Quasi-Newton Acceleration of EM and MM Algorithms via Broyden's Method with Extrapolation

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Summary.

The principle of majorization-minimization (MM) provides a general framework for eliciting effective algorithms to solve optimization problems. However, they often suffer from slow convergence, especially in large-scale and high-dimensional data settings. This has drawn attention to acceleration schemes designed exclusively for MM algorithms, but many existing designs are either problem-specific or rely on approximations and heuristics loosely inspired by the optimization literature. We propose a novel, rigorous quasi-Newton method for accelerating any valid MM algorithm, cast as seeking a fixed point of the MM *algorithm map*. The method does not require specific information or computation from the objective function or its gradient, and enjoys a limited-memory variant amenable to efficient computation in high-dimensional settings. By connecting our approach to Broyden's classical root-finding methods, we establish convergence guarantees and identify conditions for linear and super-linear convergence. These results are validated numerically and compared to peer methods in a thorough empirical study, showing that it achieves state-of-the-art performance across a diverse range of problems.

1. Introduction

Iterative procedures are becoming increasingly prevalent for statistical tasks that are cast as optimization of objective functions lacking a closed form solution. The canonical setting of minimizing a measure of fit together with a penalty term sits at the heart of statistics, yet challenges still arise from high dimensionality, missing data, constraints, and other aspects of contemporary data. The principle of majorization-minimization (MM) provides a framework for designing effective algorithms well-suited for such problems. Perhaps the most well-known special case is the expectation-maximization (EM) algorithm, a workhorse for maximum likelihood estimation under missing data. The general MM principle is attractive because it admits algorithms that (1) are simple to implement and (2) provide stable performance by obeying monotonicity in the objective (Dempster et al., 1977; Laird, 1978).

However, MM algorithms typically converge at a locally linear rate, which can translate to impractically slow progress in many statistical problems, especially in high dimensions (Wu, 1983; Boyles, 1983; Meng and Rubin, 1994). To address this issue, a body of work designs general acceleration schemes for numerical optimization methods including Nesterov's schemes (Nesterov, 1983), SAG (Schmidt et al., 2017), SAGA (Defazio et al., 2014), catalyst acceleration (Lin et al., 2017), and SDCA (Shalev-Shwartz and Zhang, 2014). Special attention has also been given towards acceleration methods specifically designed for MM algorithms (Jamshidian and Jennrich, 1997, 1993; Lange, 1995; Zhou et al., 2011). Broadly, these methods seek additional information to better inform the search direction and/or step lengths of the unadorned algorithm. Improvements may come from high order differentials of the objective or algorithm map that incur additional computational cost. Therefore, it becomes necessary to balance these tradeoffs.

So-called *hybrid* accelerators (Jamshidian and Jennrich, 1997) rely on working directly on the original objective function (Lange, 1995; Jamshidian and Jennrich, 1997, 1993). Approximate second order information can then be obtained via Fisher scoring in the case of EM. Outside of the context of missing data, classical tools such as quasi-Newton and conjugate gradient methods can be applied to the objective to similar effect. However, an advantage of MM algorithms lies in sidestepping unwieldy objectives in favor of operating on simpler surrogates—for instance, EM works well because it bypasses the need to consider the observed data log-likelihood. These hybrid methods unfortunately fail to preserve this key advantage of MM algorithms.

An alternative is to instead consider accelerating the MM algorithm map directly in a way that is largely agnostic to the optimization objective. These have been classified as *pure* accelerators; see Jamshidian and Jennrich (1997). One class of *pure* first-order accelerators is given by quasi-Newton algorithms, which utilize approximate first-order information to find roots of the MM residuals. Jamshidian and Jennrich (1997) explicitly apply Broyden's classical root-finding algorithm for this purpose (Broyden, 1965). As we outlay our method, we will demonstrate that further improvement can be achieved by modifying a general Broyden-type method (Broyden et al., 1973) that leverages extra information from the MM map. The STEM and SQUAREM methods of Varadhan and Roland (2008) approximate the Jacobian matrix of MM residuals by a scalar multiple of the identity matrix. The quasi-Newton method of Zhou et al. (2011) involves an assumption based on nearness to the stationary point, rendering it sensitive to initialization. These pure accelerators tend to preserve the simplicity, convergence properties, and low computational cost of the original algorithm. However, they often rely on heuristic approximations or derivations that potentially ignore a large amount of crucial first-order information. While loosely inspired by the theory behind classical quasi-Newton methods, it can be argued that these methods do not fully and formally take advantage of the prior optimization literature.

This paper seeks to fill the methodological gap by proposing a generic accelerator for any MM algorithm map F via a quasi-Newton approximation to the Jacobian of the fixed point equation $G(x) = F(x) - x$. We build off of the wisdom in Zhou et al. (2011), referring to their method as ZAL in this paper, that seeks a root of $G(x)$ without imposing positive definiteness constraints. Casting the problem in this way leads to robustness against numerical instabilities. Our method differs from ZAL in several important ways. While ZAL minimizes the norm of the Jacobian near the fixed point, we optimize a richer objective that directly ties into the classical approach of minimizing the change in the Jacobian across iterations. This standard quasi-Newton recipe demands storing the approximate Jacobian matrices in each iteration, which can be computationally ineffective for high dimensions. To address this issue, we further propose a limited-memory variant of our method amenable to high-dimensional settings.

2. Background: EM, MM, and Acceleration

MM algorithms are increasingly popular toward solving large-scale and high-dimensional optimization problems in statistics and machine learning (Lange and Wu, 2008; Zhou et al., 2015; Xu and Lange, 2019). Consider $\boldsymbol{x} \in \mathbb{R}^p$ and the goal of minimizing a "difficult" objective function $f : \mathbb{R}^p \to \mathbb{R}$, i.e. of finding $\boldsymbol{x}^* = \text{argmin}_{\boldsymbol{x}} f(\boldsymbol{x})$. An MM algorithm transfers this task onto an iterative scheme, successively minimizing a sequence of surrogate functions $g(\boldsymbol{x} \mid \boldsymbol{x}_k)$ which dominate the objective function $f(\boldsymbol{x})$ and are tangent to it at the current iterate $\boldsymbol{x}_k$. That is, they require that $g(\boldsymbol{x}_k \mid \boldsymbol{x}_k) = f(\boldsymbol{x}_k)$ and $g(\boldsymbol{x} \mid \boldsymbol{x}_k) \geq f(\boldsymbol{x})$ for all $\boldsymbol{x}$ at each iteration k. Decreasing $g(\boldsymbol{x} \mid \boldsymbol{x}_k)$ automatically engenders a decrease in $f(\boldsymbol{x})$. The resulting update $\boldsymbol{x}_{k+1} = \text{argmin}_{\boldsymbol{x}} g(\boldsymbol{x} \mid \boldsymbol{x}_k)$ implies the string of inequalities

$$f(\boldsymbol{x}_{k+1}) \leq g(\boldsymbol{x}_{k+1} \mid \boldsymbol{x}_k) \leq g(\boldsymbol{x}_k \mid \boldsymbol{x}_k) = f(\boldsymbol{x}_k), \tag{1}$$

validating the descent property. Examining this short proof of descent in Eq.(1) reveals that exact minimization of $g(\boldsymbol{x} \mid \boldsymbol{x}_k)$ is not strictly necessary, and any update that decreases g is sufficient. A local optimum of $f(\boldsymbol{x})$ is found by successively minimizing the sequence of surrogates. Our method will make use of this practically useful observation.

The celebrated EM method for maximum likelihood estimation is a special case of this principle that relies on the notion of missing data to define the surrogate $g(\boldsymbol{x} \mid \boldsymbol{x}_k)$. Besides EM, instances of MM abound in statistics, ranging from matrix factorization (Lee and Seung, 1999) to nonconcave penalized likelihood estimation (Zou and Li, 2008).

