Almost multisecant BFGS quasi-Newton method

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***Abstract*—In convex optimization, Quasi-Newton (QN) methods provide an alternative to second-order techniques for solving minimization problems by approximating curvature of a given target function. This approach reduces computational complexity as it relies solely on first-order information, and satisfying the secant condition. This paper focuses on multi-secant (MS) extensions of QN, which enhances the Hessian approximation at low cost. Specifically, we use a low-rank perturbation strategy to construct an almost-secant QN method that maintains positive definiteness of the Hessian estimate, which in turn helps ensure constant descent direction and reduces method divergence. Our results show that our perturbations can greatly improve stability and effectiveness of multisecant updates.**

***Index Terms*—Hessian approximation, low-rank approximation, multisecant, quasi-Newton, second order method**

I. Introduction

We consider the unconstrained minimization problem

$$\underset{x}{\text{minimize}} \quad f(x) \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}$ is convex, twice-differentiable everywhere, and bounded below. Newton's method iteratively solves the linear system of order n to get a search direction p_k,

$$\nabla^2 f(x_k) d_k = -\nabla f(x_k), \quad k = 1, ... \tag{2}$$

where $\nabla^2 f(x_k)$ is the Hessian and $\nabla f(x_k)$ is the gradient of the kth iterate. In this case, the next iterate is updated as

$$x_{k+1} = x_k + \alpha d_k$$

where $\alpha > 0$ is a step length parameter. However, while this method is foundational in continuous optimization, when dealing with large-scale problems, getting the Hessian matrix and solving (2) is not computationally scalable. For this reason, quasi-Newton (QN) methods, like BFGS (13), are introduced and become good substitutes which efficiently approximate the Hessian with simple operations performed on successive gradient vectors.

a) QN methods: The usual QN method involves forcing the satisfaction of a single secant equation

$$B_{k+1}(x_{k+1} - x_k) = \nabla f(x_{k+1}) - \nabla f(x_k). \tag{3}$$

where where B_k serves as a Hessian approximation of f at x_k, and (3) is the 2nd-order Taylor approximation of f at x_k. The iterates are then updated via an approximate Newton step

$$x_{k+1} = x_k - \alpha B_k^{-1} \nabla f(x_k). \tag{4}$$

b) Multi-secant QN methods: A stronger, lesser-explored family of approximations are the *multi-secant QN methods*, which satisfy

$$B_k(x_i - x_j) = \nabla f(x_i) - \nabla f(x_j) \tag{5}$$

for some subset of $i \neq j \in \{k, k-1, ..., k-p+1\}$ where p is the number of previous information taken into account. While multi-secant extensions have been explored in past literature (5), and are shown to be more powerful approximations than single-secant approaches, there are several key challenges that prevent them from mainstream usage:

1) The rank of the update is p (the number of secant conditions), and thus multisecant approaches have a constant factor overhead in computational complexity.
2) Multisecant versions of QN methods often struggle with stability. Specifically, in the case of DFP and BFGS, a single-secant update is guaranteed to be a descent direction; however, incorporating more secant conditions destroys this valuable property, and can lead to divergence.

While the first deficiency presents an annoyance, in general linear scaling of complexity is usually not prohibitive. However, the second deficiency is severe; for this reason, multi-secant QN methods seem popular only in quadratic optimization, and are not easily generalizable even for convex functions. Therefore, in this paper we target the second deficiency, by presenting a method with nearly identical runtime as the usual multisecant QN updates, but with a perturbation that ensures descent directions. By exploiting important linear algebra properties, our strategy is low in computational cost, and adds the necessary perturbation to accelerate multisecant QN methods on important ill-conditioned problems.

A. Related works.

Perhaps the most well-known family of single-secant quasi-Newton methods are Broyden's method (1), Powell's method (11), Davidson-Fletcher-Powell (DFP) (7), and BFGS named after the concurrent works of (1), (2), (3), and (4). These methods, though distinct, form a progression; Broyden's method is first, then Powell's method introduces symmetric updates, and DFP and BFGS simultaneously introduce positive semidefiniteness (PSD) in B_k. These qualities (symmetric and PSD) are often desired to ensure that $d_k = -B_k^{-1} \nabla f(x_k)$ is indeed

a descent direction; these advanced methods are often more stable in practice.

