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On the Derivation of Quasi-Newton Formulas for Optimization in Function Spaces

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ABSTRACT

Newton's method is usually preferred when solving optimization problems due to its superior convergence properties compared to gradient-based or derivative-free optimization algorithms. However, deriving and computing second-order derivatives needed by Newton's method often is not trivial and, in some cases, not possible. In such cases quasi-Newton algorithms are a great alternative. In this paper, we provide a new derivation of well-known quasi-Newton formulas in an infinite-dimensional Hilbert space setting. It is known that quasi-Newton update formulas are solutions to certain variational problems over the space of symmetric matrices. In this paper, we formulate similar variational problems over the space of bounded symmetric operators in Hilbert spaces. By changing the constraints of the variational problem we obtain updates (for the Hessian and Hessian inverse) not only for the Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi-Newton method but also for Davidon–Fletcher–Powell (DFP), Symmetric Rank One (SR1), and Powell-Symmetric-Broyden (PSB). In addition, for an inverse problem governed by a partial differential equation (PDE), we derive DFP and BFGS "structured" secant formulas that explicitly use the derivative of the regularization and only approximates the second derivative of the misfit term. We show numerical results that demonstrate the desired mesh-independence property and superior performance of the resulting quasi-Newton methods.

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1. Introduction

In optimization, quasi-Newton methods are a pragmatic alternative to Newton-type methods for problems where the Hessian of the objective

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function is difficult to derive (*e.g.*, for optimization problems constrained by differential equations, which requires a considerable amount of work to setup the numerical evaluation of the second-order derivatives) or is computationally expensive to evaluate. In computational practice, it is often the case that quasi-Newton performs similarly or even outperforms Newton's method: while the iteration count is generally higher for quasi-Newton methods than for Newton-type methods, the cost of one iteration of quasi-Newton methods is generally lower than the cost of a Newton iteration, which may offset the disadvantage of a higher iteration count.

Quasi-Newton methods received considerable attention in the optimization community in the last decades [1]. When applied to the minimization of a twice continuously differentiable function $f(x) : \mathbb{R}^n \to \mathbb{R},$ that is

$$\min_{x \in \mathbb{R}^n} f(x), \tag{1.1}$$

a quasi-Newton method generates a sequence of iterates x_k, $k = \{0, 1, \ldots\},$ by computing a search direction of the form $\Delta x_k = \alpha_k B_k^{-1} \nabla f(x_k),$ and by choosing an appropriate scalar step size α_k that ensures a mininum decrease of the objective *f*(*x*) along the direction Δx_k. Alternatively, the search direction can be in the form $\Delta x_k = \alpha_k H_k \nabla f(x_k)$. The $n \times n$ matrices B_k and H_k are approximations of the Hessian $\nabla^2 f(x_k)$ and its inverse, respectively. The salient idea of quasi-Newton methods is to maintain these approximations by enforcing the secant condition in the form $B_k s_k = y_k$ or $H_k y_k = s_k,$ where

$$s_k = x_{k+1} - x_k \text{ and } y_k = \nabla f(x_{k+1}) - \nabla f(x_k).$$

The Davidon–Fletcher–Powell (DFP) and the Broyden–Fletcher–Goldfarb–Shanno (BFGS) rank-two update formulas have emerged in the last decades [1] as the most efficient and, as a consequence, most comonly used Hessian approximations in a quasi-Newton framework. These formulas have closed-form algebraic forms, namely,

$$\begin{aligned}
B_{k+1}^{DFP} &= (I - \gamma_k y_k s_k^T) B_k (I - \gamma_k s_k y_k^T) + \gamma_k y_k y_k^T, \\
H_{k+1}^{DFP} &= H_k - \frac{H_k y_k y_k^T H_k}{y_k^T H_k y_k} + \gamma_k s_k s_k^T, \\
B_{k+1}^{BFGS} &= B_k - \frac{B_k s_k s_k^T B_k}{s_k^T B_k s_k} + \gamma_k y_k y_k^T, \text{ and} \\
H_{k+1}^{BFGS} &= (I - \gamma_k s_k y_k^T) H_k (I - \gamma_k y_k s_k^T) + \gamma_k s_k s_k^T,
\end{aligned}$$

where $\gamma_k = \frac{1}{s_k^T y_k}$. Other secant formulas that have been proposed and investigated in the past are the symmetric rank-one (SR1) [1] and

Powell–Symmetric–Broyden (PSB) updates [2]. They also have closed-form expressions in the form of

$$B_{k+1}^{PSB} = B_k + \frac{s_k(y_k - B_k s_k)^T + (y_k - B_k s_k)s_k^T}{\langle s_k, s_k\rangle} - \frac{\langle y_k - B_k s_k, s_k\rangle}{\langle s_k, s_k\rangle^2} s_k s_k^T,$$

$$H_{k+1}^{PSB} = H_k + \frac{y_k(s_k - H_k y_k)^T + (s_k - H_k y_k)y_k^T}{\langle y_k, y_k\rangle} - \frac{\langle s_k - H_k y_k, y_k\rangle}{\langle y_k, y_k\rangle^2} y_k y_k^T,$$

$$B_{k+1}^{SR1} = B_k + \frac{(y_k - B_k s_k)(y_k - B_k s_k)^T}{\langle s_k, y_k - B_k s_k\rangle}, \text{ and}$$

$$H_{k+1}^{SR1} = H_k + \frac{(s_k - H_k y_k)(s_k - H_k y_k)^T}{\langle y_k, s_k - H_k y_k\rangle}.$$

Related work. In this paper we consider the optimization problem (1.1) over a separable Hilbert space $\mathcal{H}$, possibly infinite-dimensional, *e.g.*, a function space such as L^2, and derive infinite-dimensional versions of the update formulas above. Central to our derivation is the use of a variational, least-squares approach that was first introduced by Güler et al. for finite-dimensional optimization problems [3]. To this extent the present work can be seen as a generalization of the work presented in [3] to an infinite-dimensional optimization setting. Some of the infinite-dimensional quasi-Newton formulas we derive in this work have previously appeared in the literature. In [4], for example, the authors use the class of variable metric methods, of which the BFGS, DFP, and Symmetric Rank One (SR1) formulas are members, for control problems over function spaces, while Broyden updates are proposed in [5] for solving nonlinear operator equations in Hilbert spaces. In [6] the authors derive the BFGS formula in infinite dimension starting from finite-rank updates and by imposing symmetry and positivity to arrive to desired form. More recently, a survey of quasi-Newton methods in Hilbert spaces is given in [7] with a case study for Riccati matrix equations. The BFGS and DFP formulas are used for optimization problems in a Hilbert space setting also in [8,9]. In [8–10] the authors present an instructive example of the impact of taking into account the infinite-dimensional nature of the underlying optimization problem on the performance of the numerical algorithm leading to mesh-independence. However, these quasi-Newton formulas are typically simply constructed/conjectured in analogy with the finite-dimensional counterparts.

Contributions. To the best of our knowledge, the present work is the first to introduce a formal derivation of BFGS, DFP, SR1, and PSB formulas for infinite-dimensional optimization problems. We note that our derivation can be also used to formally generalize the finite-dimensional limited-memory compact quasi-Newton representations of Byrd et al. [11] to Hilbert spaces. We succinctly do so in Section 4.1. Furthermore, in this paper we also illustrate how the infinite-dimensional least-square variational approach can be used to derive new and improved quasi-Newton formulas that exploit structured Hessians present in some specific classes of optimization problems; in particular, we look at inverse problems governed by partial-differential equations, derive new structured updates that explicitly incorporate the computationally affordable part of Hessian, and show that the new "structured" quasi-Newton formulas improve considerably over the unstructured counterparts.

The remaining sections of this paper are organized as follows. After presenting the requisite background material in section 2, we derive a series of technical results that are crucial for the main results in section 3. In section 4, we derive formally the update formulas for various standard secant formulas over infinite-dimensional Hilbert spaces. In the same section we also show that the limited-memory compact representations for BFGS and DFP can be generalized to Hilbert spaces using the technical results presented in section 3. Finally, in section 5 we exploit the structure present in certain classes of infinite-dimensional inverse problems and show how *structured*, more efficient secant formulas, can be obtained using the variational approach developed in sections 3 and 4. Here we also show numerical results. Section 6 provides concluding remarks.

