_k^T \boldsymbol{H}^k}{\boldsymbol{r}_k^T \boldsymbol{H}^k \boldsymbol{r}_k} + \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k} \tag{3}$$

it has been shown in [7] that the flowing representation is valid although it is not so straightforward

$$\boldsymbol{H}^{k+1} = \left(\boldsymbol{P}^k\right)^T \boldsymbol{H}^k \boldsymbol{P}^k + \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k}, \quad \text{where} \quad \boldsymbol{P}^k = \boldsymbol{I} - \frac{\boldsymbol{r}_k \boldsymbol{r}_k^T \boldsymbol{H}^k}{\boldsymbol{r}_k^T \boldsymbol{H}^k \boldsymbol{r}_k}. \tag{4}$$

The conclusion is that both BFGS and DFP updates have the same structure – they consist of the projection part and the second term (the same for both updates) $\frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k}$, which ensures verifcation of the so-called quasi-Newton condition

$$\boldsymbol{H}^{k+1}\boldsymbol{r}_k = \boldsymbol{s}_k\,.$$

The same conclusion is valid for the Broyden's Θ-family of updates

$$\begin{aligned}\boldsymbol{H}^{k+1} \;=\; & \boldsymbol{H}^k + \left(1 + \Theta^k \frac{\boldsymbol{r}_k^T \boldsymbol{H}^k \boldsymbol{r}_k}{\boldsymbol{r}_k^T \boldsymbol{s}k}\right) \frac{\boldsymbol{s}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k} \\ & - \left(1 - \Theta^k\right) \frac{\boldsymbol{H}^k \boldsymbol{r}_k \boldsymbol{r}_k^T \boldsymbol{H}^k}{\boldsymbol{r}_k^T \boldsymbol{s}_k} - \Theta^k \frac{\boldsymbol{s}_k \boldsymbol{r}_k^T \boldsymbol{H}^k + \boldsymbol{H}^k \boldsymbol{r}_k \boldsymbol{s}_k^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k}\end{aligned} \tag{5}$$

because it is the convex linear combination of the BFGS and DFP updating formulae.

One can use any other projection $\boldsymbol{P}$ in the updating formula of the BFGS update and obtain a new family of variable metric methods

$$\boldsymbol{H}^{k+1} = \left(\boldsymbol{P}^k\right)^T \boldsymbol{H}^k \boldsymbol{P}^k + \frac{\boldsymbol{s}_k \left(\boldsymbol{s}_k\right)^T}{\boldsymbol{r}_k^T \boldsymbol{s}_k}\,. \tag{6}$$

In particular one may apply projection $\boldsymbol{P}^k$ of a similar structure as in BFGS and DFP updates

$$\boldsymbol{P}^k = \boldsymbol{I} - \frac{\boldsymbol{r}_k \boldsymbol{a}^T}{\boldsymbol{r}_k^T \boldsymbol{a}}\,. \tag{7}$$

As $\boldsymbol{a}$ one may take any vector which is not parallel to $\boldsymbol{r}_k$. BFGS update is represented by vector $\boldsymbol{a} = \boldsymbol{s}_k$ and DFP update corresponds to $\boldsymbol{a} = \boldsymbol{H}^k \boldsymbol{r}_k$. Therefore it is suggested to use linear combination of those vectors and take

$$\boldsymbol{P}^k = \boldsymbol{I} - \frac{\boldsymbol{r}_k \left(\alpha_1 \boldsymbol{s}_k + \alpha_2 \boldsymbol{H}^k \boldsymbol{r}_k\right)^T}{\left(\boldsymbol{r}_k\right)^T \left(\alpha_1 \boldsymbol{s}_k + \alpha_2 \boldsymbol{H}^k \boldsymbol{r}_k\right)}\,. \tag{8}$$

In contrary to the orthogonal projection proposed and analysed in Stachurski [7] this family of updates preserves the conjugacy property in the case of quadratic programming problems and exact directional minimization.