The MM principle thus offers a general recipe for converting a hard optimization problem into a stable and simpler sequence of manageable subproblems, which can be expressed as an algorithm map in a p-dimensional space, denoted by F, that updates

$$\boldsymbol{x}_{k+1} = F(\boldsymbol{x}_k).$$

The iteration terminates when a chosen vector norm (usually L_2 norm) of differences between two consecutive iterates is small enough, i.e. $\|\Delta \boldsymbol{x}_k\| = \|\boldsymbol{x}_{k+1} - \boldsymbol{x}_k\| \leq \epsilon$ for some tolerance $\epsilon > 0$. From the perspective of the algorithm map, the MM algorithm amounts to seeking the fixed point $\boldsymbol{x}^*$ of F; an equivalent formulation that appears in the literature is to seek the root of $G(\boldsymbol{x}) := F(\boldsymbol{x}) - \boldsymbol{x}$. This approach has paved the way for quasi-Newton acceleration regimes that attempt to well-approximate the inverse of the Jacobian of G at $\boldsymbol{x}_k$; see Luenberger et al. (1984); Dennis Jr and Schnabel (1996) for a more detailed discussion. Let $dG(\boldsymbol{x})$ be the differential of G at $\boldsymbol{x}$, then $dG(\boldsymbol{x}) = (dF(\boldsymbol{x}_k) - I_p)$ where I_p is the $p \times p$ identity matrix. Denoting the approximation to $dG(\boldsymbol{x}_k)^{-1}$ by H_k, the quasi-Newton update of $\boldsymbol{x}_k$ is given by

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - H_k G(\boldsymbol{x}_k) \,. \tag{2}$$

Various quasi-Newton methods differ from one another in the way $dG(\boldsymbol{x})^{-1}$ is approximated. The thread that ties them together is a *secant condition*, which states that H_k is the exact inverse Jacobian of a linear function joining $(\boldsymbol{x}_k, G(\boldsymbol{x}_k))$ and some other point of choice, say $(\boldsymbol{y}, G(\boldsymbol{y}))$. That is, the secant constraint mandates that H_k satisfies

$$\boldsymbol{y} - \boldsymbol{x}_k = H_k(G(\boldsymbol{y}) - G(\boldsymbol{x}_k)) \,. \tag{3}$$

In the classical Broyden's method, $\boldsymbol{y}$ is taken to be $\boldsymbol{x}_{k+1}$ obtained using Eq.(2), whereas Zhou et al. (2011) assume the function G to be linear between the iterate $\boldsymbol{x}_k$ and its image $F(\boldsymbol{x}_k)$ under the MM map. For $\boldsymbol{x} \in \mathbb{R}^p$, H_k is a $p \times p$ matrix and the secant constraint fixes p degrees of freedom. The remaining $p^2 - p$ degrees entail that Eq.(3) is underdetermined, satisfied by infinitely many solutions H_k. At this juncture, deriving quasi-Newton methods proceeds by specifying an additional criterion to admit a well-defined procedure. We now survey various popular approaches along this line of thought.

2.1. Existing MM Acceleration Schemes

Perhaps the most transparent and well-studied quasi-Newton acceleration scheme was proposed by Jamshidian and Jennrich (1997). Their method directly applies the quasi-Newton method for root finding by Broyden (1965), maintaining the inverse Jacobian approximation H_k by the update

$$\Delta H_k = \frac{(\Delta \boldsymbol{x}_k - H_k \Delta G_k)\Delta \boldsymbol{x}_k^T H_k}{\Delta \boldsymbol{x}_k^T H_k \Delta \boldsymbol{x}_k} \,,$$

where $\Delta \boldsymbol{x}_k = -H_k G(\boldsymbol{x}_k)$, $\Delta G_k = G(\boldsymbol{x}_k + \Delta \boldsymbol{x}_k) - G(\boldsymbol{x}_k)$, and $\Delta H_k = H_{k+1} - H_k$ for any time point k. Contributions since have noted that this dense matrix update becomes computationally prohibitive in high dimensions typical of contemporary data. The STEM method by Varadhan and Roland (2008) instead provides a simpler approximation of H_k as only a scalar multiple of the identity matrix. Assuming $H_k = \alpha_k I_p$, three variants of STEM entail slightly different inverse Jacobian approximations under

$$\alpha_k^{(1)} = \frac{\boldsymbol{u}_k^T \boldsymbol{v}_k}{\boldsymbol{v}_k^T \boldsymbol{v}_k}, \qquad \alpha_k^{(2)} = \frac{\boldsymbol{u}_k^T \boldsymbol{u}_k}{\boldsymbol{u}_k^T \boldsymbol{v}_k}, \qquad \alpha_k^{(3)} = -\frac{\|\boldsymbol{u}_k\|}{\|\boldsymbol{v}_k\|}, \tag{4}$$

where

$$\boldsymbol{u}_k = F(\boldsymbol{x}_k) - \boldsymbol{x}_k, \quad \text{and} \quad \boldsymbol{v}_k = G(F(\boldsymbol{x}_k)) - G(\boldsymbol{x}_k) = F^2(\boldsymbol{x}_k) - 2F(\boldsymbol{x}_k) + \boldsymbol{x}_k.$$

The scalars α_k in (4) can be understood as various steplengths for each update rule. An extension to STEM known as SQUAREM was later proposed by the same authors (Varadhan and Roland, 2008), using the idea of a "squared" Cauchy method which may outperform traditional Cauchy methods. SQUAREM makes use of the following update

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - 2\alpha_k \boldsymbol{u}_k + \alpha_k^2 \boldsymbol{v}_k \,.$$

While SQUAREM outperforms many acceleration methods and is chiefly regarded for its simplicity, the loss of information due to the identity matrix approximation can remain severe, especially in high dimensional cases.

More recently, an acceleration scheme, referred to as ZAL, was proposed by Zhou et al. (2011). It enjoys the same computational complexity as SQUAREM by avoiding matrix approximation of $dG(\boldsymbol{x}_k)^{-1}$ in the quasi-Newton update formulation in Eq.(2) at each step, with update rule

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \left(I_p - \frac{\boldsymbol{v}_k \boldsymbol{u}_k^T}{\boldsymbol{u}_k^T \boldsymbol{u}_k}\right)^{-1} G(\boldsymbol{x}_k) = (1 - c_k) F(\boldsymbol{x}_k) + c_k F^2(\boldsymbol{x}_k)$$

where $c_k = \boldsymbol{u}_k^T \boldsymbol{u}_k / \boldsymbol{u}_k^T \boldsymbol{v}_k$ and the differences $\boldsymbol{u}_k, \boldsymbol{v}_k$ are as defined earlier. It is worth mentioning the secant constraint used in ZAL, as we will motivate a similar constraint in terms of the end points for our method in the next section. Let $M := dF(\boldsymbol{x}^*)$. A key assumption made is that $\boldsymbol{x}_k$ is close to the optimal point $\boldsymbol{x}^*$ so that the following linear approximation is reasonable:

$$F \circ F(\boldsymbol{x}_k) - F(\boldsymbol{x}_k) \approx M(F(\boldsymbol{x}_k) - \boldsymbol{x}_k)\,. \tag{5}$$

As these methods too operate only with reference to the algorithm map, largely ignoring the objective function to be minimized, they will serve as comparisons for our proposed method. We next examine the merits of defining secant endpoints using (5) within Broyden's quasi-Newton paradigm in the following section.

3. A novel Broyden quasi-Newton method

Illustrative Example. We begin by accelerating a classic MM example of minimizing the cosine function $f(x) = \cos(x)$, using quasi-Newton to find the root of MM residual. The goal is to highlight the difference between our secant approximation made using end points in (5) and Broyden's standard method, providing concrete intuition on why the former approach improves performance. In particular, it shows explicitly how our approach leverages information from the geometry of the MM map toward a nonlinear update. To derive a surrogate, consider the following quadratic expansion about $y \in \mathbb{R}$:

$$\begin{aligned} \cos(x) &= \cos(y) - \sin(y)(x-y) - \frac{1}{2}\cos(z)(x-y)^2 \\ &\leq \cos(y) - \sin(y)(x-y) + \frac{1}{2}(x-y)^2 \ := \ g(x \mid y), \end{aligned}$$

where z lies between x, y and the inequality follows since $|\cos(z)| \leq 1$ (Lange, 2016). Thus, $g(x \mid y)$ majorizes the original objective. It is straightforward to minimize g and see that the resulting MM step is given by the nonlinear update formula

$$x_{k+1} = F(x_k) = x_k + \sin(x_k)\,.$$

We are interested in finding the root of $G(x) = F(x) - x = \sin(x)$. Consider a scenario in Figure 1, where the previous and current iterates, labeled A and B respectively, lie on opposite sides of the root $x^* = \pi$ of the function G, denoted by the vertical dashed line. Let C^* denote the next iterate obtained by the standard MM update from point B without acceleration.