2. Preliminaries

In this section, we summarize the terminology and background material required for the derivation of the quasi-Newton formulas in infinite-dimensional setting. In what follows, we consider $\mathcal{H}$ and $\mathcal{K}$ separable Hilbert spaces, *i.e.*, they have a countable basis [12].

Definition 2.1. [13, p. 187] The space of all bounded linear operators from $\mathcal{H}$ to $\mathcal{K}$ is denoted by $\mathcal{B}(\mathcal{H},\mathcal{K})$. In particular, the space of all bounded linear operators from $\mathcal{H}$ to itself is denoted by $\mathcal{B}(\mathcal{H})$.

Definition 2.2. [14, p. 60] Let $\mathcal{H}$ be a separable Hilbert space and $\{e_i\}_{i\in I}$ be an orthonormal basis for $\mathcal{H}$. A bounded operator $A\in\mathcal{B}(\mathcal{H})$ is a Hilbert–Schmidt (HS) operator if

$$||A||_{HS} = \sum_{i\in I} ||Ae_i||^2 < \infty. \tag{2.1}$$

We denote the set of all Hilbert–Schmidt operators by $\mathcal{B}_{00}(\mathcal{H})$.

Definition 2.3. [14, p. 60] For any A and $B\in\mathcal{B}_{00}(\mathcal{H})$, the Hilbert–Schmidt inner product is defined as

$$\langle A, B\rangle_{HS} = \sum_{i\in I}\langle Ae_i, Be_i\rangle, \tag{2.2}$$

where $\{e_i\}_{i\in I}$ is an orthonormal basis of $\mathcal{H}$.

Definition 2.4. [15, p. 97] The adjoint of an operator $A \in \mathcal{B}(\mathcal{H})$ is denoted by A^* and is defined as an operator from $\mathcal{B}(\mathcal{H})$ that allows the transformation $\langle Ax, y\rangle = \langle x, A^*y\rangle$ for all x and y in $\mathcal{H}$.

Proposition 2.5. *[14, p. 62] The Hilbert–Schmidt operators form a two-sided ideal in the Banach algebra of bounded operators on $\mathcal{H}$, that is, for any $A \in \mathcal{B}_{00}(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$, one must necessarily have $AB \in \mathcal{B}_{00}(\mathcal{H}), BA \in \mathcal{B}_{00}(\mathcal{H})$, and $A^* \in \mathcal{B}_{00}(\mathcal{H})$.*

Definition 2.6. [16, p. 132] A linear bounded operator $A \in \mathcal{B}(\mathcal{H})$ is positive if $\langle x, Ax\rangle \geq 0$ for all $x \in \mathcal{H}$.

Definition 2.7. [16, p. 263] The square root operator R of symmetric positive A is defined as a symmetric operator such that $R^2 = A$.

Theorem 2.8. *[16, p. 265] If $A \in \mathcal{B}(\mathcal{H})$ is a symmetric positive operator, then there exists a unique positive square root R of A. Furthermore, R commutes with any bounded operator that commutes with A.*

Theorem 2.9. *[16, p. 266] Given any $A \in \mathcal{B}(\mathcal{H})$, the following conditions are equivalent:*

i) *A is invertible;*
ii) *there exists a constant $\alpha > 0$ such that $A^*A \geq \alpha I_{\mathcal{H}}$ and $AA^* \geq \alpha I_{\mathcal{H}}$;*
iii) *there exists a constant $\alpha > 0$ such that*
$$\langle A^*Ax, x\rangle \geq \alpha||x|| \text{ and } \langle AA^*x, x\rangle \geq \alpha||x||;$$
iv) *both operators $A^*A \in \mathcal{B}(\mathcal{H})$ and $AA^* \in \mathcal{B}(\mathcal{H})$ are invertible.*

Following [5, 7, 17], we next define the outer (dyadic) product, which is the correspondent of the rank-one update used with finite-dimensional secant formulas.

Definition 2.10. [14, p. 55] Let $x, y \in \mathcal{H}$. The outer or dyadic product of x and y is the (linear) operator, denoted by $x \otimes y$, that satisfies
$$(x \otimes y)z = \langle y, z\rangle x, \forall z \in \mathcal{H}. \tag{2.3}$$

We note that $x \otimes y$ is a bounded linear operator.

Definition 2.11. [18, p. 41] An operator T is of finite-rank if its range is finite-dimensional.

Example 2.12. The operator $x \otimes y$ is a rank-one operator since it has the range equal to the one-dimensional subspace of $\mathcal{H}$ that is spanned by x.

Remark 2.13. For the vectors $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$, the operator $\sum_{i=1}^n x_i \otimes y_i$ has finite rank of most n.

Remark 2.14. It can be proven that every finite-rank operator is a Hilbert–Schmidt operator [14].

Definition 2.15. [13, p. 110] A linear operator $T : \mathcal{H} \to \mathcal{K}$ is compact if and only if for every bounded sequence $\{x_n\} \in \mathcal{H}$ there exists a subsequence $\{x_{n_k}\}$ such that $T(\{x_{n_k}\})$ converges in $\mathcal{K}$.

Theorem 2.16. *[18, p. 41] If T is a compact operator, then there exists a sequence of finite rank operators $\{T_n\}$ such that $||T - T_n|| \to 0$.*

We now state the Hilbert Projection Theorem, which is one of the key results used by our least-squares variational approach.

Theorem 2.17. *[19, p. 50] Let $\mathcal{H}$ be a Hilbert space and M a closed subspace of $\mathcal{H}$. For any vector $x \in \mathcal{H}$, there is a unique vector $m_0 \in M$ such that $||x - m_0|| \le ||x - m||$ for all $m \in M$. Furthermore, a necessary and sufficient condition to characterize $m_0 \in M$ is that $x - m_0$ is orthogonal to M.*

Finally, the following Theorem states the Sherman–Morrison–Woodbury formula in Banach spaces of linear operators [20]; for compactness, we consider such linear operators to be defined over Hilbert spaces $\mathcal{H}$ and $\mathcal{K}$, however, they can be defined in general over Banach spaces.

Theorem 2.18. *[20, p. 1] Let $A \in \mathcal{B}(\mathcal{H})$ and $G \in \mathcal{B}(\mathcal{K})$ both be invertible and $Y, Z \in \mathcal{B}(\mathcal{K}, \mathcal{H})$. The operator $A + YGZ^*$ is invertible if and only if $G^{-1} + Z^* A^{-1} Y$ is invertible. Furthermore,*

$$(A + YGZ^*)^{-1} = A^{-1} - A^{-1} Y (G^{-1} + Z^* A^{-1} Y)^{-1} Z^* A^{-1}. \tag{2.4}$$

3. Least-squares variational characterization framework for deriving quasi-Newton updates

This section derives intermediary results needed in Section 4 to derive various quasi-Newton update formulas as analytical solutions to infinite-dimensional variational problems. Let us first denote by $\mathcal{B}^s(\mathcal{H})$ the set of bounded linear operators that are *self-adjoint* and consider the linear subspace $\mathcal{L} = \{X \in \mathcal{B}^s(\mathcal{H}) : Xs = 0\}$, which corresponds to the affine subspace given by the secant equation, namely to $\mathcal{A} = \{X \in \mathcal{B}^s(\mathcal{H}) : Xs = y\}$. Furthermore, we define the operators $S_i = s \otimes e_i + e_i \otimes s$ for each $i \in I$, where $\{e_i\}_{i \in I}$ is an (countable) orthonormal basis of the (separable) Hilbert space $\mathcal{H}$.

Lemma 3.1. *If $s, y \in \mathcal{H}$ with $s \neq 0$, then the following statements are true:*

i) $\mathcal{L} = \{X \in \mathcal{B}^s(\mathcal{H}) : \ \langle X, S_i \rangle_{HS} = 0, \ \forall i \in I\}$;
ii) $\mathcal{L}^\perp = \operatorname{span}\{\{S_i\}_{i \in I}\}$;
iii) $\mathcal{L}^\perp = \{s \otimes \lambda + \lambda \otimes s \ : \ \lambda \in \mathcal{H}\}$.

Proof.