The *multi-secant* extensions were first explored not long later; (5) for Broyden's method, and (6) for extensions of Broyden's, Powell's method, DFP, and BFGS updates. These methods also attempt to progressively include desired features, such as 1. fast and cheap updates, 2. symmetry, and 3. positive definiteness. However, the addition of these features is much less straightforward in the multisecant case; for this reason, multisecant methods are primarily used to solve quadratic systems, where symmetric PSD updates of multi-secant DFP and BFGS are easier to guarantee. *However, for general convex optimization problems, multi-secant quasi-Newton methods do not ensure descent.*

An important extension is the l-BFGS (9) method is a limited memory version of the BFGS algorithm and is widely used in machine learning. Additionally, Fang and Saad (8) also proposed the generalization of Broyden's and Multisecant family with several successful techniques for handling QN-type problems. More recently, closely related works include (14), (15), and (16). These are higher rank update schemes that use only first-order information, and are shown to achieve q-superlinear convergence, at least in the local sense.

In this work, we explore various techniques to impose symmetric and PSD updates in multisecant DFP and BFGS through carefully tuned perturbations, for ill-conditioned non-quadratic problems. We compare these techniques against the perturbation methods presented in the seminal work (6).

II. Preliminaries

Consider the goal of identifying B_k such that the following linear equations are satisfied

$$B_{k+1}(x_i - x_j) = \nabla f(x_i) - \nabla f(x_j), \quad i, j \leq k. \tag{6}$$

If $x_k \in \mathbb{R}^n$, then a symmetric Hessian estimate B_{k+1} has $n(n+1)/2$ degrees of freedom. In other words, for a reasonable number of secant constraints (fewer than $n(n+1)/2$), the system (13) is underdetermined, thus leading to the construction of a variety of QN methods. We first present a brief overview of four historically important methods, first in the single-secant framework, and then the multi-secant generalization.

A. Single-secant QN equations

In this section, the Hessian approximations B_{k+1} satisfy the single-secant condition

$$B_{k+1} \underbrace{(x_{k+1} - x_k)}_{s_k} \approx \underbrace{\nabla f(x_{k+1}) - \nabla f(x_k)}_{y_k}. \tag{7}$$

which is derived from the Taylor's second order expansion and its differential

$$\nabla f(x_{k+1}) \approx \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k).$$

where $B_{k+1} \approx \nabla^2 f(x_{k+1})$. If we restrict B_{k+1} to be symmetric, then the (7) has $\frac{n(n+1)}{2}$ degrees of freedom but only n constraints, where $n \geq 1$. If $n = 1$, then (7) has a unique solution; however, when $n > 1$, there are many variations of quasi-Newton methods that equally satisfy (7). After computing B_{k+1}, each quasi-Newton method will update x_{k+1} at each iteration

$$x_{k+1} = x_k - \alpha B_k^{-1} \nabla f(x_k).$$

To guarantee that each step taken is in a descent direction, the following

$$-\nabla f_k^T B_k^{-1} \nabla f_k < 0 \tag{8}$$

should be satisfied. If B_{k+1} is not PSD, (8) is not necessarily satisfied and hence the algorithm will not be guaranteed to monotonically decrease at each iteration. Therefore, maintaining B_{k+1} PSD is an important key for quasi-Newton methods.

B. Single-secant QN methods

The most well-known four single-secant quasi-Newton methods are described below. First, the Broyden's update (10) is given as

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k) s_k^T}{s_k^T s_k}. \tag{Broyden}$$

Here, we generally start with $B_1 = I$. It is a simple exercise to show that $B_{k+1} s_k = y_k$. However, there is no guarantee that such an update will maintain B_k to be symmetric or PSD. This is done by a series of follow-up updates; Powell's (11) gives symmetry

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k) s_k^T + s_k (y_k - B_k s_k)^T}{s_k^T s_k} + \frac{1}{2} \frac{(y_k - B_k s_k)^T s_k}{(s_k^T s_k)^2} s_k s_k^T \tag{Powell}$$

and DFP (7) and BFGS (1; 2; 3; 4) give symmetry and PSD:

$$B_{k+1} = B_k + \frac{(y_k - B s_k) y_k^T + y_k (y_k - B_k s_k)^T}{y_k^T s_k} - \frac{y_k (y_k - B_k s_k)^T s_k y_k^T}{(y_k^T s_k)^2} \tag{DFP}$$

$$B_{k+1} = B_k + \frac{y_k y_k^T}{y_k^T s_k} - \frac{B_k s_k s_k^T B_k}{(s_k^T B_k s_k)}. \tag{BFGS}$$

It has previously been shown that DFP and BFGS achieve q-superlinear convergence (17).