Rather than moving to C^*, the standard Broyden's method approximates the Newton search direction as the slope of the line joining A and B (dotted red), whereas our update

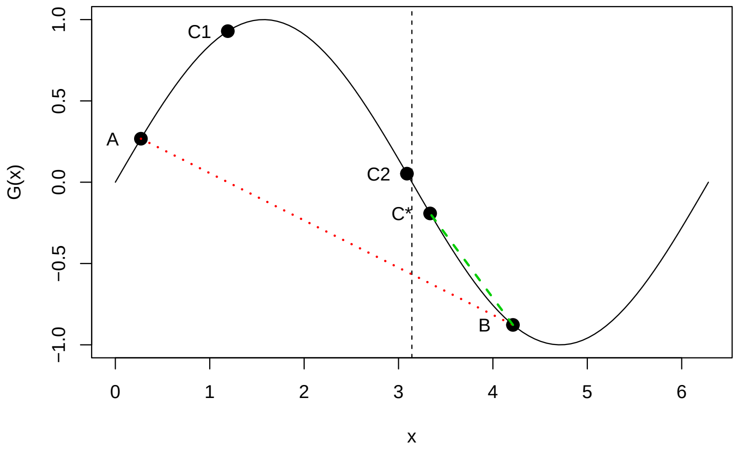


Fig. 1. Comparison of secant approximations.

derived below will use the line joining B and C^* as the search direction (dashed green). As a result, the next iterate from standard Broyden's method would yield C_1 whereas our update, described in the next section, leads to C_2, much closer to the optimum. Denoting the corresponding points on the x-axes as a, b, c^*, c_1, and c_2, the formulation for both the updates is

$$c_1 = b - G(b)\frac{b-a}{G(b)-G(a)} \qquad \text{and} \qquad c_2 = b - G(b)\frac{c^*-b}{G(c^*)-G(b)} .$$

Even in a univariate setting, where H_k can be completely determined from the secant condition, the advantage provided by our novel secant approximation is clear when the current state does not render a good search direction. The additional information can act as a correction when the original algorithm leads us to a *bad* current state (here B). Because the secants drawn in the standard version of Broyden's method rely only linearly on the current and previous state, a bad quasi-Newton step propagates to a poor secant approximation that produces an update straying far from the fixed point. Our proposed method avoids this by drawing a secant that incorporates information at the current state together with an extrapolation from the next MM step, as we detail below. While this example would have been trivial to optimize directly, it illustrates an advantage that tends to become more pronounced in higher dimensions where the added directional information we harness from the MM extrapolation is richer.

Deriving the proposed method. Recall that seeking the fixed points of the MM map amounts to finding the roots of $G(\boldsymbol{x})$ numerically. The quasi-Newton update is given by Eq.(2). Drawing inspiration from the secant approximation in (5), we propose the linear approximation

$$dG(\boldsymbol{x}_k)^{-1}\left[G(F(\boldsymbol{x}_k)) - G(\boldsymbol{x}_k)\right] \approx F(\boldsymbol{x}_k) - \boldsymbol{x}_k \,. \tag{6}$$

Using the differences $\boldsymbol{u}_k, \boldsymbol{v}_k$ as introduced in the previous section and recalling H_k denotes the approximation to $dG(\boldsymbol{x}_k)^{-1}$ that satisfies (6), the secant condition can be expressed as $H_k\boldsymbol{v}_k = \boldsymbol{u}_k$. Note that one may impose several secant approximations $H_k(\boldsymbol{v}_k^i) = \boldsymbol{u}_k^i$ for $i \in \{1, ..., q\}$ for any choice such that $q < p$. These can be generated at the current iterate $\boldsymbol{x}_k$ and previous $(q-1)$ iterates, and may yield better performance at the cost of extra computation. To this end, let $U_k = (\boldsymbol{u}_1\ \boldsymbol{u}_2 \ldots \boldsymbol{u}_q)$ and $V_k = (\boldsymbol{v}_1\ \boldsymbol{v}_2 \ldots \boldsymbol{v}_q)$ be two $p \times q$ matrices; the corresponding linear constraint for H_k in the multiple secant conditions case is

$$H_k V_k = U_k \,. \tag{7}$$

The $p \times p$ inverse Jacobian matrix H_k has p^2 degrees of freedom, of which pq degrees of freedom are fixed by the secant approximation. To derive a well-defined update, one must choose how to fix the remaining $p^2 - pq$ degrees of freedom. We follow classical intuitions that yield a connection to Broyden's method for finding roots of nonlinear functions. The idea behind this and several of the most successful quasi-Newton methods seeks the smallest perturbation to H_{k-1} when updating to H_k, which can also be viewed as imposing a degree of smoothness in the sequence of iterates. The resulting optimization problem can be formulated as

$$\begin{aligned} \text{Minimize} : &\ \|H_k - H_{k-1}\|_F \\ \text{subject to} : &\ H_k V_k = U_k \ , \end{aligned} \tag{8}$$

where $\|\cdot\|_F$ denotes the Frobenius norm. To proceed, we take partial derivatives of the Lagrangian

$$\mathcal{L} = \frac{1}{2}\|H_k - H_{k-1}\|_F^2 + \Lambda^T(H_kV_k - U_k)$$

with respect to h_k^{ij} and set to 0. Here h_k^{ij} denotes the ij^{th} element of the matrix H_k. As a consequence, we obtain the Lagrange multiplier equation

$$0 = h_k^{ij} - h_{k-1}^{ij} + \sum_{k=1}^{p} \lambda_{ik} v_{jk},$$

which can be expressed in matrix form as

$$H_k - H_{k-1} + \Lambda V_k^T = \mathbf{0}. \tag{9}$$

Right-multiplying Eq.(9) by V_k and imposing the constraint from Eq.(7) gives the solution for Λ as

$$\Lambda = (H_{k-1}V_k - U_k)(V_k^TV_k)^{-1}.$$

Therefore,

$$H_k = H_{k-1}\left(I_p - V_k(V_k^TV_k)^{-1}V_k^T\right) + U_k(V_k^TV_k)^{-1}V_k^T. \tag{10}$$

We remark that as the problem dimension increases, a larger choice of q fixes more information and may improve acceleration, but also risks numerical singularity for the matrix $V_k^TV_k$. We draw attention to the special case of $q = 1$ where

$$H_k = H_{k-1} - H_{k-1}\frac{\boldsymbol{v}_k\boldsymbol{v}_k^T}{\boldsymbol{v}_k^T\boldsymbol{v}_k} + \frac{\boldsymbol{u}_k\boldsymbol{v}_k^T}{\boldsymbol{v}_k^T\boldsymbol{v}_k}. \tag{11}$$

We see (11) can be written as $H_k = H_{k-1} + A_k + B_k$ where both A_k and B_k are rank-1 matrices, yielding a rank-2 update as expected. Also note that the symmetry condition on H_k assumed in classical Broyden-Fletcher-Goldfarb-Shanno (BFGS) updates for minimization is *not* necessary, as here we are approximating an inverse Jacobian rather than a Hessian/inverse Hessian matrix.

The search direction $\boldsymbol{p}_k$ at iteration k is given by $\boldsymbol{p}_k = -H_kG(\boldsymbol{x}_k)$, with a corrected update formula $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k + \gamma_k\boldsymbol{p}_k$, where $\gamma_k = \omega_k/\|\boldsymbol{p}_k\|$ is an appropriate scaling factor in the search direction. Here ω_k is the steplength and $\|\cdot\|$ denotes the L_2 vector norm. The corresponding steplength for the unaccelerated MM algorithm is $\|F(\boldsymbol{x}_k) - \boldsymbol{x}_k\| = \|\boldsymbol{u}_k\|$, and for a SQUAREM algorithm is $|\alpha_k^{(i)}|\|\boldsymbol{u}_k\|$ for $i \in \{1, 2, 3\}$. We choose the steplength $|\alpha_k^{(3)}|\|\boldsymbol{u}_k\| = \|\boldsymbol{u}_k\|^2/\|\boldsymbol{v}_k\|$ from (4) for our experiments in this paper due to its intuitive explanation (Varadhan and Roland, 2008). While the behavior of each of the three variants of SQUAREM varies widely, we will see that our method in contrast performs consistently well in a range of scenarios fixing $\omega_k = \|\boldsymbol{u}_k\|^2/\|\boldsymbol{v}_k\|$.

Intuition and relation to existing methods. ZAL and SQUAREM are perhaps the most widely used quasi-Newton acceleration methods for MM algorithms. The point of departure in these methods is to cast acceleration as seeking a zero of G. We delve a little further into the connection between quasi-Newton root-finding methods and MM acceleration; in particular, we ground our approach in the wisdom behind Broyden's method, and improve upon it by designing a novel secant approximation with endpoints as $\boldsymbol{x}_k$ and $F(\boldsymbol{x}_k)$. As illustrated in the demonstrative example, the benefits of this extrapolation step are twofold. By the descent property of the MM map, $F(\boldsymbol{x}_k) - \boldsymbol{x}_k$ gives a more reliable direction to move along, especially when $\boldsymbol{x}_k$ was a poor update from $\boldsymbol{x}_{k-1}$. Second, instead of only one constraint, the MM map enables us to impose multiple linear constraints that become increasingly accurate as iterates $\boldsymbol{x}_k$ approaches $\boldsymbol{x}^*$.

In contrast, the STEM and SQUAREM methods employ scalar multiples of the identity as approximations to the Jacobian matrix, which can ignore much valuable curvature information compared to a dense approximation. Unlike traditional root finders for nonlinear functionals (Broyden, 1965; Pearson, 1969), their convergence properties are not as rigorously established. The ZAL method makes an assumption that $\boldsymbol{x}_k$ is close to the stationary point $\boldsymbol{x}^*$, validating the linear approximation in Eq.(5). If M_k denotes the approximation to $dF(\boldsymbol{x}^*)$ at step k, then using the principle of parsimony, the objective in ZAL seeks to minimize $\|M_k\|_F$ subject to the constraint $V_k = (M_k - I_p)U_k$. This criterion yields a computationally elegant update, but unlike Eq.(8) for BQN, effects a disconnect from the theory and intuition behind quasi-Newton methods based on minimally perturbing H_k, i.e. Eq. (8). It is unclear how convergence is affected when initiated far from a stationary point where the linear approximation is not reasonably valid. It is our understanding that this approach may fail or converge slowly in such cases, since penalizing M_k discourages large steps even when the current estimate is far from stationarity.