(i) We first remark that

$$XS_ie_j = X(s \otimes e_i)e_j + X(e_i \otimes s)e_j = \langle e_i, e_j \rangle Xs + \langle s, e_j \rangle Xe_i \tag{3.1}$$

for any $X \in \mathcal{B}^s(\mathcal{H})$ and $i \in I$. Since $\langle X, S_i \rangle_{HS} = \sum_{j=1}^\infty \langle Xe_j, S_ie_j \rangle = \sum_j \langle e_j, XS_ie_j \rangle$, identity (3.1) allows us to write

$$\langle X, S_i \rangle_{HS} = \sum_{j=1}^\infty \left[\langle e_i, e_j \rangle \langle e_j, Xs \rangle + \langle s, e_j \rangle \langle e_j, Xe_i \rangle \right]. \tag{3.2}$$

Since X is self-adjoint, $\langle e_i, e_j \rangle = 0$ for $i \neq j$, and $\langle e_j, e_j \rangle = 1$, one can subsequently write that

$$\begin{aligned} \langle X, S_i \rangle_{HS} &= \langle e_i, Xs \rangle + \left\langle \sum_{j=1}^\infty \langle s, e_j \rangle e_j, Xe_i \right\rangle \\ &= \langle e_i, Xs \rangle + \langle s, Xe_i \rangle = \langle e_i, Xs \rangle + \langle Xs, e_i \rangle = 2\langle Xs, e_i \rangle. \end{aligned}$$

This shows that $X \in \mathcal{L}$ if and only if $\langle X, S_i \rangle_{HS} = 0$ for all $i \in I$.

(ii) Let $Y \in \operatorname{span}\{\{S_i\}_{i=1}^\infty\}$, namely $Y = \sum_{i=1}^\infty \alpha_i S_i$. Then consider $\langle X, Y \rangle$ for any $X \in \mathcal{L}$, one can write

$$\langle X, Y \rangle = \left\langle X, \sum_{i=1}^\infty \alpha_i S_i \right\rangle = \sum_{i=1}^\infty \alpha_i \langle X, S_i \rangle = 0$$

obtaining $\mathcal{L}^\perp \supseteq \operatorname{span}\{\{S_i\}_{i=1}^\infty\}$. For the other inclusion, let $Y \in \operatorname{span}\{\{S_i\}_{i=1}^\infty\}^\perp$, this implies $\langle Y, S_i \rangle = 0$ for all S_i, *i.e.*, $Y \in \mathcal{L}$. This shows that $\operatorname{span}\{\{S_i\}_{i=1}^\infty\}^\perp \subseteq \mathcal{L}$, taking the orthogonal complement we obtain $\operatorname{span}\{\{S_i\}_{i=1}^\infty\} \supseteq \mathcal{L}^\perp$.

(iii) Consider $Y \in \mathcal{L}^\perp, Y = \sum_{i=1}^\infty \alpha_i S_i$, which we can rewrite as

$$\sum_{i=1}^\infty \alpha_i S_i = \sum_{i=1}^\infty \alpha_i (s \otimes e_i + e_i \otimes s) = (s \otimes \lambda + \lambda \otimes s) \tag{3.3}$$

for some $\lambda = \sum_{i=1}^\infty \alpha_i e_i$. This shows that $\mathcal{L}^\perp \subseteq \{s \otimes \lambda + \lambda \otimes s \ : \ \lambda \in \mathcal{H}\}$. On the other hand, if $Y \in \{s \otimes \lambda + \lambda \otimes s \ : \ \lambda \in \mathcal{H}\}$ and $X \in \mathcal{L}$ we have

$$\langle X,Y\rangle = \langle X, s\otimes\lambda + \lambda\otimes s\rangle = \left\langle X, s\otimes\sum_{i=1}^{\infty}\alpha_i e_i + \sum_{i=1}^{\infty}\alpha_i e_i\otimes s\right\rangle$$
$$= \sum_{i=1}^{\infty}\alpha_i\langle X, s\otimes e_i + e_i\otimes s\rangle = \sum_{i=1}^{\infty}\alpha_i\langle X, S_i\rangle = 0.$$

This completes the proof that $\mathcal{L}^{\perp} = \{s\otimes\lambda + \lambda\otimes s \;:\; \lambda\in\mathcal{H}\}$. □

We now consider a generic least-squares problem that is closely related to the variational problem used to derive the various quasi-Newton formulas in Sections 4 and 5.

Theorem 3.2. *Given $s, y\in\mathcal{H}$, the variational problem*

$$\min_{X\in\mathcal{B}(\mathcal{H})} \frac{1}{2}||X||_{HS}^2 \tag{3.4}$$
$$\text{s.t. } Xs = y \tag{3.5}$$

has a self-adjoint solution operator $\overline{X}\in\mathcal{B}_{00}(\mathcal{H})$ given by

$$\overline{X} = \frac{s\otimes y + y\otimes s}{\langle s,s\rangle} - \frac{\langle y,s\rangle}{\langle s,s\rangle^2}s\otimes s. \tag{3.6}$$

Proof. We note that the set $\mathcal{A} = \{X\in\mathcal{B}(\mathcal{H}) \mid Xs = y\}$ is closed. Let $\overline{X}$ denote a solution of (3.4)-(3.5); such solution necessarily exists per Hilbert projection Theorem [21, p. 80]. We remark that for any $A\in\mathcal{L}$ and for any $t\in\mathbb{R}$, the function $\overline{X}+tA$ satisfies the secant equation (3.5). Let us consider an arbitrary $A\in\mathcal{L}$. Then we obtain by the minimality of $\overline{X}$ that $||\overline{X}||_{HS}^2 \le ||\overline{X}+tA||_{HS}^2$, or, equivalently, that $\langle\overline{X},\overline{X}\rangle_{HS} \le \langle\overline{X}+tA, \overline{X}+tA\rangle_{HS}$ for any $t\in\mathbb{R}$. A simple manipulation of this inequality reveals that one must necessarily have $-2t\langle\overline{X},A\rangle_{HS} \le t^2\langle A,A\rangle_{HS}$ for any $t\in\mathbb{R}$. For positive t, the previous inequality is equivalent to $\langle\overline{X},A\rangle_{HS} \ge -\frac{t}{2}\langle A,A\rangle_{HS}$ and can hold for arbitrarily small t only if $\langle\overline{X},A\rangle_{HS}\ge 0$. Similarly, by taking t to be negative and arbitrarily close to zero, one must necessarily have $\langle\overline{X},A\rangle_{HS}\le 0$. Therefore, we have that $\langle\overline{X},A\rangle_{HS} = 0$. Since A was chosen arbitrary from $\mathcal{L}$, this implies that $\overline{X}\in L^{\perp}$ and thus, based on iii) of Lemma 3.1 that $\overline{X} = s\otimes\lambda+\lambda\otimes s$, for some $\lambda\in\mathcal{H}$.

Next we find an explicit expression for λ. Since $\overline{X}s = y$, we can write

$$\begin{aligned}\langle y,s\rangle = \langle\overline{X}s,s\rangle &= \langle[s\otimes\lambda+\lambda\otimes s]s,s\rangle\\ &= \langle[s\otimes\lambda]s,s\rangle + \langle[\lambda\otimes s]s,s\rangle = \langle\langle\lambda,s\rangle s,s\rangle + \langle\langle s,s\rangle\lambda,s\rangle\\ &= \langle\langle\lambda,s\rangle s,s\rangle + ||s||^2\langle\lambda,s\rangle = 2||s||^2\langle\lambda,s\rangle,\end{aligned}$$

to obtain that $\langle \lambda, s\rangle = \frac{\langle y, s\rangle}{2||s||^2}$. This can be used in conjunction with the secant equation to write that $y = \overline{X}s = [s \otimes \lambda + \lambda \otimes s]s = \langle s, s\rangle\lambda + \langle \lambda, s\rangle s = ||s||^2\lambda + \frac{\langle y, s\rangle}{2||s||^2}s$, from which λ is obtained to be

$$\lambda = \frac{1}{||s||^2}y - \frac{\langle y, s\rangle}{2||s||^4}s.$$

Equation (3.6) follows readily by substituting the above expression for λ in $\overline{X} = \lambda \otimes s + s \otimes \lambda$. Finally, we remark that $\overline{X}$ given by (3.6) is self-adjoint; also, one can easily verify that has rank two, which implies that $\overline{X} \in \mathcal{B}_{00}$ [22]. □

The following corollary offers an analytical expression for the solution of a prototype variational problem and will be the basis of the derivation of quasi-Newton update formulas in generic Hilbert spaces.