3. Properties of the New Class of Updates

Under mild assumptions matrices generated according to formula (6) preserve positive definiteness. This is stated as the following lemma.

Lemma 1. *Let vectors $\boldsymbol{r}_k$ and $\boldsymbol{s}_k$ verify the inequality $\boldsymbol{r}_k^T \boldsymbol{s}_k > 0$ and let the matrix $\boldsymbol{H}^k$ be strictly positive definite.*

Then for any form of a well-defined projection $\boldsymbol{P}^k$ the new update $\boldsymbol{H}^{k+1}$ is also strictly positive definite.

Proof. Let us take any nonzero vector $\boldsymbol{x} \in R^n$ and split it into two parts – $\boldsymbol{x}_1$ orthogonal to vector $\boldsymbol{r}_k$ and $\boldsymbol{x}_2 = \beta \boldsymbol{r}_k$ parallel to $\boldsymbol{r}_k$.

Then making use of the $\boldsymbol{x}$ splitting and projection $\boldsymbol{P}^k$ definition implies

$$\boldsymbol{x}^T \boldsymbol{H}^{k+1} \boldsymbol{x} = \boldsymbol{x}^T \left(\boldsymbol{P}^k\right)^T \boldsymbol{H}^k \boldsymbol{P}^k \boldsymbol{x} + \frac{\left(\boldsymbol{x}^T \boldsymbol{s}\right)^2}{\boldsymbol{r}_k^T \boldsymbol{s}_k} = \boldsymbol{x}_1^T \boldsymbol{H}^k \boldsymbol{x}_1 + \frac{\left(\boldsymbol{x}^T \boldsymbol{s}\right)^2}{\boldsymbol{r}_k^T \boldsymbol{s}_k} .$$

Both terms are greater than or equal to 0. If $\boldsymbol{x}_1 \neq \mathbf{0}$ strict positive definiteness of $\boldsymbol{H}^k$ implies that the first term s greater than 0. In the opposite case $\boldsymbol{x}_2$ should be nonzero and consequently $\beta \neq 0$. Therefore the second term will assume the form

$$\frac{\left(\boldsymbol{x}^T \boldsymbol{s}\right)^2}{\boldsymbol{r}_k^T \boldsymbol{s}} = \beta^2 \frac{\left[\boldsymbol{r}_k^T \boldsymbol{s}\right]^2}{\boldsymbol{r}_k^T \boldsymbol{s}} = \beta^2 \boldsymbol{r}_k^T \boldsymbol{s}$$

which is greater than 0 by the assumption.

Hence in both cases $\boldsymbol{x}^T \boldsymbol{H}^{k+1} \boldsymbol{x} > 0$. □

In the proof above the particular form of the projection operator $\boldsymbol{P}^k$ is not important. Therefore thesis of Lemma 1 will be valid for any well-derfined projection operator. Projection given by formula (8) is well-defined if and only if $\boldsymbol{r}_k^T \left(\alpha_1 \boldsymbol{s}_k + \alpha_2 \boldsymbol{H}^k \boldsymbol{r}_k\right) \neq 0$.

Corollary 2. *Search directions generated as* $\boldsymbol{d}^k = -\boldsymbol{H}^k \nabla f\left(\boldsymbol{x}^k\right)$ *with* $\boldsymbol{H}^k$ *updated according to the formula (6) are descent directions.*

3.1. Case of Strictly Convex Quadratic Problems

Let us consider the problem of minimizing a strictly convex quadratic function

$$\min \left\{ f(\boldsymbol{x}) = \frac{1}{2} \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{t}^T \boldsymbol{x} \right\} , \tag{9}$$

where $\boldsymbol{Q}$ is a symmetric, stricty positive definite matrix, i.e.

$$\boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} > 0, \quad \text{for all } \boldsymbol{x} \in R^n, \quad \boldsymbol{x} \neq \mathbf{0} .$$

The theorem below states that directions $\boldsymbol{d}^1, \boldsymbol{d}^2, \ldots, \boldsymbol{d}^n$ generated by the quasi-Newton method with updates defined by (6)-(7) are $\boldsymbol{Q}$-conjugate.