It can be argued that a chief advantage of these prior methods is their computational simplicity. In particular, they are quite scalable to high-dimensional problems as their space complexity only grows linearly in the number of variables. While bringing us closer to established optimization theory, our method produces Jacobians that may become computationally unwieldy as the number of variables grows. To ameliorate this, we next propose a low-memory variant based on the ideas in limited-memory BFGS.

3.1. A limited memory variant for high-dimensional settings

Examining Eq.(11) reveals that our algorithm requires the $p \times p$ matrix H_k to perform a rank-two update at each step, which can be computationally prohibitive in high dimensions. Additionally, storing the full $p \times p$ matrix at each step can be very challenging. Fortunately, many limited memory variants of quasi-Newton algorithms have been proposed (Shanno, 1978; Nocedal, 1980; Griewank and Toint, 1982), and rooting our method in Broyden's framework allows us to immediately import these ideas.

We will construct the limited memory version of our algorithm denoted by L-BQN by analogy to the way BFGS algorithm is made scalable using L-BFGS (Liu and Nocedal, 1989). BFGS (Fletcher, 2013) is a quasi-Newton optimization method that stores an approximation of the inverse Hessian matrix of the objective function at each iteration. For computationally challenging high-dimensional cases, L-BFGS surpasses this problem by instead storing only a few vectors that represent the inverse Hessian approximation implicitly. Likewise, we will also store a pre-defined m number of vectors that will approximate the inverse Jacobian at each step. Recall that our update is given by $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - H_k G(\boldsymbol{x}_k)$, where H_k is updated by the formula

$$H_{k+1} \quad = \quad H_k \left(I_p - \frac{\boldsymbol{v}_k \boldsymbol{v}_k^T}{\boldsymbol{v}_k^T \boldsymbol{v}_k} \right) + \frac{\boldsymbol{u}_k \boldsymbol{v}_k^T}{\boldsymbol{v}_k^T \boldsymbol{v}_k} \quad = \quad H_k W_k + \frac{\boldsymbol{u}_k \boldsymbol{v}_k^T}{\boldsymbol{v}_k^T \boldsymbol{v}_k},$$

where $W_k = \left(I - \boldsymbol{v}_k \boldsymbol{v}_k^T / \boldsymbol{v}_k^T \boldsymbol{v}_k \right)$. Akin to the L-BFGS method, we may store m previous pairs of $\{\boldsymbol{u}_i, \boldsymbol{v}_i\}$, $i = k-1, \ldots, k-m$, where m typically is chosen between 3 and 20. The matrix product required at each step $H_k G(\boldsymbol{x}_k)$ can be obtained by performing a sequence of inner products and vector summations involving only $G(\boldsymbol{x}_k)$ and the pairs $\{\boldsymbol{u}_i, \boldsymbol{v}_i\}$, $i = k, \ldots, k-m$. After the new iterate is computed, the oldest pair $\{\boldsymbol{u}_{(k-m)}, \boldsymbol{v}_{(k-m)}\}$ is dropped and replaced by the pair $\{\boldsymbol{u}_{k+1}, \boldsymbol{v}_{k+1}\}$ obtained from the current step.

A limited memory variant proceeds by recursion at each iteration. At the k^{th} step, an initial estimate of the inverse Jacobian is taken to be a scalar multiple of identity matrix $H_k^0 = \nu_k I_p$. The scale factor ν_k attempts to capture the size of the true inverse Jacobian matrix along the most recent search direction. Next, H_k^0 is updated $(m+1)$ times via Eq.(11) in a nested manner to obtain the relation

$$\begin{aligned} H_k &= H_k^0(W_{k-m} \ldots W_k) + \frac{\boldsymbol{u}_{k-m}\boldsymbol{v}_{k-m}^T}{\boldsymbol{v}_{k-m}^T\boldsymbol{v}_{k-m}}(W_{k-m+1} \ldots W_k) \\ &+ \frac{\boldsymbol{u}_{k-m+1}\boldsymbol{v}_{k-m+1}^T}{\boldsymbol{v}_{k-m+1}^T\boldsymbol{v}_{k-m+1}}(W_{k-m+2} \ldots W_k) + \ \ldots + \ \frac{\boldsymbol{u}_k\boldsymbol{v}_k^T}{\boldsymbol{v}_k^T\boldsymbol{v}_k}\,. \end{aligned}$$

Details on obtaining the nested formula above can be found in Chapter 6 of Nocedal and Wright (2006). There the authors suggest that an effective choice for the scaling factor is given by $\nu_k = \boldsymbol{u}_k^T\boldsymbol{v}_k/\boldsymbol{v}_k^T\boldsymbol{v}_k$. Through this choice, our L-BQN algorithm can be understood as a generalization of the STEM method (Varadhan and Roland, 2008): STEM corresponds to the special case where $m = 0$. However, the approximate inverse Jacobian $\nu_k I_p$ for STEM is derived by minimizing the distance between the zeros of two linear secant-like approximations for $G(\boldsymbol{x})$— one centered around $\boldsymbol{x}_k$, and another at $F(\boldsymbol{x}_k)$. While the approaches that lead to this approximation are quite different, it accords more confidence in L-BQN as for non-zero m, the inverse Jacobian approximation is made *more* robust by leveraging curvature information from the last m iterates.

3.2. Convergence

We now analyze the convergence properties of the proposed method. The two essential components are 1) convergence of the base MM algorithm to the stationary point $\boldsymbol{x}^*$, and 2) convergence of Broyden's root finding quasi-Newton method to the stationary point $\boldsymbol{x}^*$ of the map G. Our study bridges careful analyses of these two facets.

Naturally, establishing convergence guarantees for our proposed acceleration scheme rests on the convergence of the underlying MM map, which typically exhibits a locally linear rate of convergence (Lange, 2016). We will assume the base algorithm to be locally convergent in a neighborhood S of $\boldsymbol{x}^*$ with rate of convergence denoted by $\tau > 0$. In this section, we prove that BQN is also locally convergent to $\boldsymbol{x}^*$ in a subset of this neighborhood, and further identify conditions that establish its convergence rate. Recall $\{\boldsymbol{x}_k\}$ converges to $\boldsymbol{x}^*$ at a *linear* rate if, for some chosen vector norm $\|\cdot\|$,

$$\frac{\|\boldsymbol{x}_{k+1}-\boldsymbol{x}^*\|}{\|\boldsymbol{x}_k-\boldsymbol{x}^*\|} \leq r$$

for some rate of convergence $r \in (0,1)$. The convergence rate is *superlinear* if

$$\frac{\|\boldsymbol{x}_{k+1}-\boldsymbol{x}^*\|}{\|\boldsymbol{x}_k-\boldsymbol{x}^*\|} \to 0 \qquad \text{as } k \to \infty\,.$$

A seminal work of Broyden et al. (1973) derives local linear and Q-superlinear convergence results for several single and double rank quasi-Newton root finding methods. Our approach stands close to Broyden's second method, while the improved secant approximation through MM extrapolation will be incorporated into the analysis. We assume that G is differentiable in a neighborhood of $\boldsymbol{x}^*$, in that the Jacobian matrix $dG(\boldsymbol{x}^*)$ exists and is non-singular. At many instances, we will treat $(\boldsymbol{x}, dG(\boldsymbol{x})^{-1})$ as a tuple whose individual components are updated via Eq.(2) and (11). It is crucial to prove that the update function in Eq.(2) is well defined in some neighborhood of the limit point $(\boldsymbol{x}^*, dG(\boldsymbol{x}^*)^{-1})$. To this end, we first prove by induction local convergence of our algorithm under certain conditions. We then carefully construct a neighborhood of $(\boldsymbol{x}^*, dG(\boldsymbol{x}^*)^{-1})$ to satisfy these conditions explicitly.

To ease notation, our current iterate is denoted by $(\boldsymbol{x}, H)$ in a neighborhood of $(\boldsymbol{x}^*, dG(\boldsymbol{x}^*)^{-1})$. We use $\bar{\boldsymbol{x}}$ to denote the update on $\boldsymbol{x}$ given by Eq.(2), $\bar{H}$ to denote the update on H from Eq.(11), and introduce further notations:

$$\boldsymbol{s} = \bar{\boldsymbol{x}} - \boldsymbol{x}, \quad \boldsymbol{y} = G(\bar{\boldsymbol{x}}) - G(\boldsymbol{x}), \quad \boldsymbol{u} = F(\boldsymbol{x}) - \boldsymbol{x}, \quad \text{and} \quad \boldsymbol{v} = G(F(\boldsymbol{x})) - G(\boldsymbol{x}).$$

In the subsequent discussion, suppose $\|\cdot\|$ denotes a chosen vector norm on $\mathbb{R}^p$, then for a $p \times p$ matrix A, $\|A\|$ denotes the corresponding induced operator norm. The lemma below supplies useful inequalities to be applied in proving the main theorem.