C. Multi-secant quasi-Newton methods

Equation (6) explained four typical multisecant quasi-Newton methods. Firstly, we consider two choices for s_i and y_i: the "curve-hugging" version for $i = k, ..., k-p+1$ such that

$$s_i = x_{i+1} - x_i, \quad y_i = \nabla f(x_{i+1}) - \nabla f(x_i) \tag{9}$$

and the "anchored at most recent" version for $i = k-1, ..., k-p$ such that

$$s_i = x_{k+1} - x_i, \quad y_i = \nabla f(x_{k+1}) - \nabla f(x_i). \tag{10}$$

The two interpolating schemes have different benefits. For the simplicity, we will use the former 'curve-hugging' version. We represent these choices with matrices S_k and Y_k as

$$S_k = \begin{bmatrix} | & | & & | \\ s_{k-p} & s_{k-p+1} & \dots & s_k \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n\times p} \tag{11}$$

$$Y_k = \begin{bmatrix} | & | & & | \\ y_{k-p} & y_{k-p+1} & \dots & y_k \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n\times p} \tag{12}$$

where $s_i = x_{i+1} - x_i$ and $y_i = \nabla f(x_{i+1}) - \nabla f(x_i)$. Then, we can define multisecant condition

$$B_{k+1}S_k = Y_k \tag{13}$$

which interpolates p number of previous iterates. Given the matrices S_k and Y_k, the number of free variables in B_{k+1} in (13) is still $n(n+1)/2 > pn$, so (13) is still an underdetermined problem when $p < n/2$ (usual regime). Reference (6) presented the following four multisecant generalizations of QN methods:

$$B_{k+1} = B_k + (Y_k - B_kS_k)(S_k^TS_k)^{-1}S_k^T \quad \text{(MS Broyden)}$$

$$\begin{aligned} B_{k+1} = {} & B_k + (Y_k - B_kS_k)(S_k^TS_k)^{-1}S_k^T \\ & + S_k(S_k^TS_k)^{-1}(Y_k - B_kS_k)^T \\ & - S_k(S_k^TS_k)^{-1}(Y_k - B_kS_k)^TS_k(S_k^TS_k)^{-1}S_k^T \end{aligned} \quad \text{(MS PSB)}$$

$$\begin{aligned} B_{k+1} = {} & B_k + (Y_k - B_kS_k)(Y_k^TS_k)^{-1}Y_k^T \\ & + Y_k(Y_k^TS_k)^{-1}(Y_k - B_kS_k)^T \\ & - Y_k(Y_k^TS_k)^{-1}(Y_k - B_kS_k)^TS_k(Y_k^TS_k)^{-1}Y_k^T \end{aligned} \quad \text{(MS DFP)}$$

$$\begin{aligned} B_{k+1} = {} & B_k + Y_k(Y_k^TS_k)^{-1}Y_k^T \\ & - B_kS_k(S_k^TB_kS_k)^{-1}S_k^TB_k \end{aligned} \quad \text{(MS BFGS)}$$

In (6), it is noted that Powell's B_{k+1} is guaranteed to be symmetric only if $S_k^TY_k$ is symmetric, and DFP's and BFGS's B_{k+1} is symmetric+PSD only if $Y_k^TS_k$ is symmetric+PSD. To see this, note that the constraint (13) enforces $S_k^TB_{k+1}S_k = S_k^TY_k$, so the symmetry / PSD-ness of B_{k+1} is not possible if $S_k^TY_k$ does not have the same corresponding properties. *However, this assumption is too strong for general convex functions f.* In fact, outside of f being a quadratic function, it is usually untrue. In (6), the problem is addressed using perturbations of an estimated Cholesky factorization of B_k. Here, we investigate simple diagonal perturbations.

D. Update of B_k^{-1}

A key feature of a successful quasi-Newton method is avoiding inverting matrices, or solving full linear systems, at each iteration. Therefore, it is desirable to have a closed-form update of the matrix inverse at each step. In the unique case of BFGS, using the "Woodbury inversion formula", we may write succinctly for $H_k = B_k^{-1}$, and we iteratively update the approximate Hessian (MS BFGS) as

TABLE I: Quasi-Newton method comparison. Our method, applied on any of the multisecant QN methods, sacrifices the multisecant condition for PSD.

Method	Symm.	PSD	MS cond.	update rank
Broyden's	×	×	×	1
PSB	✓	×	×	3
DFP	✓	✓	×	3
BFGS	✓	✓	×	2
Multisecant QN	×	×	✓	$2p$
Ours	✓	✓	≈	$2p$

$$\begin{aligned} H_{k+1} = {} & H_k - \\ & \begin{bmatrix} H_kY_k & S_k \end{bmatrix} \begin{bmatrix} Y_k^TS_k + Y_k^TH_kY_k & Y_k^TS_k \\ S_k^TY_k & 0 \end{bmatrix}^{-1} \begin{bmatrix} Y_k^TH_k \\ S_k^T \end{bmatrix}. \end{aligned}$$

Importantly, the term B_k is never needed in the update. This is not true for Broyden's, PSB, or DFP; that is, in their Woodbury inversions, B_k is not canceled. Therefore, in these three methods, backsolve is still required at each iteration.