Theorem 3. *Let us consider the QP problem (9) with* $\boldsymbol{Q}$ *strictly positive definite. Suppose that the problem is solved by the quasi-Newton method with updates defined by* (6)-(8), *starting with an initial point* $\boldsymbol{x}^1$ *and a symmetric, strictly positive definite matrix* $\boldsymbol{H}^1$. *Let for* $k = 1, 2, \ldots, n$ τ^k *be an optimal solution to the directional minimization problem* $\min_{\tau \in R^1} f\left(x^j + \tau * \boldsymbol{d}^k\right)$ *and let* $\boldsymbol{x}^{k+1} = \boldsymbol{x}^k + \tau^k \boldsymbol{d}^k$, *where* $\boldsymbol{d}^k = -\boldsymbol{H}^k \nabla f(\boldsymbol{x}^k)$ *and* $\boldsymbol{H}^k$ *is updated using* *formulae* (6)-(8). *If* $\nabla f(\boldsymbol{x}^k) \neq \mathbf{0}$ *for each* k, *then the directions* $\boldsymbol{d}^1, \boldsymbol{d}^2, \ldots, \boldsymbol{d}^n$ *are* $\boldsymbol{Q}$*-conjugate and* $\boldsymbol{H}^{n+1} = \boldsymbol{Q}^{-1}$. *Furthermore,* $\boldsymbol{x}^{n+1}$ *is the optimal solution to the problem.*

Proof. We first prove by induction that the following conditions are verified for every k, $1 \leq k \leq n$:

1. $\boldsymbol{d}^1, \ldots, \boldsymbol{d}^k$ are linearly independent,
2. $\left(\boldsymbol{d}^i\right)^T \boldsymbol{Q}\boldsymbol{d}^j = 0$ for $i \neq j$, $i, j \leq k$,
3. $\boldsymbol{H}^{k+1}\boldsymbol{Q}\boldsymbol{s}_i = \boldsymbol{H}^{k+1}\boldsymbol{r}_i = \boldsymbol{s}_i$ or, equivalently, $\boldsymbol{H}^{k+1}\boldsymbol{Q}\boldsymbol{d}^i = \boldsymbol{d}^i$ for $1 \leq i \leq k$, where $\boldsymbol{s}_i = \tau^i \boldsymbol{d}^i$.

For $k = 1$, parts 1 and 2 are obvious. To prove part 3, let us set $k = 1$ in formulas (6)-(8)

$$\boldsymbol{H}^2\boldsymbol{Q}\boldsymbol{s}_1 = \left(\boldsymbol{P}^1\right)^T \boldsymbol{H}^1\boldsymbol{P}^1\boldsymbol{r}_1 + \frac{\boldsymbol{s}_1\boldsymbol{s}_1^T}{\boldsymbol{r}_1^T\boldsymbol{s}_1}\boldsymbol{r}_1 = \mathbf{0} + \frac{\boldsymbol{s}_1^T\boldsymbol{r}_1}{\boldsymbol{r}_1^T\boldsymbol{s}_1}\boldsymbol{s}_1 = \boldsymbol{s}_1$$

and therefore part 3 is valid for $i = 1$.