Lemma 1. *Assume $G : \mathbb{R}^p \to \mathbb{R}^p$ is differentiable in the open convex set D, and suppose that for some $\widehat{\boldsymbol{x}}$ in D and $d > 0$,*

$$\|dG(\boldsymbol{x}) - dG(\widehat{\boldsymbol{x}})\| \leq K\|\boldsymbol{x} - \widehat{\boldsymbol{x}}\|^d\,, \tag{12}$$

where $K \in \mathbb{R}$ is a constant. Assuming $dG(\widehat{\boldsymbol{x}})$ is invertible, we have for each $\boldsymbol{y}, \boldsymbol{z}$ in D,

$$\begin{aligned} \|G(\boldsymbol{y}) - G(\boldsymbol{z}) - dG(\widehat{\boldsymbol{x}})(\boldsymbol{y}-\boldsymbol{z})\| &\leq K \max\{\|\boldsymbol{y}-\widehat{\boldsymbol{x}}\|^d, \|\boldsymbol{z}-\widehat{\boldsymbol{x}}\|^d\}\|\boldsymbol{y}-\boldsymbol{z}\| \\ \|dG(\widehat{\boldsymbol{x}})^{-1}(G(\boldsymbol{y}) - G(\boldsymbol{z})) - (\boldsymbol{y}-\boldsymbol{z})\| &\leq K\|dG(\widehat{\boldsymbol{x}})^{-1}\| \max\{\|\boldsymbol{y}-\widehat{\boldsymbol{x}}\|^d, \|\boldsymbol{z}-\widehat{\boldsymbol{x}}\|^d\}\|\boldsymbol{y}-\boldsymbol{z}\| \,. \end{aligned} \tag{13}$$

Moreover, there exists $\epsilon > 0$ and $\rho > 0$ such that

$$\max\{\|\boldsymbol{y}-\widehat{\boldsymbol{x}}\|^d, \|\boldsymbol{z}-\widehat{\boldsymbol{x}}\|^d\} < \epsilon$$

implies that $\boldsymbol{y}$ and $\boldsymbol{z}$ belong to D, and

$$(1/\rho)\|\boldsymbol{y}-\boldsymbol{z}\| \leq \|G(\boldsymbol{y}) - G(\boldsymbol{z})\| \leq \rho\|\boldsymbol{y}-\boldsymbol{z}\| \,. \tag{14}$$

Inequalities (13) follow from standard arguments using Taylor's expansion (Ortega and Rheinboldt, 2000), while inequality (14) is an immediate consequence of continuity and non-singularity of dG at $\widehat{\boldsymbol{x}}$. In the subsequent analysis, we will use a matrix norm $\|\cdot\|_M$, not related to the vector norm $\|\cdot\|$ described earlier. Here, $\|A\|_M := \|MAM\|_F$ where M is a matrix and $\|\cdot\|_F$ is the Frobenius norm. However, there is a constant $\eta > 0$ such that $\|A\| \leq \eta\|A\|_M$ by the equivalence of norms in finite-dimensional vector spaces.

We now derive general sufficient conditions for local convergence in the spirit of a classic result by Broyden et al. (1973). Since we require the inverse of dG, we posit the following conditions before proving convergence, with S and D as defined earlier.

Assumption 1. *(A1) Let the function $G : \mathbb{R}^p \to \mathbb{R}^p$ be differentiable in the open convex set D containing $\boldsymbol{x}^*$ such that $G(\boldsymbol{x}^*) = 0$ and $dG(\boldsymbol{x}^*)$ is non-singular. Assume that for some $d > 0$, G satisfies Inequality (12) inside D.*

Assumption 2. *(A2) Let the update function in Eq.(2) be well-defined in a neighborhood $N1$ of $\boldsymbol{x}^*$ where $N_1 \subset D \cap S$, and inverse Jacobian update from Eq.(11) be well-defined in a neighborhood N_2 of $dG(\boldsymbol{x}^*)^{-1}$ containing non-singular matrices. Assume that there are non-negative constants α_1 and α_2 such that for each tuple $(\boldsymbol{x}, H)$ in $N1 \times N2$, the following is satisfied,*

$$\begin{aligned} \|\bar{H} - dG(\boldsymbol{x}^*)^{-1}\|_M \leq &\left[1 + \alpha_1 \max\left\{\|F(\boldsymbol{x}) - \boldsymbol{x}^*\|^d, \|\boldsymbol{x}-\boldsymbol{x}^*\|^d\right\}\right] \|H - dG(\boldsymbol{x}^*)^{-1}\|_M \\ &+ \alpha_2 \max\left\{\|F(\boldsymbol{x}) - \boldsymbol{x}^*\|^d, \|\boldsymbol{x}-\boldsymbol{x}^*\|^d\right\} \,. \end{aligned} \tag{15}$$

The first assumption warrants the application of Lemma 1 on G, and the second assumption lends a key error bound on the inverse Jacobian estimation. The notion of well-defined used in Assumption 2 will be qualified for BQN later in Theorem 2.

THEOREM 1. *Let A1 hold true for the function G and A2 be satisfied for some neighborhoods N_1 and N_2 and non-negative constants α_1 and α_2. Then for each $r \in (0,1)$ there exist positive constants $\epsilon(r)$ and $\delta(r)$ such that the sequence with $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - H_k G(\boldsymbol{x}_k)$ is well-defined and converges to $\boldsymbol{x}^*$ whenever $\|\boldsymbol{x}_0 - \boldsymbol{x}^*\| < \epsilon(r)$ and $\|H_0 - dG(\boldsymbol{x}^*)^{-1}\|_M < \delta(r)$. Furthermore,*

$$\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\| \leq r\|\boldsymbol{x}_k - \boldsymbol{x}^*\| \qquad \textit{for each } k \geq 0,$$

and the sequences $\{\|H_k\|\}$ and $\{\|H_k^{-1}\|\}$ are uniformly bounded.

A detailed proof appears is in the Appendix. Under Theorem 1, we inherit the following property by an identical argument of Broyden et al. (1973), with proof omitted here.

COROLLARY 1. *Assume that the conditions of Theorem 1 hold. If some subsequence of $\{\|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M\}$ converges to zero, then $\{\boldsymbol{x}_k\}$ converges Q-superlinearly to $\boldsymbol{x}^*$.*

It remains to show that our acceleration algorithm satisfies the assumptions of Theorem 1 and Corollary 1. The following result and subsequent corollary identify concrete conditions on the update functions F and G that ensure this.

THEOREM 2. *Let A1 hold true for the function G. If*

$$\frac{\|M\boldsymbol{v} - M^{-1}\boldsymbol{v}\|}{\|M^{-1}\boldsymbol{v}\|} \leq \mu_2\|\boldsymbol{v}\|^p, \qquad \boldsymbol{v} \neq 0\,, \tag{16}$$

for a constant $\mu_2 \geq 0$, non-singular and symmetric matrix $M \in \mathbb{R}^{p\times p}$, and all $(\boldsymbol{x}, H)$ in a neighborhood N' of $(\boldsymbol{x}^*, dG(\boldsymbol{x}^*)^{-1})$, then the update functions (11) *is well-defined in a neighborhood N of $(\boldsymbol{x}^*, dG(\boldsymbol{x}^*)^{-1})$ and the corresponding iteration*

$$\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - H_k G(\boldsymbol{x}_k)$$

is locally convergent to the limit point $\boldsymbol{x}^*$.

We emphasize that this result does not require stronger conditions than those imposed in the classical results pertaining to Broyden acceleration, which have endured as reasonable mild assumptions in the optimization literature.

COROLLARY 2. *If further* $\lim_{k\to\infty} \|\boldsymbol{x}_{k+1} - F(\boldsymbol{x}_k)\|/\|\boldsymbol{x}_k - \boldsymbol{x}^*\| = 0$ *holds, then the convergence rate of* $\{\boldsymbol{x}_k\}$ *to* $\boldsymbol{x}^*$ *is Q-superlinear.*

The complete technical proofs of these results are detailed in the Appendix.

4. Results and Empirical Performance

We now turn to a performance assessment on a variety of real and simulated data examples, including (a) quadratic minimization using Landweber's method, (b) maximum likelihood estimation in a truncated beta-binomial model, (c) the largest (and smallest) eigenvalue problem for symmetric matrices, and (d) location-scale estimation of a multivariate t-distribution. These problems were selected as examples in the prior studies that introduced the competing methods we benchmark against, thus offering a conservative comparison. As peer methods, we consider (1) unaccelerated MM, (2) the ZAL accelerator, (3) the three variants of SQUAREM, and (4) our proposed BQN method as well as (5) its limited memory variant L-BQN.