III. An almost-multi-secant method

We first summarize all the existing multisecant QN methods as

$$B_{k+1} = B_k - D_1W^{-1}D_2^T \tag{14}$$

for some D_1, D_2, W, specified in Table II. (Note that W is not assumed to be symmetric nor PSD.) The natural perturbation to enforce symmetry and positive semidefiniteness is to

$$B_{k+1} = B_k - \frac{D_1W^{-1}D_2^T + (D_1W^{-1}D_2^T)^T}{2} + \mu I \tag{15}$$

where μ is the smallest positive value needed to ensure that $B_{k+1} \succeq 0$. That is, defining

$$\Delta = -\frac{1}{2}\begin{bmatrix} D_1 & D_2 \end{bmatrix} \begin{bmatrix} 0 & W_k^{-1} \\ W_k^{-T} & 0 \end{bmatrix} \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix} \in \mathbb{R}^{n\times n}$$

then the goal is to find $\mu = \max\{0, -\lambda_{\min}(B_k + \Delta)\}$. Note that the multisecant condition $B_{k+1}S_k = Y_k$ cannot be exact when we perturb B_{k+1}, and this is the reason of being an 'almost multisecant' scheme.

However, in general, finding $\lambda_{\min}(B_k)$ may not be computationally cheap. The obvious approach is to use a fast power method or Lanczos method, but there is no reason to assume that B_k is sparse, nor low rank after n iterations. Therefore, we assume that this operation is prohibitive, or at least can only be used rarely. Instead, we use low-rank operations to simply find $\mu = \max\{0, -\lambda_{\min}(\Delta)\}$. This is an overapproximation, and guarantees that B_{k+1} is symmetric and PSD. In cases where μ is too large, at worst the method behaves like gradient descent. However, in our numerical results, our method always outperforms gradient descent.

We now provide the main theorem that describes how to compute μ using only low rank updates. Note that A, c, and F are explicitly chosen such that $H_1 = \Delta$ in the following Theorem 1.

TABLE II: All four MS methods can be written in form (14), with the following choices of D_1, D_2, and W, where W is related to the Schur complement of the update matrix. Here, we write $Z_k = Y_k - B_k S_k$. We also show the update of $H_k = B_k^{-1}$ for BFGS. *= update is consistent only if B_k is symmetric PSD at each iteration.

	D_1	D_2	W
Broyden's	Z_k	S_k	$-S_k^T S_k \in \mathbb{R}^{p\times p}$
PSB	$\begin{bmatrix} Z_k & S_k & S_k \end{bmatrix}$	$\begin{bmatrix} S_k & Z_k & S_k \end{bmatrix}$	$\begin{bmatrix} -S_k^T S_k & 0 & 0 \\ 0 & -S_k^T S_k & 0 \\ 0 & 0 & S_k^T S_k (Z_k^T S_k)^{-1} S_k^T S_k \end{bmatrix} \in \mathbb{R}^{3p\times 3p}$
DFP	$\begin{bmatrix} Z_k & Y_k & Y_k \end{bmatrix}$	$\begin{bmatrix} Y_k & Z_k & Y_k \end{bmatrix}$	$\begin{bmatrix} -Y_k^T S_k & 0 & 0 \\ 0 & -Y_k^T S_k & 0 \\ 0 & 0 & (Y_k^T S_k)(Z_k^T S_k)^{-1}(Y_k^T S_k) \end{bmatrix} \in \mathbb{R}^{3p\times 3p}$
BFGS	$\begin{bmatrix} Y_k & B_k S_k \end{bmatrix}$	$\begin{bmatrix} Y_k & B_k S_k \end{bmatrix}$	$\begin{bmatrix} -Y_k^T S_k & 0 \\ 0 & S_k^T B_k S_k \end{bmatrix} \in \mathbb{R}^{2p\times 2p}$
BFGS inv*	$[H_k Y_k \quad S_k]$	$[H_k^T Y_k \quad S_k]$	$\begin{bmatrix} Y_k^T H_k Y_k + Y_k^T S & Y_k^T S_k \\ S_k^T Y_k & 0 \end{bmatrix} \in \mathbb{R}^{2p\times 2p}$