Corollary 3.3. *For any given operator $X_0 \in \mathcal{B}^s(\mathcal{H})$ and positive and invertible "weight" operator $W \in \mathcal{B}^s(\mathcal{H})$, the variational problem*

$$\min_{X \in \mathcal{B}(\mathcal{H})} \frac{1}{2}||W^{1/2}(X - X_0)W^{1/2}||_{HS}^2 \tag{3.7}$$

$$\text{s.t.} Xs = y \tag{3.8}$$

admits a solution $\overline{X} \in \mathcal{B}^s(\mathcal{H})$ in the form

$$\overline{X} = X_0 + \frac{W^{-1}s \otimes (y - X_0 s) + (y - X_0 s) \otimes W^{-1}s}{\langle s, W^{-1}s\rangle} - \frac{\langle y - X_0 s, s\rangle}{\langle s, W^{-1}s\rangle^2}W^{-1}s \otimes W^{-1}s.$$

Furthermore, the operator $\overline{X} - X_0$ lies in $\mathcal{B}_{00}(\mathcal{H})$.

Proof. The corollary is a direct consequence of Theorem 3.2. More specifically, since W is invertible and positive, we can write the secant equation (3.8) as

$$W^{1/2}(X - X_0)W^{1/2}(W^{-1/2}s) = W^{1/2}(y - X_0 s).$$

Then Theorem 3.2 implies that a minimizer $\overline{X}$ of (3.7)-(3.8) exists and satisfies

$$W^{1/2}(\overline{X} - X_0)W^{1/2} = \frac{W^{-1/2}s \otimes W^{1/2}(y - X_0 s) + W^{1/2}(y - X_0 s) \otimes W^{-1/2}s}{\langle W^{-1/2}s, W^{-1/2}s\rangle} - \frac{\langle W^{1/2}(y - X_0 s), W^{-1/2}s\rangle}{\langle W^{-1/2}s, W^{-1/2}s\rangle^2}W^{-1/2}s \otimes W^{-1/2}s.$$

The form of $\overline{X}$ from the corollary follows from the above identity by multiplying from left and right with $W^{-1/2}$ and performing appropriate simple algebraic manipulations. We remark that Theorem 3.2 also implies that $W^{1/2}(\overline{X}-X_0)W^{1/2} \in \mathcal{B}_{00}(\mathcal{H})$. This implies that $\overline{X}-X_0 = W^{-1/2}W^{1/2}(\overline{X}-X_0)W^{1/2}W^{-1/2} \in \mathcal{B}_{00}(\mathcal{H})$ since Hilbert–Schmidt operators form an ideal in $\mathcal{B}(\mathcal{H})$ (see Proposition 2.5). □

4. Derivation of various secant update formulas

In this section we derive the quasi-Newton update formulas for approximating a second-order derivative operators defined over generic Hilbert spaces. Corollary 3.3 is used with specific choices for the "weight" operator W to obtain in this section the classical BFGS, DFP, PSB, and SR1 formulas in their operator form.

Proposition 4.1 (DFP formula for Hessian operator). *Let us consider an operator $B_k \in \mathcal{B}^s(\mathcal{H})$, a positive and invertible operator $W \in \mathcal{B}^s(\mathcal{H})$ such that $Wy_k = s_k$, and s_k and y_k nonzero elements of $\mathcal{H}$.*

i. *The solution to the variational problem*

$$\begin{aligned} \min_{B\in\mathcal{B}(\mathcal{H})} \quad & \frac{1}{2}||W^{1/2}(B-B_k)W^{1/2}||^2_{HS} \\ s.t \quad & Bs_k = y_k \end{aligned} \tag{4.1}$$

is given by

$$B_{k+1} = (I-\gamma(y_k\otimes s_k))B_k(I-\gamma(s_k\otimes y_k)) + \gamma(y_k\otimes y_k), \tag{4.2}$$

where $\gamma = \frac{1}{\langle s_k, y_k\rangle}$; in addition, $B_{k+1} \in \mathcal{B}^s(\mathcal{H})$ and $B_{k+1} - B_k \in \mathcal{B}_{00}(\mathcal{H})$.

ii. *If B_k is positive and invertible, and the positive curvature condition $\langle s_k, y_k\rangle > 0$ holds, then B_{k+1} is positive and invertible.*

Proof.

i. By Corollary 3.3, we have that

$$\begin{aligned} B_{k+1} = B_k &+ \frac{W^{-1}s_k\otimes(y_k-B_ks_k) + (y_k-B_ks_k)\otimes W^{-1}s_k}{\langle s_k, W^{-1}s_k\rangle} \\ &- \frac{\langle y_k - B_ks_k, s_k\rangle}{\langle s_k, W^{-1}s_k\rangle^2} W^{-1}s_k\otimes W^{-1}s_k. \end{aligned}$$

Since $y_k = W^{-1}s_k$ and by letting $\gamma = \frac{1}{\langle s_k, y_k\rangle}$, the above identity becomes

$$\begin{aligned} B_{k+1} = B_k &+ \gamma\left[y_k\otimes(y_k-B_ks_k) + (y_k-B_ks_k)\otimes y_k\right] \\ &- \gamma^2\langle y_k - B_ks_k, s_k\rangle(y_k\otimes y_k). \end{aligned} \tag{4.3}$$

We note that the last term in the above equality can be simplified as follows

$$\begin{aligned}\gamma^2\langle y_k - B_k s_k, s_k\rangle(y_k \otimes y_k) &= \gamma^2\left[\langle y_k, s_k\rangle - \langle B_k s_k, s_k\rangle\right](y_k \otimes y_k)\\ &= \gamma(y_k \otimes y_k) - \gamma^2\langle B_k s_k, s_k\rangle(y_k \otimes y_k).\end{aligned} \tag{4.4}$$

With the above simplification, Equation (4.3) above can be manipulated to obtain the following

$$\begin{aligned}B_{k+1} = B_k + \gamma\big[&y_k \otimes (y_k - B_k s_k) + (y_k - B_k s_k) \otimes y_k - (y_k \otimes y_k)\big]\\ &+ \gamma^2\langle B_k s_k, s_k\rangle(y_k \otimes y_k),\end{aligned}$$

and hence

$$\begin{aligned}B_{k+1} = \big[&B_k - \gamma(y_k \otimes B_k s_k) - \gamma(B_k s_k \otimes y_k) + \gamma^2\langle B_k s_k, s_k\rangle(y_k \otimes y_k)\big]\\ &+ \gamma(y_k \otimes y_k).\end{aligned} \tag{4.5}$$

One can further manipulate the last identity to get the desired Equation (4.2) as follows

$$\begin{aligned}B_{k+1} &= (B_k - \gamma y_k \otimes B_k s_k)(I - \gamma s_k \otimes y_k) + \gamma(y_k \otimes y_k)\\ &= \big(I - \gamma y_k \otimes s_k\big)B_k\big(I - \gamma s_k \otimes y_k\big) + \gamma(y_k \otimes y_k).\end{aligned} \tag{4.6}$$

From (4.5) we note that $B_{k+1} - B_k$ is a finite rank operator as it has at most rank four, therefore it is a Hilbert-Schmidt operator [14]. Finally, since $y_k \otimes B_k s_k$ is the adjoint of $B_k s_k \otimes y_k$, and $y_k \otimes y_k$ is self-adjoint, by using the properties of the dyadic product and the fact that B_k is self-adjoint we conclude that B_{k+1} is self-adjoint.

ii. Let us write $B_{k+1} = G^*G + F$ where $G = B_k^{1/2}(I - \gamma s_k \otimes y_k)$, and $F = \gamma(y_k \otimes y_k)$. Since B_k is positive, one can prove that $\langle x, G^*Gx\rangle \geq 0$ for all $x \in \mathcal{H}$. Furthermore, $0 = \langle x, G^*Gx\rangle$, or equivalently, $0 = \langle Gx, Gx\rangle$ if and only if $Gx = 0$, which in turn holds if and only if $x - \gamma(s_k \otimes y_k)x = 0$ by the positiveness of B_k. We leave the proof of the fact that $\{x \in \mathcal{H} : x - \gamma(s_k \otimes y_k)x = 0\} = \{\alpha s_k : \alpha \in \mathbb{R}\}$ as an exercise to the reader, and conclude that $0 = \langle x, G^*Gx\rangle$ if and only if $x = \alpha s_k$ for some real scalar α. On the other hand, it is straightforward to prove that $\langle x, Fx\rangle \geq 0$ for all $x \in \mathcal{H}$ when the positive curvature holds (and, as a result, $\gamma > 0$). Furthermore, we remark that $\langle \alpha s_k, F\alpha s_k\rangle = \alpha^2\langle s_k, y_k\rangle > 0$ for all nonzero $\alpha \in \mathbb{R}$.