All methods are implemented using `R`; we use the implementation of ZAL and SQUAREM in the `R` package `turboEM`. Throughout our examples, we use the first-order ($K = 1$) scheme for SQUAREM as proposed by Varadhan and Roland (2008) as the standard of comparison, since the $K = 2$ and $K = 3$ schemes are deemed less reliable by the original authors. The implementation of the proposed accelerators, BQN and L-BQN, and all data examples are implemented as an `R` package `quasiNewtonMM` †. We consider $q = 1$ and $q = 2$ secant conditions for the proposed method as well ZAL.

Stopping criteria are matched across all methods, declaring convergence at $\boldsymbol{x}^*$ when $\|F(\boldsymbol{x}^*) - \boldsymbol{x}^*\| \leq \epsilon$ for a specified tolerance ϵ. For ZAL and BQN, we revert to the original MM step whenever updates violate monotonicity, following Zhou et al. (2011). In most cases, we observe that BQN performs strikingly well and at least on par with its

†`https://github.com/medhaaga/quasiNewtonMM`

Table 1. Quadratic minimization of $f(\theta) = \theta^T A\theta/2 + b^T\theta$ for 100 random starting points.

Algorithm	F evals	Time (in sec)	Objective
MM	194872.5 (179472.5, 207076.8)	4.218 (3.870, 4.470)	-24.0591 (-24.0591, -24.0591)
BQN, $q = 1$	5724.0 (4719.5, 6510.0)	0.400 (0.330, 0.450)	-24.0602 (-24.0612, -24.0596)
BQN, $q = 2$	2953.0 (2616.5, 3501.0)	0.226 (0.196, 0.274)	-24.0604 (-24.0614, -24.0599)
L-BQN	12856.0 (11260.0, 13772.5)	0.631 (0.562, 0.698)	-24.0592 (-24.0598, -24.0591)
SqS1	2150.0 (1926.5, 2412.0)	0.140 (0.127, 0.156)	-24.1067 (-24.1081, -24.1052)
SqS2	12665.0 (11515.5, 13855.0)	0.833 (0.745, 0.909)	-24.0974 (-24.0983, -24.0968)
SqS3	5911.0 (5092.0, 6374.5)	0.410 (0.348, 0.445)	-24.1062 (-24.1064, -24.1060)
ZAL	23015.50 (21638.25, 24150.75)	1.655 (1.544, 1.741)	-24.1081 (-24.1081, -24.1080)

competitors. An overall theme is that existing methods may outpace our approach on some examples but then falter on a case-by-case basis, while BQN succeeds consistently.

4.1. Landweber's method for quadratic minimization

We begin with the "well-behaved" problem of minimizing a quadratic function $f : \mathbb{R}^p \to \mathbb{R}$ using an MM iterative scheme. For $\theta \in \mathbb{R}^p$, consider a quadratic objective function

$$f(\theta) = \frac{1}{2}\theta^T A\theta + b^T\theta\,,$$

where A is a $p \times p$ positive definite matrix and $b \in \mathbb{R}^p$. The exact solution is available by solving the linear equation $A\theta = -b$, but incurs a complexity of $\mathcal{O}(p^3)$. To avoid this computational cost, Landweber's method instead effects an iterative scheme, making use of the Lipschitz property of gradient of $f(\theta)$. The method can be viewed from the lens of majorization-minimization (Lange, 2016): since $\nabla f(\theta) = A\theta + b$, we can write the gradient inequality

$$\|\nabla f(\theta) - \nabla f(\Phi)\| = \|A(\theta - \Phi)\| \leq \|A\|\|\theta - \Phi\|.$$

As a consequence, the spectral norm of A is the Lipschitz constant for $\nabla f(\theta)$. Let the constant $L > \|A\|$. Landweber's method gives the following majorization for $f(\theta)$:

$$f(\theta) \leq f(\Phi) + \nabla f(\Phi)^T(\theta - \Phi) + \frac{L}{2}\|\theta - \Phi\|^2.$$

Minimizing the above surrogate function then yields the MM update formula

$$\theta_{n+1} = \theta_n - \frac{1}{L}\nabla f(\theta_n) = \theta_n - \frac{1}{L}(A\theta_n + b).$$

Consider the problem dimension to be $p = 100$ and tolerance to be $\epsilon = 10^{-5}$. We use a randomly generated A and b such that at true minima, the value of objective function is -24.10846. Due to the simple structure of the optimization problem, we might expect all algorithms to perform reasonably well, while we already see the unaccelerated MM algorithm converges very slowly. Table 1 reports performance in terms of the median and (interquartile range), comparing the number of F function evaluations (F evals), wall-clock time, and objective values at convergence over 100 random initializations centered at the true mean, perturbing each component by normal noise with variance 1000. Figure 2 displays runtime and function evaluations as boxplots for BQN with $q = 1$ (B1), BQN with $q = 2$ (B2), L-BQN (L-B), SQUAREM-3, and ZAL. Initial values are matched across methods for each trial. Given the strongly convex objective, all methods successfully deliver the minimum here.

Our proposed BQN method with $q = 1$ performs on par with the default SQUAREM-3, while using $q = 2$ secant conditions provides further improvement. However, we notice that SQUAREM-1 outpaces our method in this case. This may be unsurprising as this "easy" problem is favorable to methods that do not need to fully utilize curvature information, but are simple and fast. It is also worth noting that the variations of SQUAREM already perform quite differently from one another, suggesting significant sensitivity to the choice of step-length. As mentioned earlier, the performance of ZAL tends to depend on the starting point, and we observe it tends to converge more slowly in this case when initialized with large perturbations of the true value.

4.2. Truncated Beta Binomial

We next consider a more difficult statistical optimization problem, turning to the cold incidence dataset by Lidwell and Sommerville (1951). These data have been modeled as a zero-truncated beta binomial model as the reported households have at least one cold incidence. The data includes four different household types. We analyze the subset of data corresponding to all adult households here; further details on the data and results

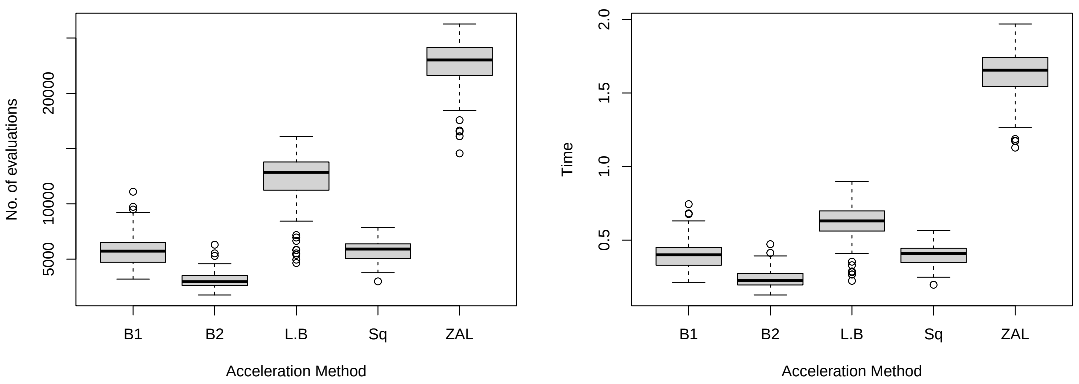


Fig. 2. Quadratic minimization: number of function evaluations and runtime over 100 random starting points.

for other subsets of the data appear in Table 6 in the Appendix. Among adults, the number of households with $1, 2, 3,$ and 4 cases are $15, 5, 2,$ and 2 respectively.

Suppose n is the total number of independent observations (households) and x_i denotes the number of cold cases in the i^{th} household. This can be modeled as a discrete probability model (Zhou et al., 2011) with likelihood given by

$$L(\theta|X) = \prod_{i=1}^{n} \frac{d(x_i|\theta)}{1 - d(0|\theta)} .$$

Here $d(x|\theta)$ is the probability density function for a beta binomial distribution with parameter vector θ and maximum count of $m = 4$. Here $\theta = (\alpha, \pi)$ such that $\pi \in (0, 1)$ and $\alpha > 0$. We use MM algorithm to numerically maximize the likelihood function. The MM updates are given by

$$\alpha_{t+1} = \frac{\sum_{j=0}^{m-1} (\dfrac{s_{1j} j \alpha_t}{\pi_t + j\alpha_t} + \dfrac{s_{2j} j \alpha_t}{1 - \pi_t + j\alpha_t})}{\sum_{j=0}^{m-1} \dfrac{r_j j}{1 + j\alpha_t}}$$

$$\pi_{t+1} = \frac{\sum_{j=0}^{m-1} \dfrac{s_{1j} \pi_t}{\pi_t + j\alpha_t}}{\sum_{j=0}^{m-1} (\dfrac{s_{1j\pi_t}}{\pi_t + j\alpha_t} + \dfrac{s_{2j}(1 - \pi_t)}{1 - \pi_t + j\alpha_t})}$$