Theorem 1. *Consider W a nonsymmetric matrix, and*

$$\Delta = \mu I - \frac{1}{2}\begin{bmatrix} D_1 & D_2 \end{bmatrix} \begin{bmatrix} 0 & W^{-1} \\ W^{-T} & 0 \end{bmatrix} \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix}. \tag{16}$$

We take the eigenvalue decomposition of the $p \times p$ matrix $W^{-1} = U\Sigma V^T$, and for any $c > 0$, $0 \le \epsilon \le 1$, construct

$$\begin{aligned} &\Sigma = (S^2 - c^2 I)^{-1} S, \qquad F = \frac{c\epsilon}{c + \|W\|_2} V S U^T, \\ &P = (cI - c^{-1} F F^T)^{-1}, \qquad Q = (cI - c^{-1} F^T F)^{-1}, \end{aligned} \tag{17}$$

$$A = \begin{bmatrix} D_1 & D_2 \end{bmatrix} \begin{bmatrix} P & -cQF^T - W^{-1} \\ -cFQ - W^{-T} & Q \end{bmatrix} \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix}.$$

Then Δ is PSD if and only if

$$H_2 = \begin{bmatrix} cI & F \\ F^T & cI \end{bmatrix} - \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix} (A + 2\mu I)^{-1} \begin{bmatrix} D_1 & D_2 \end{bmatrix}$$

is PSD.

Proof of Thm. 1. First, we verify that by this construction,

$$A = \begin{bmatrix} D_1 & D_2 \end{bmatrix} \begin{bmatrix} P & -cQF^T - W^{-1} \\ -cFQ - W^{-T} & Q \end{bmatrix} \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix}.$$

is PSD. Based on our construction, A can be written as

$$\begin{aligned} A &= \begin{bmatrix} D_1 & D_2 \end{bmatrix} \begin{bmatrix} P & -cFQ - W^{-1} \\ -cQF^T - W^{-T} & Q \end{bmatrix} \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix} \\ &= \begin{bmatrix} D_1 U & D_2 V \end{bmatrix} \underbrace{\begin{bmatrix} R & -c\delta SR - \Sigma \\ -c\delta RS - \Sigma & R \end{bmatrix}}_{=:E} \begin{bmatrix} U^T D_1^T \\ V^T D_2^T \end{bmatrix} \end{aligned}$$

where

$$R = (cI - c^{-1}\delta^2 S^2)^{-1}, \qquad \delta = \frac{c\epsilon}{c + \|W\|_2}.$$

Also, from (17), the first equation is a quadratic equation involving S_{ii} satisfying

$$S_{ii} = \frac{1 + \sqrt{1 + 4\Sigma_i^2 c^2}}{2\Sigma_i} \le \frac{1}{\Sigma_i} + c.$$

Note that since Σ_i are the singular values of W^{-1}, $\frac{1}{\Sigma_i} \le \|W\|_2$, which implies $S_{ii} \le \|W\|_2 + c$.

We are left to show if E is PSD. Note that we may partition E into 4 blocks of diagonal matrices, which means there exists a permutation PEP^T which is block diagonal, with 2x2 symmetric blocks

$$E_{ii} = \begin{bmatrix} (c - \frac{1}{c}\delta^2 S_{ii}^2)^{-1} & \frac{\delta S_{ii}}{\delta^2 S_{ii}^2 - c^2} - \Sigma_{ii} \\ \frac{\delta S_{ii}}{\delta^2 S_{ii}^2 - c^2} - \Sigma_{ii} & (c - \frac{1}{c}\delta^2 S_{ii}^2)^{-1}. \end{bmatrix}$$

The (1,1) and (2,2) blocks can be shown to be positive since

$$\delta S_{ii} \le \frac{c}{c + \|W\|_2}(\|W\|_2 + c) = c. \tag{18}$$

Therefore, E_{ii} is PSD iff the (2,1) element has magnitude smaller than both diagonal elements; that is,

$$E_{ii} \succeq 0 \iff \frac{1}{c - \frac{1}{c}\delta^2 S_{ii}^2} \ge \frac{\delta S_{ii}}{\delta^2 S_{ii}^2 - c^2} - \Sigma_{ii}.$$

Since (18), this is equivalent to

$$c \ge -c_3 S_{ii} - \underbrace{(c^2 - c_3^2 S_{ii}^2)}_{\ge 0} \Sigma_{ii}$$

which is true since the right hand side is negative.