With the above, we have that $\langle x, B_{k+1}x\rangle > 0$ for all nonzero x, which shows the positive definiteness of B_{k+1}. Finally, the invertibility of B_{k+1} follows from the Sherman–Morrison–Woodbury formula. We note that the latter is shown in detail in the proof of Proposition 4.5. □

Proposition 4.2 (BFGS formula for the inverse Hessian operator). *Let us consider an operator $H_k \in \mathcal{B}^s(\mathcal{H})$, a positive and invertible operator $W \in \mathcal{B}^s(\mathcal{H})$ such that $Ws_k = y_k$, and s_k and y_k nonzero elements of $\mathcal{H}$.*

i. *The solution to the variational problem*

$$\min_{H \in \mathcal{B}(\mathcal{H})} \quad \frac{1}{2} ||W^{1/2}(H - H_k)W^{1/2}||_{HS}^2 \tag{4.7}$$

$$s.t \quad \mathrm{Hy_k = s_k} \tag{4.8}$$

is given by

$$H_{k+1} = (I - \gamma(s_k \otimes y_k))H_k(I - \gamma(y_k \otimes s_k)) + \gamma(s_k \otimes s_k), \tag{4.9}$$

where $\gamma = \frac{1}{\langle s_k, y_k \rangle}$; *in addition,* $H_{k+1} \in B^s(\mathcal{H})$ *and* $H_{k+1} - H_k$ *lies in* $\mathcal{B}_{00}(\mathcal{H})$.

ii. *If H_k is positive and invertible, and the positive curvature condition $\langle y_k, s_k \rangle > 0$ holds, then H_{k+1} is positive and invertible.*

Proof. The proof is identical to the proof of Proposition 4.1. □

We next show that different choices of the "weight" operator W inside the Hilbert-Schmidt norm lead to different quasi-Newton formulas for the Hessian or its inverse. The Powell–Symmetric–Broyden formula is obtained using the trivial weight $W = I$ as we show next in Proposition 4.3. Surprisingly, the symmetric rank-one update can be also obtained (when it exists) with a particular choice of W, as shown in Proposition 4.4. Furthermore, notable from these two examples is that W does not have to satisfy the secant equation (as it does in Propositions 4.1 and 4.2 for the DFP and BFGS formulas).

Proposition 4.3 (Powell–Symmetric–Broyden Update). *Let us consider an operator $B_k \in \mathcal{B}^s(\mathcal{H})$ and s_k and y_k nonzero elements of $\mathcal{H}$. The solution to the variational problem*

$$\min_{B \in \mathcal{B}(\mathcal{H})} \quad \frac{1}{2} ||B - B_k||_{HS}^2$$

$$s.t \quad Bs_k = y_k$$

is given by

$$B_{k+1} = B_k + \frac{s_k \otimes (y_k - B_k s_k) + (y_k - B_k s_k) \otimes s_k}{\langle s_k, s_k \rangle} - \frac{\langle y_k - B_k s_k, s_k \rangle}{\langle s_k, s_k \rangle^2} s_k \otimes s_k.$$

Furthermore, B_{k+1} is self-adjoint and $B_{k+1} - B_k \in \mathcal{B}_{00}(\mathcal{H})$.

Proof. The proof follows by taking W to be the identity in Corollary 3.3. □

Proposition 4.4 (Symmetric Rank-One Update). *Let us consider an operator $B_k \in \mathcal{B}^s(\mathcal{H})$ and assume that a positive and invertible operator $W \in \mathcal{B}^s(\mathcal{H})$ exists such that $W^{-1}s_k = y_k - B_k s_k$ for s_k and y_k nonzero elements of $\mathcal{H}$. The solution to the variational problem*

$$\begin{aligned} \min_{B \in \mathcal{B}(\mathcal{H})} \quad & \frac{1}{2}||W^{1/2}(B - B_k)W^{1/2}||^2_{HS} \\ s.t \quad & Bs_k = y_k \end{aligned}$$

is the operator

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k) \otimes (y_k - B_k s_k)}{\langle s_k, y_k - B_k s_k \rangle},$$

which is self-adjoint and satisfies $B_{k+1} - B_k \in \mathcal{B}_{00}(\mathcal{H})$.

Proof. By Corollary 3.3 we have that

$$\begin{aligned} B_{k+1} = B_k &+ \frac{W^{-1}s_k \otimes (y_k - B_k s_k) + (y_k - B_k s_k) \otimes W^{-1}s_k}{\langle s_k, W^{-1}s_k \rangle} \\ &- \frac{\langle y_k - B_k s_k, s_k \rangle}{\langle s_k, W^{-1}s_k \rangle^2} W^{-1}s_k \otimes W^{-1}s_k. \end{aligned}$$

Since $W^{-1}s_k = y_k - B_k s_k$, we simplify the above identity as follows:

$$\begin{aligned} B_{k+1} = B_k &+ \frac{(y_k - B_k s_k) \otimes (y_k - B_k s_k) + (y_k - B_k s_k) \otimes (y_k - B_k s_k)}{\langle s_k, y_k - B_k s_k \rangle} \\ &- \frac{\langle y_k - B_k s_k, s_k \rangle}{\langle s_k, y_k - B_k s_k \rangle^2} (y_k - B_k s_k) \otimes (y_k - B_k s_k) \\ = B_k &+ \frac{(y_k - B_k s_k) \otimes (y_k - B_k s_k)}{\langle s_k, y_k - B_k s_k \rangle}, \end{aligned}$$

which completes the proof. □

In the remainder of this section we derive the inverse formulas for the DFP and BFGS formulas presented above in Propositions 4.1 and 4.2 using a generalization of Sherman–Morrison–Woodbury formula [20] given in Theorem 2.18.

Proposition 4.5 (BFGS formula for Hessian operator). *Let us consider the positive definite and invertible operators $B_k \in \mathcal{B}^s(\mathcal{H})$ and $W \in \mathcal{B}^s(\mathcal{H})$ such that $Wy_k = s_k$, where s_k and y_k are nonzero elements of $\mathcal{H}$.*

i. *The solution to the variational problem*

$$\begin{aligned} \min_{B \in \mathcal{B}(\mathcal{H})} \quad & \frac{1}{2}||W^{1/2}(B^{-1} - B_k^{-1})W^{1/2}||^2_{HS} \\ s.t \quad & Bs_k = y_k \end{aligned} \tag{4.10}$$

is given by

$$B_{k+1} = B_k - \frac{B_k s_k \otimes B_k s_k}{\langle s_k, B_k s_k \rangle} + \frac{y_k \otimes y_k}{\langle s_k, y_k \rangle}; \tag{4.11}$$

in addition, $B_{k+1} \in \mathcal{B}^s(\mathcal{H}), B_{k+1} - B_k \in \mathcal{B}_{00}(\mathcal{H})$, *and* B_{k+1} *is invertible.*

ii. *If the positive curvature condition* $\langle s_k, y_k \rangle > 0$ *holds, then* B_{k+1} *is positive.*

Proof.

i. The salient idea of the proof is to obtain (4.11) by inverting the inverse Hessian BFGS formula $B_{k+1}^{-1} = H_{k+1}$ from Proposition 4.2 using the Sherman–Morrison–Woodbury (SMW) formula of Theorem 2.18.