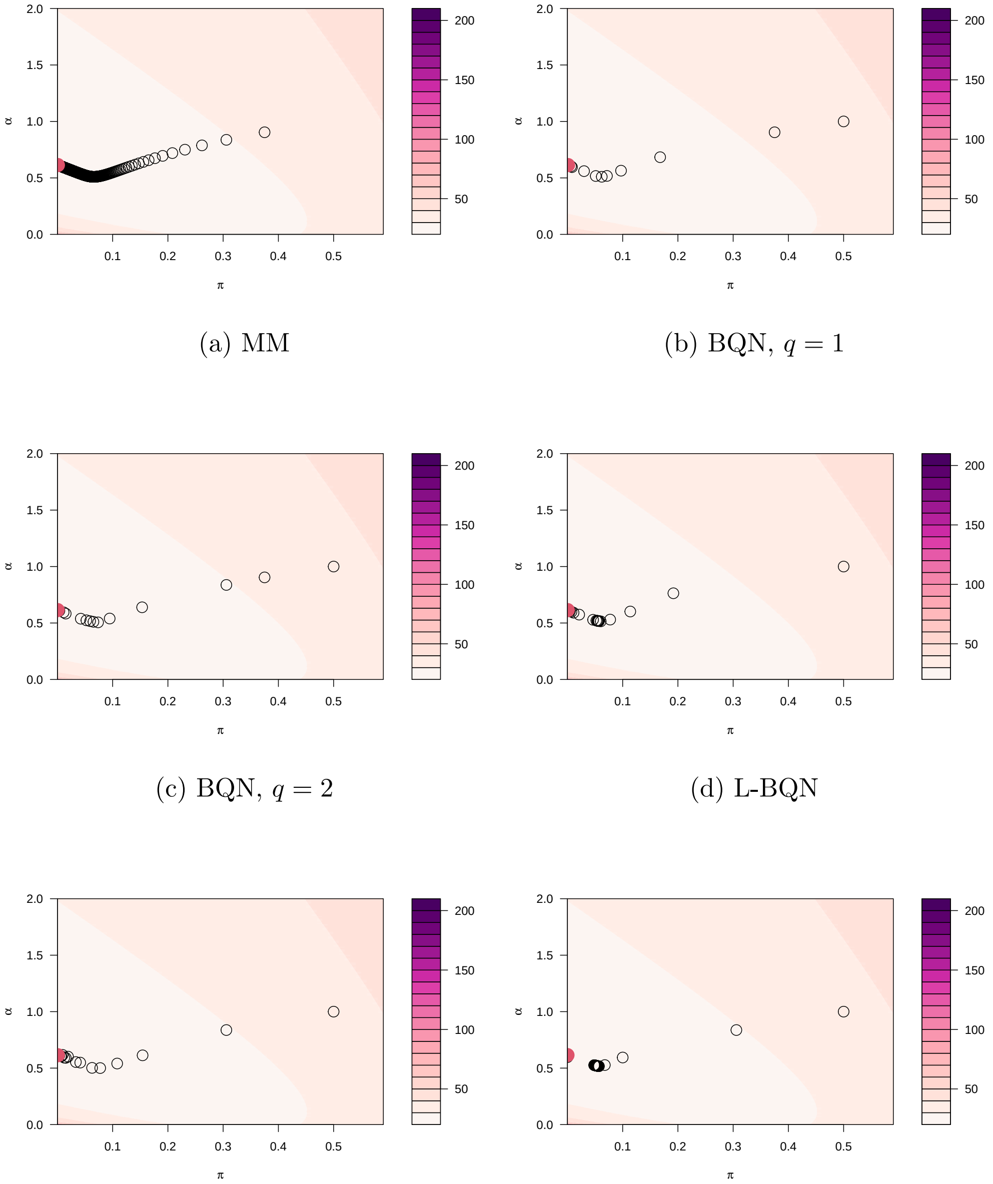
Table 2. Truncated beta binomial: performance on Lidwell and Somerville data, from initial point $(\pi, \alpha) = (0.5, 1)$.

Algorithm	-ln L	F Evals	Iterations	Time (in sec)
MM	25.2283	17898	17898	0.114
BQN ($q = 1$)	25.2287	26	14	0.001
BQN ($q = 2$)	25.2277	29	16	0.001
L-BQN	25.2288	73	37	0.002
SqS1	25.2274	1797	1769	0.160
SqS2	25.2277	36	19	0.004
SqS3	25.2269	69	35	0.005
ZAL	25.2269	28	24	0.003

where s_{1j}, s_{2j}, r_j can be interpreted as pseudocounts, given by

$$\begin{aligned} s_{1j} &= \sum_{i=1}^{n} 1_{x_i \geq j+1} \\ s_{2j} &= \sum_{i=1}^{n} \left[1_{x_i \leq m-j-1} + \frac{g(0|\pi_t, \alpha_t)}{1 - g(0|\pi_t, \alpha_t)} \right] \\ r_j &= \sum_{i=1}^{n} \left[1 + \frac{g(0|\pi_t, \alpha_t)}{1 - g(0|\pi_t, \alpha_t)} \right] 1_{t \geq j+1} . \end{aligned}$$

Following Zhou et al. (2011), each algorithm is initializated at $(\pi, \alpha) = (0.5, 1)$. Table 2 lists the negative log-likelihood values, number of MM evaluations (F evals), number of algorithm iterations, and runtime until convergence for each algorithm. Figure 3 provides a closer look, showing the progress path of each algorithm on a contour plot of the objective. SQUAREM methods, though achieving significant acceleration, tend to exhibit slow tail behavior near the optimal value. In particular, SQUAREM-1 leads to orders of magnitude slower convergence than the others, while it outpaced other choices of steplength among variants of SQUAREM in the simple example; we again focus on visualizing the progress of the default SQUAREM-3. In all cases, our method converges in fewer iterations and requires fewer function evaluations than its competitors despite a naive implementation. From Figure 3, we can visualize the advantage of our extrapolation-based steps making steady progress, in contrast to the more congested



(a) MM

(b) BQN, $q = 1$

(c) BQN, $q = 2$

(d) L-BQN

(e) SQUAREM-3

(f) ZAL, $q = 1$

Fig. 3. Truncated beta binomial: ascent paths of peer methods on the Lidwell and Somerville household incidence data in a truncated beta binomial model, with optimum marked in red.

updates near the optimum under existing methods. While the small problem dimension does not call for a limited-memory method, we see L-BQN also compares favorably despite its streamlined updates.

4.3. Generalized eigenvalues

In this example, we consider a more complicated objective function that exhibits a zig-zag descent path under the naïve MM algorithm, rendering progress excruciatingly slow. For two $p \times p$ matrices A and B, the generalized eigenvalue problem refers to finding a scalar λ and a nontrivial vector x such that $Ax = \lambda Bx$. We consider the case where A is symmetric and B is symmetric and positive definite, so that the generalized eigenvalues and eigenvectors are real (Zhou et al., 2011). A simple alternative for finding the generalized eigenvalues iteratively is by optimizing the Rayleigh quotient