Let us assume now that parts 1, 2 and 3 hold for $k < n$. To show that they are valid also for $k+1$, let us recall first that $\nabla f\left(\boldsymbol{x}^{k+1}\right)^T \boldsymbol{d}^i = 0$ for all $i \leq k$ due to the conjugacy assumption and the exact directional minimization (see Fletcher [2]). By the induction hypothesis of part 3, $\boldsymbol{d}^i = \boldsymbol{H}^{k+1}\boldsymbol{Q}\boldsymbol{d}^i$ for $i \leq k$. Multiplying both sides of this equality by $\nabla f\left(\boldsymbol{x}^{k+1}\right)^T$ we obtain the following equality

$$0 = \nabla f\left(\boldsymbol{x}^{k+1}\right)^T \boldsymbol{d}^i = \nabla f\left(\boldsymbol{x}^{k+1}\right)^T \boldsymbol{H}^{k+1}\boldsymbol{Q}\boldsymbol{d}^i = -\boldsymbol{d}^{k+1}\boldsymbol{Q}\boldsymbol{d}^i$$

valid for all $i \leq k$. In view of the induction hypothesis part 2, it shows that part 2 is also valid for $k+1$.

Now, we show, that part 3 holds for $k+1$. Let us take $i \leq k+1$

$$\boldsymbol{H}^{k+2}\boldsymbol{Q}\boldsymbol{s}_i = \left(\boldsymbol{P}^{k+1}\right)^T \boldsymbol{H}^{k+1}\boldsymbol{P}^{k+1}\boldsymbol{Q}\boldsymbol{s}_i + \frac{\boldsymbol{s}_{k+1}\boldsymbol{s}_{k+1}^T}{\boldsymbol{r}_{k+1}^T\boldsymbol{s}_{k+1}}\boldsymbol{Q}\boldsymbol{s}_i\,. \tag{10}$$

For $i = k+1$ the first term in (10) is equal to $\mathbf{0}$, while the second to the desired $\boldsymbol{s}_{k+1}$. Now let us take $i \leq k$. Since part 2 is valid for $k+1$, the second term is equal to $\mathbf{0}$. In the first term

$$\boldsymbol{P}^{k+1}\boldsymbol{Q}\boldsymbol{s}_i = \left(\boldsymbol{I} - \frac{\boldsymbol{r}_{k+1}\left(\alpha_1\boldsymbol{s}_{k+1} + \alpha_2\boldsymbol{H}^{k+1}\boldsymbol{r}_{k+1}\right)^T}{\left(\boldsymbol{r}_{k+1}\right)^T\left(\alpha_1\boldsymbol{s}_{k+1} + \alpha_2\boldsymbol{H}^{k+1}\boldsymbol{r}_{k+1}\right)}\right)\boldsymbol{Q}\boldsymbol{s}_i = \boldsymbol{r}_i$$

because $\boldsymbol{s}_{k+1}^T\boldsymbol{Q}\boldsymbol{s}_i = 0$ and

$$\boldsymbol{r}_{k+1}\boldsymbol{H}^{k+1}\boldsymbol{Q}\boldsymbol{s}_i = \boldsymbol{r}_{k+1}\boldsymbol{s}_i = \boldsymbol{s}_{k+1}\boldsymbol{Q}\boldsymbol{s}_i = 0$$

due to the induction assumption. Hence the first term in (10) becomes

$$\begin{aligned} \left(\boldsymbol{P}^{k+1}\right)^T \boldsymbol{H}^{k+1}\boldsymbol{Q}\boldsymbol{s}_i &= \left(\boldsymbol{P}^{k+1}\right)^T \boldsymbol{s}_i \\ &= \left(\boldsymbol{I} - \frac{\left(\alpha_1 \boldsymbol{s}_{k+1} + \alpha_2 \boldsymbol{H}^{k+1}\boldsymbol{r}_{k+1}\right)\boldsymbol{r}_{k+1}^T}{\boldsymbol{r}_{k+1}^T\left(\alpha_1 \boldsymbol{s}_{k+1} + \alpha_2 \boldsymbol{H}^{k+1}\boldsymbol{r}_{k+1}\right)}\right)\boldsymbol{s}_i = \boldsymbol{s_i} \end{aligned}$$

Hence, part 3 holds for $k+1$.