Let the linear operator $Y : \mathbb{R} \times \mathbb{R} \to \mathcal{H}$ be defined by $Y(\alpha, \beta) = \alpha s_k + \beta H_k y_k$. We remark that $Y \in \mathcal{B}(\mathbb{R} \times \mathbb{R}, \mathcal{H})$ and that the adjoint operator $Y^* \in \mathcal{B}(\mathcal{H}, \mathbb{R} \times \mathbb{R})$ is given by

$$Y^* x = \begin{bmatrix} \langle s_k, x \rangle \\ \langle H_k y_k, x \rangle \end{bmatrix}. \tag{4.12}$$

Also, let $G : \mathbb{R} \times \mathbb{R} \to \mathbb{R} \times \mathbb{R}$ be given by

$$G(\alpha, \beta) = \begin{bmatrix} \gamma\alpha + \gamma^2 \langle H_k y_k, y_k \rangle \alpha - \gamma\beta \\ -\gamma\alpha \end{bmatrix}.$$

Above, we used the notation $\gamma = (\langle s_k, y_k \rangle)^{-1}$. We remark that G is a linear bounded invertible operator and has a bounded inverse in the form of

$$G^{-1}(\omega, \nu) = \begin{bmatrix} -\dfrac{\nu}{\gamma} \\ -\dfrac{\omega}{\gamma} - \dfrac{\nu}{\gamma}(1 + \gamma \langle H_k y_k, y_k \rangle) \end{bmatrix}.$$

One can show that $[G^{-1} + Y^* H_k^{-1} Y](\alpha, \beta) = \left[\alpha \langle s, B_k s \rangle \ - \frac{\beta}{\gamma}\right]$, which implies that $G^{-1} + Y^* H_k^{-1} Y$ is invertible and

$$(G^{-1} + Z^* H_k^{-1} Y)^{-1} = \begin{bmatrix} \dfrac{1}{\langle s_k, B_k s_k \rangle} & 0 \\ 0 & -\gamma \end{bmatrix}. \tag{4.13}$$

Note we chose $Z = Y$. In the above we used the matrix notation to be close to the the standard finite dimensional notation, but one can write this in operator notation as well. We next notice that

$$
\begin{aligned}
[H_k + YGY^*]x &= H_kx + Y(G(Y^*x)) = H_kx + Y\left(G\left(\begin{bmatrix} \langle s_k, x\rangle \\ \langle H_ky_k, x\rangle \end{bmatrix}\right)\right) \\
&= H_kx + Y\left(\begin{bmatrix} \gamma\langle s_k, x\rangle + \gamma^2\langle H_ky_k, y_k\rangle\langle s_k, x\rangle - \gamma\langle H_ky, x\rangle \\ -\gamma\langle s_k, x\rangle \end{bmatrix}\right) \\
&= H_kx + \left(\gamma\langle s_k, x\rangle + \gamma^2\langle H_ky_k, y\rangle\langle s_k, x\rangle \ - \ \gamma\langle H_ky_k, x\rangle\right)s_k \\
&\quad - \gamma\langle s_k, x\rangle H_ky \\
&= H_kx - \gamma(s_k \otimes H_ky_k)(x) - \gamma(H_ky_k \otimes s_k)(x) \\
&\quad + (s_k \otimes \gamma^2\langle H_ky_k, y_k\rangle s_k)(x) + \gamma(s_k \otimes s_k)(x).
\end{aligned}
$$

On the other hand, the inverse Hessian BFGS formula from Proposition 4.2 can be manipulated as follows:

$$
\begin{aligned}
H_{k+1} &= (I - \gamma(s_k \otimes y_k))H_k(I - \gamma(y_k \otimes s_k)) + \gamma(s_k \otimes s_k) \\
&= H_k - \gamma(s_k \otimes y_k)H_k - \gamma(H_ky_k \otimes s_k) + \gamma^2(s_k \otimes y_k)H_k(y_k \otimes s_k) + \gamma(s_k \otimes s_k).
\end{aligned}
$$

Therefore $H_k + YGY^* = H_{k+1}$. Finally, from the Sherman–Morrison– Woodbury formula formula and by using the fact that $H_k^{-1} = B_k$ we obtain that

$$
\begin{aligned}
B_{k+1} &= H_{k+1}^{-1} = H_k^{-1} - H_k^{-1}Y(G^{-1} + Y^*H_k^{-1}Y)^{-1}Y^*H_k^{-1} \\
&= B_k - B_kY(G^{-1} + Y^*B_kY)^{-1}Y^*B_k.
\end{aligned}
$$

The definition of Y, Equations (4.12) and (4.13), and the properties of dyadic products can be used to write for any $x \in \mathcal{H}$ that

$$
\begin{aligned}
B_{k+1}x &= B_kx - B_kY\begin{bmatrix} \dfrac{1}{\langle s_k, B_ks_k\rangle} & 0 \\ 0 & -\gamma \end{bmatrix}\begin{bmatrix} \langle s_k, B_kx\rangle \\ \langle H_ky_k, B_kx\rangle \end{bmatrix} \\
&= B_kx - B_kY\begin{bmatrix} \dfrac{\langle s_k, B_kx\rangle}{\langle s_k, B_ks_k\rangle} \\ -\dfrac{\langle H_ky_k, B_kx\rangle}{\langle s_k, y_k\rangle} \end{bmatrix} \\
&= B_kx - B_k\left(\frac{\langle s_k, B_kx\rangle}{\langle s_k, B_ksv\rangle}s_k \ - \ \frac{\langle H_ky_k, B_kx\rangle}{\langle s_k, y_k\rangle}H_ky_k\right) \\
&= B_kx - \frac{\langle s_k, B_kx\rangle}{\langle s_k, B_ks\rangle}B_ks_k + \frac{\langle H_ky_k, B_kx\rangle}{\langle s_k, y_k\rangle}y_k \\
&= B_kx - \frac{B_ks_k \otimes s_k}{\langle s_k, B_ks_k\rangle}B_kx + \frac{y_k \otimes y_k}{\langle s_k, y_k\rangle}x \\
&= B_kx - \frac{B_ks_k \otimes B_ks_k}{\langle s_k, B_ks_k\rangle}x + \frac{y_k \otimes y_k}{\langle s_k, y_k\rangle}x.
\end{aligned}
$$

This completes the proof of (4.11) and also shows that B_{k+1} is invertible. It remains to show $B_{k+1} \in \mathcal{B}^s(\mathcal{H}), B_{k+1} - B_k \in \mathcal{B}_{00}(\mathcal{H})$ and part *(ii) i.e.*, to show B_{k+1} is positive. Both are consequence of Proposition 4.2 which gives us $H_{k+1} \in \mathcal{B}^s(\mathcal{H})$, $H_{k+1} - H_k \in \mathcal{B}_{00}(\mathcal{H})$ and H_{k+1} is positive. One way to show both in one step is to use the fact $B_{00}(\mathcal{H})$ and the space of positive bounded linear operators are an ideal in the space of bounded operators. □

Proposition 4.6 (DFP formula for the inverse Hessian operator). *Let us consider the positive definite and invertible operators $H_k \in \mathcal{B}^s(\mathcal{H})$ and $W \in \mathcal{B}^s(\mathcal{H})$ such that $Wy_k = s_k$, where s_k and y_k are nonzero elements of $\mathcal{H}$.*

(i) *The solution to the variational problem*

$$\min_{H \in \mathcal{B}(\mathcal{H})} \quad \frac{1}{2}||W^{1/2}(H^{-1} - H_k^{-1})W^{1/2}||_{HS}^2 \tag{4.14}$$

$$s.t \quad Hy_k = s_k \tag{4.15}$$

is given by

$$H_{k+1} = H_k - \frac{(H_k y_k \otimes H_k y_k)}{\langle y_k, H_k y_k \rangle} + \frac{(s_k \otimes s_k)}{\langle s_k, y_k \rangle}. \tag{4.16}$$

Furthermore, H_{k+1} is invertible and $H_{k+1} - H_k$ lies in $\mathcal{B}_{00}(\mathcal{H})$.