Next, we consider the matrix

$$H = \begin{bmatrix} 2\mu I + A & D_1 & D_2 \\ D_1^T & cI & F \\ D_2^T & F^T & cI \end{bmatrix}.$$

where c is a nonnegative scalar, F is a $2p \times 2p$ matrix (yet undefined), and A is some (unspecified) symmetric matrix. Then the two Schur complements of H are H_1 and H_2:

$$\begin{aligned} H_1 &:= 2\mu I + A - \begin{bmatrix} D_1 & D_2 \end{bmatrix} \begin{bmatrix} cI & F \\ F^T & cI \end{bmatrix}^{-1} \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix} \\ H_2 &= \underbrace{\begin{bmatrix} cI & F \\ F^T & cI \end{bmatrix}}_{H_3} - \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix} (A + 2\mu I)^{-1} \begin{bmatrix} D_1 & D_2 \end{bmatrix}. \end{aligned}$$

Then,

$H_1 \in \mathbb{R}^{n\times n}$ is PSD and $\begin{bmatrix} c_1 I & F \\ F^T & c_2 I \end{bmatrix}$ is PSD and invertible

if and only if

$H_2 \in \mathbb{R}^{4m\times 4m}$ is PSD and $A + 2\mu I$ is PSD and invertible.

Since we already showed that A is PSD, we see that testing H_2 for PSD is sufficient to guarantee H_1 is PSD.

□

This proposes a method for choosing μ, which is summarized in Alg. 1; the full method is summarized in Alg. 2.

Algorithm 1 Compute μ

Input: D_1, D_2, W, $i_{\max}$

Output: μ such that Δ in (16) is PSD.

$[U, \Sigma, V] = \mathbf{svd}(W)$

Define F, P, Q and S as in (17).

$\mu = 0.01$

Construct $\bar{D} = \begin{bmatrix} D_1^T \\ D_2^T \end{bmatrix} \begin{bmatrix} D_1 & D_2 \end{bmatrix}$ and

$$C = \begin{bmatrix} P & -cQF^T - W^{-1} \\ -cFQ - W^{-T} & Q \end{bmatrix}.$$

for $i = 1$ **to** $i_{\max}$ **do**

  Find H_2 where $A+2\mu I$ is inverted using the Woodbury lemma

$$H_2 = \begin{bmatrix} cI & F \\ F^T & cI \end{bmatrix} - \frac{1}{2\mu}\bar{D} + \frac{1}{2\mu}\bar{D}(2\mu C^{-1} + \bar{D})^{-1}\bar{D}$$

  if $\lambda_{\min}(H_2) > 10^{-15}$ **then**

    break.

  else

    $\mu \leftarrow 2\mu$

  end if

end for

Algorithm 2 Almost multisecant Quasi-Newton algorithm

Input: $B, x_0, \alpha, p, f(x), \nabla f(x)$

Output: $f_{k+1}(x)$

$B_0 = I$

for $k = 1, \ldots, T$ **do**

  Update s_1,...,s_p, and $y_1, ..., y_p$ using (9) or (10).

  Update S_k, Y_k using (11) and (12).

  Compute D_1, D_2, W

  Use Alg. 1 to pick μ

  Update B_{k+1}^{-1} using (15)

  Update $x_{k+1} = x_k - \alpha B_{k+1}^{-1}\nabla f(x_k)$

end for

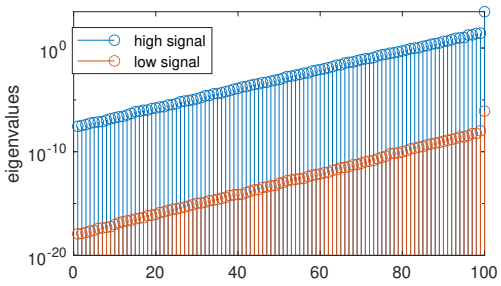

Fig. 1: Spectrum of Hessian in sensing problem

IV. Numerical Results

A. Compute μ

Table III shows the runtime of Algorithm 1 vs eigenvalue decompositions using full (`eig`) or fast partial (`eigs`) operations. By leveraging low-rank structure, we significantly reduce the runtime complexity.

B. Sensing problem

Our experiments are performed over a sensing problem that is tuned to make the Hessian ill-conditioned; that is, problems in which quasi-Newton methods (and especially MS variants) perform better than gradient or single-secant methods. Our sensing model is $\mathbf{A}x \approx \mathbf{b}$, where we construct each variable as follows:

- Labels $\mathbf{b}_i \in \{1, -1\}$ with equal probability (class balanced)
- Decay rate $c_j = \exp(-\beta j), j = 1, ..., n$
- Noise decaying with feature

$$\mathbf{N}_{i,j} = z_{i,j}^{(2)} c_j, \qquad z_{i,j} \sim \mathcal{N}(0, 1)$$

- High signal regime $\mathbf{A}_{i,j} = \mathbf{b}_i z_j^{(1)} + \mathbf{N}$
- Low signal regime: $\mathbf{A}_{i,j} = \mathbf{b}_i z_j^{(1)}(1 - c_j) + \mathbf{N}$

The spectrum of the Hessian in logistic regression, using these problem parameters and objective function (20) is shown in Fig 1.