To close the induction argument it is necessary to show that part 1 is true for $k+1$. Let us assume the existance of a linear combination of $\boldsymbol{d}^i$ vectors summng up to zero $\sum_{i=1}^{k+1} \beta_i \boldsymbol{d}^i = \boldsymbol{0}$. Now, multipication by $\left(\boldsymbol{d}^{k+1}\right)^T \boldsymbol{Q}$ and noting that part 2 is valid for $k+1$, it follows that $\beta_{k+1}\left(\boldsymbol{d}^{k+1}\right)^T \boldsymbol{Q}\boldsymbol{d}^{k+1} = 0$. By assumption $\nabla f\left(\boldsymbol{x}^{k+1}\right) \neq \boldsymbol{0}$, $\boldsymbol{H}^{k+1}$ is strictly positive definite (since $\boldsymbol{r}_{k+1}^T \boldsymbol{s}_{k+1} = \boldsymbol{s}_{k+1}^T \boldsymbol{Q}\boldsymbol{s}_{k+1} > 0$ and Lemma 1 is applicable). Therefore, $\boldsymbol{d}^{k+1} = -\boldsymbol{H}^{k+1}\nabla f\left(\boldsymbol{x}^{k+1}\right) \neq \boldsymbol{0}$. $\boldsymbol{Q}$ is strictly positive defined, hence $\beta_{k+1} = 0$. This implies that $\sum_i^k \beta_i \boldsymbol{d}^i = \boldsymbol{0}$ and $\beta_i = 0$, since vectors $\boldsymbol{d}^1, \ldots, \boldsymbol{d}^k$ are linearly independent by the inductiuon hypothesis. Thus, part 1 holds for $k+1$.

If $k = n$ then $\boldsymbol{H}^{n+1}\boldsymbol{Q}\boldsymbol{d}^i = \boldsymbol{d}^i$ for $i = 1, \ldots, n$ and hence $\boldsymbol{H}^{n+1} = \boldsymbol{Q}^{-1}$ and $\boldsymbol{x}^{n+1}$ is the optimal point of the QP problem. □

4. Preliminary Numerical Results

Program for testing has been prepared in standard *ANSI C* language and the tests were run on the PC computer equipped with the Intel(R) Pentium(R) 4 CPU 3.20GHz processor. During the tests runs the number of steps has been restricted (maximum 2000). In the directional minimization, we have accepted the first point α^i in the sequence of decreasing numbers defined as $\left\{\alpha_s \beta^i\right\}_{i=0}^{\infty}$ (with $\beta \in (0,1)$) verifying the condition

$$f(\boldsymbol{x}^k + \alpha_s \beta^i \boldsymbol{d}^k) \leq f(\boldsymbol{x}^k) + \rho\alpha_s\beta^i \left(\boldsymbol{g}^k\right)^T \boldsymbol{d}^k\,.$$

Tests were run on the first six examples from Moré [4], i.e. Rosenbrock, Freudenstein and Roth, Powell badly scaled, Brown badly scaled, Beale and Jennrich and Sampson functions.

In Table 1 we have collected numbers of iterations of particular methods.

	Function					
Method	Ros.	F&R	Pow.	Brown	Beale	J&S
Ort.Proj.	68	6	113	186	33	32
BFGS	135	5	2000	200	15	26
NPr.($\alpha_1 = 0.5$, $\alpha_2 = 0.5$	91	6	2000	2000	34	40
NPr.($\alpha_1 = 1.0$, $\alpha_2 = -1.0$	110	5	2000	2000	78	247
NPr.($\alpha_1 = 1.0$, $\alpha_2 = 0.1$	113	5	2000	2000	18	27

Table 1:

5. Conclusions

The conclusions stemming from the numerical experiments are not fully satisfactory. Propoosed class of updates is on the test problems almost equally good as of the famous BFGS formula. In our opinion, when we apply an inexact directional minimization, it seems to be necessary to reconsider in the variable metric updates also the term $\frac{\boldsymbol{s}_k(\boldsymbol{s}_k)^T}{(\boldsymbol{r}_k)^T\boldsymbol{s}_k}$ ensuring fullfillment of the quasi-Newton condition.

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