(ii) *If the curvature condition is met $\langle y_k, s_k \rangle > 0$, then $H_{k+1} \in \mathcal{B}_{00}(\mathcal{H})$ is self-adjoint and positive definite.*

Proof. The proof is similar to the proof of Proposition 4.5 and uses Theorem 2.18 for the inverse Hessian operator given by Proposition 4.1. □

4.1. Note on the limited-memory compact representation formulas

The popular limited-memory compact representations introduced by Byrd et al. [11] have similar forms for Hessian operators defined over general Hilbert spaces. For completeness, we succintly present them below. Their derivation is analogous to the finite-dimensional case [11] and relies on the Sherman–Morrison–Woodbury formula (Theorem 2.18) along the lines of the proof of Proposition 4.5. In what follows, given $s_i \in \mathcal{H}$ and $y_i \in \mathcal{H}, i = \{0, 1, ..., l-1\}$, let $S_l : \mathbb{R}^l \to \mathcal{H}$ be given by $S_l(v) = \sum_{i=0}^{l-1} v_{i+1} s_i$, and $Y_l : \mathbb{R}^l \to \mathcal{H}$ given by $Y_l(v) = \sum_{i=0}^{l-1} v_{i+1} y_i$, where v_i denotes the i^{th} component of a vector $v \in \mathbb{R}^l$. Furthermore, define R_l as a $l \times l$ matrix as

$$(R_l)_{ij} = \begin{cases} \langle s_{i-1}, y_{j-1} \rangle & \text{if} \quad i \le j, \\ 0 & \text{otherwise.} \end{cases}$$

Theorem 4.7. *Let $H_0 \in B^s(\mathcal{H})$ be positive and invertible. Furthermore, let H_l be given by updating H_0 l times using the inverse BFGS formula obtained in Proposition 4.2. If all the pairs $\{s_i, y_i\}_{i=0}^{l-1}$ satisfy the positive curvature condition $\langle s_i, y_i \rangle > 0$, then*

$$H_l = H_0 + \begin{bmatrix} S_l & H_0 Y_l \end{bmatrix} \left(\begin{bmatrix} R_l^{-T}(D_l + (H_0 Y_l)^* Y_l) R_l^{-1} & -R_l^{-T} \\ -R_l^{-1} & 0 \end{bmatrix} \begin{bmatrix} S_l^* \\ (H_0 Y_l)^* \end{bmatrix} \right),$$

where D_l is the $l \times l$ diagonal matrix given by

$$(D_l)_{ij} = \begin{cases} \langle s_i, y_j \rangle & \text{if} \quad i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Theorem 4.8. *Let $B_0 \in B^s(\mathcal{H})$ be positive and invertible. Furthermore, let B_l be given by updating B_0 l times using the BFGS formula obtained in Proposition 4.5. If all the pairs $\{s_i, y_i\}_{i=0}^{l-1}$ satisfy the positive curvature condition $\langle s_i, y_i \rangle > 0$, then*

$$B_l = B_0 - \begin{bmatrix} B_0 S_l & Y_l \end{bmatrix} \left(\begin{bmatrix} S_l^* B_0 S_l & L_l \\ L_l^T & -D_l \end{bmatrix}^{-1} \begin{bmatrix} (B_0 S_l)^* \\ Y_l^* \end{bmatrix} \right),$$

where L_l is the $l \times l$ matrix with entries

$$(L_l)_{ij} = \begin{cases} \langle s_{i-1}, y_{j-1} \rangle & \text{if} \quad i > j, \\ 0 & \text{otherwise.} \end{cases}$$

5. Incorporating hessian structure in Quasi-Newton formulas: a case study for inverse problems governed by partial differential equations

As an illustration of potential uses of the results introduced by this paper, we consider the class of regularized inverse problems governed by partial differential equations (PDEs) and derive DFP and BFGS "structured" secant formulas that explicitly use the derivative of the regularization and only approximates the second derivative of the misfit term. To this end, we consider the inversion of a coefficient field in an elliptic PDE. Depending on the interpretation of the inputs and the type of measurements, this problem arises, for instance, in inversion for the permeability field in a subsurface flow problem, for the conductivity field in a heat transfer problem, or the stiffness parameter field in a membrane deformation problem [23].

We formulate the inverse problem over $\Omega = [0, 1] \times [0, 1]$ as follows: given possibly noisy observations $\mathrm{d} \in \mathbb{R}^q$ of the state solution u in Ω, we wish to infer the coefficient field m that best reproduces the observations. Mathematically, this can be formulated as the nonlinear least-squares minimization problem

$$\min_{m} \mathcal{J}(m) := \frac{1}{2}\langle Ou(m) - \mathrm{d}, Ou(m) - \mathrm{d}\rangle_{\mathbb{R}^q} + \frac{\gamma}{2}\langle \nabla m, \nabla m\rangle_{L^2}, \tag{5.1}$$

$$\text{s.t.} \qquad \underline{m} \le m \le \overline{m}, \tag{5.2}$$

where u solves the state (or forward) problem

$$-\nabla \cdot (m\nabla u) = f \text{ in } \Omega \text{ and } u = 0 \text{ on } \partial\Omega. \tag{5.3}$$

Above, $\mathrm{d} \in \mathbb{R}^q$ denotes the observations, with q denoting the number of observation spoints, $f \in H^{-1}(\Omega)$ is a given volume force, $O : L^2(\Omega) \to \mathbb{R}^q$ is a linear observation operator that extracts measurements from u, and $\underline{m}, \overline{m} \in L^\infty(\Omega)$ are the lower and upper bounds of the unknown coefficient field m, respectively. The first term in the objective of (5.1) is the data misfit term, which we will denote by $\mathcal{M}(m)$, and the second term, which we will denote by $\mathcal{R}(m)$, is a regularization term with regularization parameter $\gamma > 0$ added to render the inverse problem well-posed [24, 25]. We note that when we discretize the regularization term, this will take the form of $\mathbf{m}^T \boldsymbol{K}\mathbf{m}$, where $\mathbf{m}$ is the vector of finite element coefficients of the parameter field m, and $\boldsymbol{K}$ is the stiffness matrix [26, 27].

We solve (5.1) using a quasi-Newton interior-point method [28]. We assume that only the second derivative of the regularization term is available, while the second derivative of the misfit term is not (e.g., we target application problems for which this terms is expensive to evaluate). Therefore, to take advantage of this structure, in what follows, we derive and apply so-called *structured* DFP and BFGS formulas.

5.1. Derivation of structured DFP and BFGS formulas

To derive structured DFP and BFGS formulas for the Hessian matrix, we consider a structured variant of Proposition 4.1. More specifically, since we are looking for a DFP update in the form $B = R + A$, where A approximates the second-derivative of the misfit term $\mathcal{M}$, in the spirit of Proposition 4.1 we require that a formula for A satisfies

$$\begin{aligned} \min_{A} \quad & \frac{1}{2}||W^{1/2}(A - A_k)W^{1/2}||_{HS}^2 \\ \text{s.t} \quad & As_k = \overline{y}_k, \end{aligned} \tag{5.4}$$

where $\overline{y}_k = \nabla\mathcal{M}(m_{k+1}) - \nabla\mathcal{M}(m_k)$. In words, the variational form (5.4) builds the structured update A based only on the change in the gradient of the misfit. Analogous to the proof of Proposition 4.1, one can show that the *structured DFP formula for the Hessian* is

$$A_{k+1} = (I - \overline{\gamma}(\overline{y}_k \otimes s_k))A_k(I - \overline{\gamma}(s_k \otimes \overline{y}_k)) + \overline{\gamma}(\overline{y}_k \otimes \overline{y}_k), \tag{5.5}$$

where $\overline{\gamma} = 1/\langle s_k, \overline{y}_k \rangle$. Similarly, the *structured BFGS formula for the Hessian* can be obtained by considering the structured version of Proposition 4.5 in the form of

$$\begin{aligned} \min_{A} \quad & \frac{1}{2} || W^{1/2} \left[(A+R)^{-1} - (A_k+R)^{-1} \right] W^{1/2} ||_{HS}^2, \\ \text{s.t} \quad & A s_k = \overline{y}_k \end{aligned} \tag{5.6}$$

which gives the structured BFGS formula

$$A_{k+1} = A_k - \frac{(A_k+R)s_k \otimes (A_k+R)s_k}{\langle s_k, Rs_k + \overline{y}_k \rangle} + \frac{(\overline{y}_k + Rs_k) \otimes (\overline{y}_k + Rs_k)}{\langle s_k, Rs_k + \overline{y}_k \rangle}. \tag{5.7}$$

We remark that the Hessian formula $B_k = R + A_k$ with A_k given by (5.7) above is identical to the unstructured BFGS given by Proposition 4.5 as long as the two formulas are initialized with $B_0 = R + A_0$ and A_0. This is not the case for the structured and unstructured DFP formulas (5.5) and (4.2), respectively.