C. Quadratic vs non-Quadratic

We compare the performance of the proposed MS-BFGS variants in Figure 2, where the quadratic and logistic regression problems minimize the following respective cost functions:

$$f_{\text{quad}}(x) := \frac{1}{2p}||\mathbf{A}x - \mathbf{b}||_2^2, \tag{19}$$

$$f_{\text{logreg}}(x) := -\frac{1}{p}\sum_{i=1}^{p} \log(\sigma(\mathbf{b}_i \mathbf{a}_i^T x)). \tag{20}$$

Specifically, for quadratic problems, while the variations and enhancement do offer improvements, up to a pretty small error most enhancements are relatively irrelevant, as $Y^T S$ is always positive semidefinite and symmetrization / perturbations are not needed to make MS methods stable. On the other hand, for logistic regression, non-perturbed MS methods are not guaranteed to be stable; they do often diverge.

TABLE III: Runtime (in seconds) comparison of Alg. 1, vs direct eigenvalue computation. Format: mean(std).

n	eig	eigs	Alg. 1 $i_{\max} = 10$	Alg. 1 $i_{\max} = 30$	Alg. 1 $i_{\max} = 50$
500	3.3e-2 (1.1e-2)	2.0e-3 (8.0e-4)	7.2e-4 (2.6e-4)	7.3e-4 (2.7e-4)	6.6e-4 (2.5e-4)
1000	8.9e-2 (3.0e-2)	4.8e-3 (2.0e-3)	1.7e-3 (5.8e-4)	1.8e-3 (6.4e-4)	1.9e-3 (6.3e-4)
2500	5.8e-1 (1.9e-1)	3.1e-2 (1.0e-2)	9.6e-3 (3.2e-3)	9.8e-3 (3.3e-3)	1.0e-2 (3.5e-3)
5000	2.3 (7.6e-1)	2.1e-01 (7.0e-2)	3.6e-2 (1.2e-02)	3.6e-2 (1.2e-2)	3.8e-02 (1.3e-2)

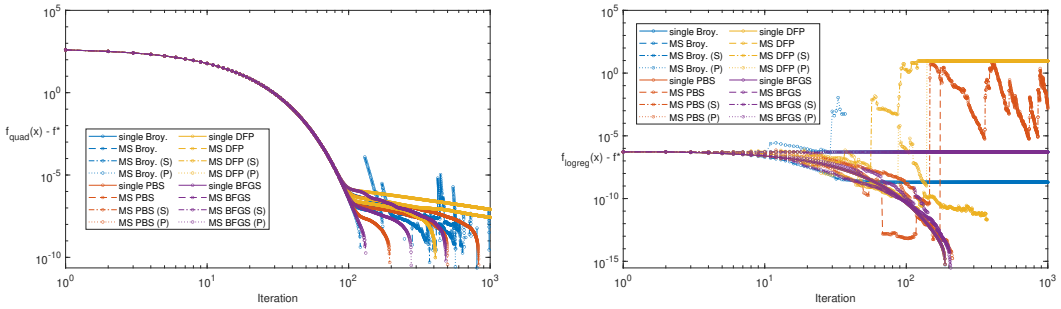

Fig. 2: Comparison of methods on quadratic (19) vs logistic regression (low signal) (20).

TABLE IV: Failure rate (diverge or did not converge in 500 iterations) over 18 problems, 10 trials each.

	sin.	(V)	(S)	(P)	our(B)	our(W)
Broyden	0	0.18	1.00	0.072	0.11	–
PSB	0	0.028	0.67	0	0.0056	–
DFP	0	0.039	0.79	0.028	0.050	–
BFGS	0	0.017	0.68	0	0.0056	0.017

TABLE V: Average number of iterations to reach $f(x_k) - f^* \leq \epsilon := 10^{-9}$, over 10 trials.