5.2. Numerical results

We compare the performance of structured update formulas derived in Section 5.1 with their unstructured counterparts for the inverse problem governed by the Poisson equation given by (5.1)-(5.3). The numerical algorithm we use is a filter line-search interior-point method for constrained optimization problems [29, 30] in which we replace the Hessian of the objective (5.1) with quasi-Newton approximations similarly to the state-of-the-art Ipopt solver [31]. The stopping criteria for the interior-point method consist of a stringent 10^{-8} tolerance for the norm of gradient (of the Lagrangian function of (5.1), for more details see [31]) and a maximum number of 100 iterations. We derive the gradient (i.e., the firs-derivative information) using an adjoint-based approach [27, 32, 33]. The underlying PDEs are solved with the finite element method using Comsol with Matlab, while the interior-point method is implemented in Matlab. The problem was solved on five uniform 2 D meshes and on one nonuniform 2 D mesh with rectangular elements. For the discretization of the state and ajoint variables we used quadratic and for the parameter linear finite elements. The state dimension was increased form 441 to 5227 and the parameter dimension (i.e., the dimension of the optimization problem) from 121 to 1328. The numerical experiments were performed on an Intel Ivy Bridge 2.5 GHz 8-Core Linux machine with 128 GB RAM memory.

In what follows, the structured quasi-Newton formulas are denoted with acronyms starting with "S-". These are compared with unstructured counterparts, which are prefixed by "U-". For a both fair play and

Table 1. Summary of the formulas investigated numerically in this section. The algorithmic parameter σ_k is the Barzilai-Borwein spectral estimate [34] discussed in the text.

Acronym	Formula for B_k	Initial Hessian	Notes
U-BFGS-U	(4.11)	$B_0 = \sigma_k M$	unstructured BFGS with uninformed initialization
U-BFGS-I	(4.11)	$B_0 = \sigma_k(M + R)$	unstructured BFGS with informed initialization
S-BFGS	$B_k = A_k + R$ A_k given by (5.7)	$A_0 = \sigma_k M$	structured BFGS
U-DFP-U	(4.2)	$B_0 = \sigma_k M$	unstructured DFP with uninformed initialization
U-DFP-I	(4.2)	$B_0 = \sigma_k(M + R)$	unstructured DFP with informed initialization
S-DFP	$B_k = A_k + R$ A_k given by (5.4)	$A_0 = \sigma_k M$	structured DFP

comprehensive comparison, the unstructured quasi-Newton formulas are used with an *uninformed* (suffixed by "-U") and *informed* (suffixed by "-I") initial Hessian approximations. The uninformed initial approximations correspond to a plain, fully unstructured formula, while the informed initial approximation correspond to unstructured formulas that take into account the known part of the Hessian (that is, the Hessian of the regularization term). Table 1 summarizes this discussion and presents the algorithmic parameters used in the numerical experiments. The parameter multiple of the identity σ_k is the Barzilai-Borwein spectral estimate [34] that changes at each optimization iteration according to $\sigma_k = \langle s_k, s_k \rangle / \langle s_k, y_k \rangle$. This estimate is also used in Ipopt; in our experiments it gave the smallest number of iterations for all formulas from Table 1.

In Table 2, we report on the number of iterations for unstructured informed and uninformed and structured BFGS and DFP formulas. We have used these formulas with (s_k, y_k) pairs from the last ℓ iteration for $\ell = 8$ (a), $\ell = 16$ (b), and $\ell = 32$ (c). Our numerical experiments reveal that the standard unstructured updates with *uninformed* initialization, namely U-BFGS-U and U-DFP-U, exhibit a number of iterations that increases for finer or non-uniform meshes. This mesh dependence behavior is present for all three memory sizes $\ell = 8, \ell = 16,$ and $\ell = 32$ we have used. On the other hand, the standard unstructured formulas with *informed* initialization, namely U-BFGS-I and U-DFP-I, do not show this mesh dependent behavior; instead, the iteration count for these updates remains relatively constant for all meshes. Our point is that in order to obtain mesh independence, one needs not only to use the infinite-dimensional BFGS and DFP formulas but also to carefully choose the initial quasi-Newton approximation operator. Intuitively, for the inverse problem we solve here, the use of an informed initialization with U-BFGS-I and U-DFP-I, namely a multiple of the identity operator plus the stiffness operator, circumvents

Table 2. Shown are the number of optimization iterations obtained with formulas from Table 1 with quasi-Newton memory for $\ell = 8$ (a), $\ell = 16$ (b), and $\ell = 32$ (c).

Mesh	U-BFGS-U	U-BFGS-I	S-BFGS	U-DFP-U	U-DFP-I	S-DFP
(a) Number of iterations for $\ell = 8$						
10×10	41	35	37	39	30	34
20×20	87	43	39	95	38	37
30×30	>100	41	38	>100	39	36
40×40	>100	42	39	>100	45	52
50×50	>100	46	39	>100	44	36
non-unif.	>100	43	40	>100	46	39
(b) Number of iterations for $\ell = 16$						
10×10	39	29	30	38	27	29
20×20	78	36	34	90	35	32
30×30	>100	36	33	>100	39	32
40×40	>100	36	33	>100	39	32
50×50	>100	39	35	>100	38	34
non-unif.	>100	36	34	>100	38	39
(c) Number of iterations for $\ell = 32$						
10×10	37	28	28	37	26	29
20×20	77	34	29	87	33	32
30×30	>100	35	30	>100	37	30
40×40	>100	38	30	>100	37	35
50×50	>100	37	30	>100	37	37
non-unif.	>100	37	30	>100	36	34

the need to approximate the stiffness operator; instead these formulas approximate only the Hessian of the misfit, which is known to be compact [35,36] and, therefore, can be approximated relatively well (both in a mesh independent manner and within a relatively small number of iterations) by the finite-rank operators built using the infinite-dimensional BFGS and DFP formulas derived in this paper.

We now turn to the *structured* BFGS and DFP formulas, *i.e.*, S-BFGS and S-DFP, which we derived in this section to explicitly incorporate additional Hessian information (namely the stiffness operator). We remark from Table 2(a)–(c) that these structured formulas improve over the unstructured informed formulas U-BFGS-I and U-DFP-I in terms of number of iterations (by up to 20%) and, also, exhibit mesh independence behavior. In particular, we remark that S-BFGS shows a more consistent iteration count over all meshes when compared to S-DFP; and, for larger quasi-Newton memory sizes ($\ell = 32$), S-BFGS seems slightly faster than S-DFP, while for smaller memory sizes the two compare similarly.

6. Conclusions

We have presented a new derivation of well-known quasi-Newton formulas in an infinite-dimensional Hilbert space setting needed for example for solving optimization problems governed by differential equations. In particular, we have generalized the variational, least-squares framework of Güler et al. [3] to operators defined over general separable Hilbert spaces.

The framework we present was used to derive classical BFGS, DFP, PSB, and SR1 formulas in operator form. Furthermore, we illustrated how the variational framework can be employed to derive improved DFP and BFGS updates for a class of inverse problems governed by PDEs. To illustrate the importance of using these infinite-dimensional quasi-Newton formulas we formulated and solved an inverse problem governed by partial differential equations (PDEs) via a quasi-Newton interior-point method on progressively finer uniform meshes and on a nonuniform mesh. In addition, we derived structured DFP and BFGS formulas for the Hessian operator, where we considered parts of the Hessian known and only approximate the remaining part (e.g., the second-derivative of the term corresponding to the misfit). Numerical results showed that in order to obtain mesh independence, it is essential not only to use the infinite-dimensional BFGS and DFP formulas but also to carefully choose the initial quasi-Newton approximation operator. In addition, we compared the performance of the structured update formulas with their unstructured counterparts and found that taking into account the structure of the problem leads to reducing further the computational cost.

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