	Low signal regime			High signal regime		
	Easy	Med.	Hard	Easy	Med.	Hard
Single Broy.	77.3	81.1	92.1	69.6	69.6	69.6
MS Broy. (V)	67.5	**65.9**	83.4	**55.7**	59.4	**51.6**
MS Broy. (S)	–	–	–	–	–	–
MS Broy. (P)	81.9	95.1	84.8	89.9	81.2	74.7
Our Broy. (B)	**60.1**	**65.9**	**71.8**	57.8	**54.6**	62.3
Single PSB	77.3	81.1	92.1	69.6	69.6	69.5
MS PSB (V)	80.5	78.0	83.4	62.3	64.1	57.9
MS PSB (S)	227.9	207.3	285.6	115.4	123.7	214.5
MS PSB (P)	**66.0**	**71.4**	**83.1**	**58.8**	**62.8**	**53.4**
Our PSB (B)	71.8	97.5	102.0	85.3	74.6	61.2
Single DFP	**77.3**	**81.1**	**92.1**	**69.6**	**69.6**	**69.6**
MS DFP (V)	133.5	169.6	151.6	108.1	128.6	107.7
MS DFP (S)	128.3	248.2	213.3	158.5	252.5	117.2
MS DFP (P)	94.3	103.8	114.7	105.7	81.7	110.8
Our DFP (B)	165.9	172.3	142.8	120.6	153.6	120.8
Single BFGS	77.3	81.1	92.1	69.6	69.6	69.6
MS BFGS (V)	69.9	84.9	72.7	67.6	57.3	59.5
MS BFGS (S)	249.7	182.9	296.6	144.2	192.0	252.6
MS BFGS (P)	76.5	75.0	92.4	64.0	68.7	76.3
Ours (B)	65.6	65.7	88.3	65.0	62.6	64.2
Ours (W)	**45.0**	**51.0**	**60.2**	**26.4**	**27.6**	**27.7**

D. Logistic regression

We now give more extensive results for minimizing (20). Here, we construct the problem specifically to make optimizing f difficult without second-order information. We use $\alpha = 0.1$ as the backoff parameter in all cases.

We compare the performance over the four base QN methods: Broyden's, PSB, DFP, and BFGS. In each case, we compare over five variants: single-secant ($p = 1$) update, vanilla MS update (V), symmetrization-only update (where $\mu = 0$ in (15)) (S), PSD-direct update (where μ is computed exactly as the smallest perturbation to make B_{k+1}^{-1} PSD), and ours (Algorithm 2). In the case of BFGS, we also include an update where the entire procedure is replaced with perturbing $H_k = B_k^{-1}$, rather than B_k. We differentiate the two as (B) (for backsolve) and (W) (for Woodbury).

Table V gives the average number of iterations to reach the tolerance under an easy ($\beta = 10/n$), medium (($\beta = 20/n$), and hard ($\beta = 30/n$) regime. In several cases, the method diverged or did not converge in 500 iterations, and was labeled a "failure"; the failure rate across all experiments is given in Table IV. Interestingly, direct symmetrization, without ensuring PSD, almost certainly guarantees failure, highlighting the delicacy of these methods; careless perturbations will not fail gracefully. We observe the following trends.

1) In Broyden's method and BFGS, our perturbation often performed best, and in the BFGS case, with the Woodbury inversion, significantly outperformed all other MS-QN methods.
2) In PSB methods, the best method is an exact computation of μ, followed by our approach. This shows that we have the right idea, but Algorithm 1 is a bit noise-prone. This is not surprising, since doubling μ at each iteration means that the final estimate is often very coarse. Note also that MS BFGS(P) in Table V is not a feasible method in practice, as it requires full spectral computations; it is only a mark of comparison.
3) In DFP, it does not look like any method is more superior than the single-secant variant. In fact, all multi-secant approaches seem to deteriorate performance significantly. This is perhaps because the family of logistic regression problems we have chosen are not the best fit for DFP.

To clarify, the method (P) adds a $-\lambda_{\min}(H)I$ term to the approximate Hessian, which is like an "oracle" because in general $\lambda_{\min}(H)$ cannot be computed at each iteration. These rows are included as unrealistic baselines. We also note that in terms of actual implementation practically, we observe that only BFGS can be useful because the others cannot update their inverse Hessian approximates in closed form, and require linear system solves at each iteration. Overall, though, Table V is meant to be comprehensive, and the four QN variants do not always behave identically.

V. Conclusion

We explore multisecant quasi-Newton methods as fast curvature-approximating methods. The time complexity of all methods is $O(n^2)$ for the matrix-vector multiplications; this is the same for all multiscant QN methods. However, Our key contribution is in the *number of steps to convergence* which is controlled by ensuring descent at each step. Specifically, we look at convex nonquadratic problems, where, because of the multisecant feature, the step directions are not always descending (Hessian approximate is not always positive semidefinite), which leads to method instability. We propose a unified fast perturbation strategy in terms of a small μ perturbation, whose update is computed efficiently, and approximates the update steps for Broyden's, Powell's, DFP, and BFGS, which introduce little overhead but offer improved convergence and stability.

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