$$R(x) = \frac{x^T Ax}{x^T Bx} \qquad\qquad x \neq 0\,.$$

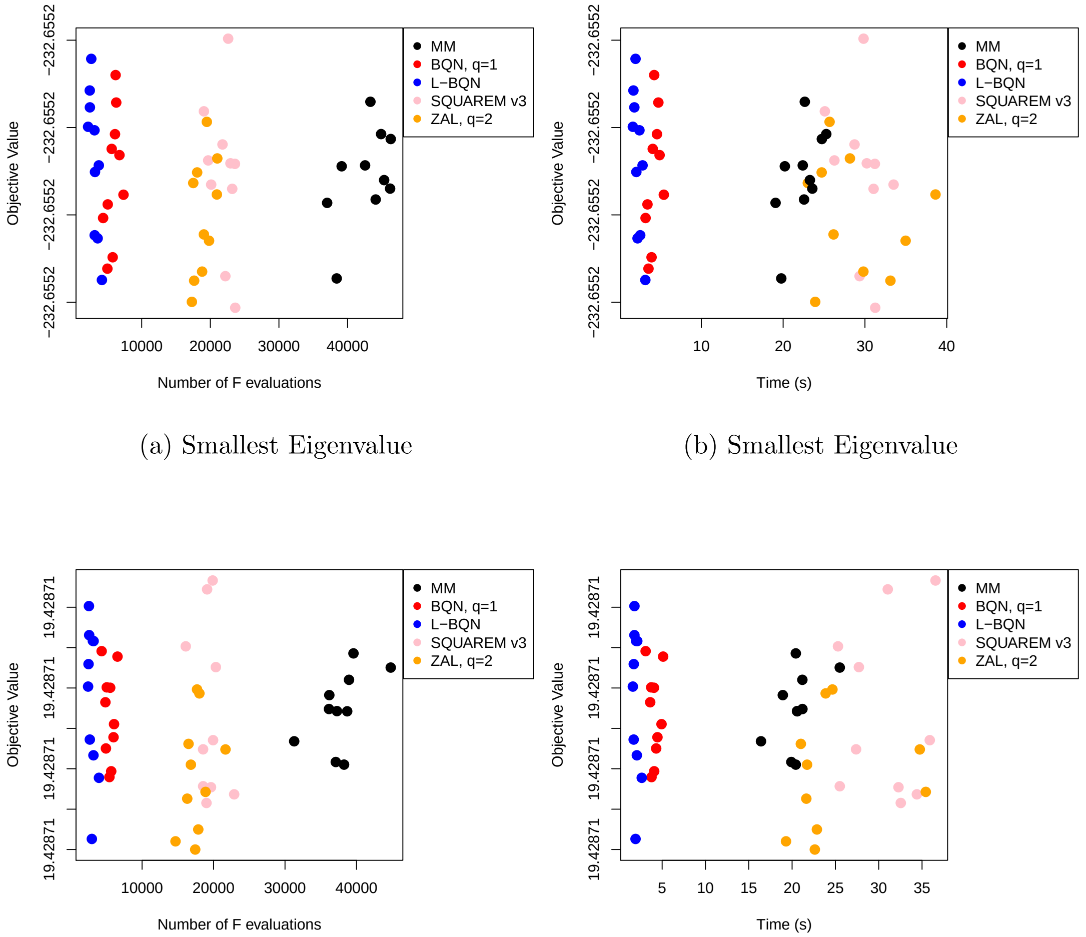
The gradient of $R(x)$ is given by

$$\nabla R(x) = \frac{2}{x^T Bx}[Ax - R(x)Bx]\,.$$

Therefore, a solution of $\nabla R(x) = 0$ corresponds to a generalized eigenpair, wherein the maximum of $R(x)$ gives the maximum generalized eigenvalue and minimum gives the minimum generalized eigenvalue. To optimize $R(x)$, we consider the line search method for steepest ascent proposed by Hestenes and Karush (1951) as the base algorithm.

Due to the zigzag nature of steepest ascent on this problem, Zhou et al. (2011) found naïve acceleration to perform poorly. Utilizing this side information, they considered instead the s-fold functional composition of the base algorithm for s even as the underlying map, improving performance. We refrain from using the same heuristic in order to illustrate the off-the-shelf applicability of our method. We consider a simulation study with symmetric matrices A and B randomly generated with $p = 100$ dimensions, and run 10 random initializations of each method from matched initial points.

Figure 4 displays objective values at convergence, and Table 3 details the results. It can be seen that without the s-fold functional composition, both SQUAREM and ZAL fails to accelerate meaningfully here. On the other hand, the curvature information



(a) Smallest Eigenvalue

(b) Smallest Eigenvalue

(c) Largest Eigenvalue

(d) Largest Eigenvalue

Fig. 4. Generalized eigenvalues: objectives at convergence over 10 restarts vs the time and number of F evaluations.

Table 3. Generalized eigenvalues: number of $F(x)$ evaluations, runtime, and eigenvalues at convergence.

	Smallest Eigenvalue			Largest Eigenvalue		
Algorithm	Time (in sec)	F Evals	Eigenvalue	Time (in sec)	F Evals	Eigenvalue
MM	10.104	42552	-232.6552	8.539	38262	19.4287
BQN, $q = 1$	2.046	6682	-232.6552	1.854	5766	19.4287
L-BQN	1.203	4046	-232.6552	0.664	2399	19.4287
SqS1	11.850	21777	-232.6552	11.397	19642	19.4287
SqS2	12.391	21777	-232.6552	11.003	19642	19.4287
SqS3	12.525	21777	-232.6552	11.021	19642	19.4287
ZAL	9.979	17920	-232.6552	9.665	17415	19.4287

is crucial toward informing a good search direction in such cases, and our formulation successfully leverages this information. This information is largely ignored in the scalar based methods SQUAREM, while ZAL attempts to make use of curvature information under an assumption that it is close to the stationary point.

4.4. Multivariate t-distribution

Our last example turns to estimation under a multivariate t-distribution, a robust alternative to multivariate normal modeling when the errors involve heavy tails (Lange et al., 1989). Varadhan and Roland (2008) considered this example to compare SQUAREM to standard EM as well as PX-EM, an efficient data augmentation method (Meng and Van Dyk, 1997).

Suppose we have p-dimensional data $Y = (y_1, ..., y_N)$ that we wish to fit to a multivariate t-distribution with unknown degrees of freedom ν. The density is given by

$$f(y|\mu, \Sigma) \propto |\Sigma|^{-1/2} \left(\nu + (y - \mu)^T \Sigma^{-1} (y - \mu)\right)^{(\nu+p)/2},$$

and so the data likelihood is givein by $\prod_{i=1}^{N} f(y_i|\mu, \Sigma)$. There is no closed form solution to find (μ, Σ) which maximize the likelihood, but we can make progress by augmenting the missing data with latent variables. That is, we obtain the complete data $\{(y_i, q_i); i = 1, ..., N\}$ where q are IID from χ^2_ν/ν; the maximum likelihood estimator (MLE) now

Table 4. Multivariate t-distribution: maximum likelihood estimation of a 25-dimensional multivariate t-distribution.

Algorithm	F Evals	Time (in sec)	$-\ln L$
EM	744	1.086	8608.993
PX-EM	38	0.063	8608.993
BQN, $q=1$	112	0.215	8608.993
BQN, $q=2$	223	0.457	8608.993
L-BQN	89	0.114	8608.993
SqS1	64	0.156	8608.993
SqS2	65	0.148	8608.993
SqS3	63	0.155	8608.993
ZAL, $q=2$	383	1.383	8608.993

follows from weighted least squares. In an EM algorithm, the E-step finds the expected complete data log-likelihood conditional on parameters from the previous iteration k. Conditional on Y and (μ_k, Σ_k), the latent variables are distributed as $q_i \sim \chi^2_{\nu+p}/(\nu + d_i^{(k)})$, where $d_i^{(k)} = (y_i - \mu_k)^T \Sigma_k^{-1}(y_i - \mu_k); i = 1, ..., N$. As the complete-data log-likelihood is linear in q_i, the E-step amounts to defining

$$w_i = E[q_i | y_i, \mu_k, \Sigma_k] = (\nu + p)/(\nu + d_i^{(k)}); \qquad i = 1, ..., N\,.$$

The M-step then yields:

$$\mu_{k+1} = \sum_i w_i y_i \Big/ \sum_i w_i\,, \qquad \Sigma_{k+1} \;=\; \frac{1}{N} w_i (y_i - \mu)(y_i - \mu)^T\,.$$

The PX-EM method of Meng and Van Dyk (1997) differs only in the Σ update, replacing the denominator N by $\sum_i w_i$. We randomly generate synthetic data with $\nu = 1$ (a multivariate Cauchy distribution) and parameters $\mu = 0$, $\Sigma = V$, where V is a symmetric randomly generated matrix with dimension $p = 25$, which corresponds to 350 parameters (25 for μ and 325 for Σ). We report results obtained from following the initial values suggested by Meng and Van Dyk (1997):

$$\mu_0 = \frac{1}{N}\sum_{i=1}^{N} y_i, \qquad \Sigma_0 = \frac{1}{N}\sum_{i=1}^{N}(y_i - \overline{y})(y_i - \overline{y})^T\,.$$

Table 4 displays runtime, number of F evaluations (F evals), and negative log likelihood of all acceleration schemes at convergence. Our method achieves significant acceleration compared to the standard EM algorithm and performs on par with SQUAREM while outpacing ZAL. Here ZAL fails to provide meaningful acceleration under its implementation in `turboEM`—we observe it frequently proposes an update such that Σ_k is not positive-definite. In these cases, the algorithm reverts to the default MM update, adding additional computational effort, though the implementation in Zhou et al. (2011) achieves more success. Though performance is always quite dependent on implementations, we echo the overall theme in the findings of Varadhan and Roland (2008); Zhou et al. (2011) that model-specific augmentation under PX-EM performs remarkably well, outpacing all of the more general methods. This example illustrates that despite the robust performance of our proposed method across settings, it is worthwhile to exploit problem-specific structure as does PX-EM whenever possible.

5. Conclusion

This article presents a novel quasi-Newton acceleration of MM algorithms that extends recent ideas, but lends them new intuition as well as theoretical guarantees. The method retains gradient information across all components, which is often ignored in other *pure* MM accelerators. A key advantage of MM algorithms is their transfer of difficulty away from the original objective function, obtained by the construction of surrogates. While the *hybrid* quasi-Newton MM accelerators (Lange, 1995; Heiser, 1995; Lange et al., 2000) are rigorously analyzed in the literature, they lose this appeal in part by requiring information from the original objective through their iterates. Our approach seeks to embody the best of both worlds, retaining the simplicity of pure accelerators without restrictive assumptions, maintaining computational tractability so that it is amenable for large and high-dimensional problems, and taking advantage of richer curvature information that yields classical convergence guarantees which may not hold for its peer methods.

The limited-memory version of our method performs well on our representative, but not exhaustive, set of examples. As this shows promise toward high-dimensional problems, a fruitful line of research may seek to study the convergence properties of L-BQN explicitly, building on prior analyses on convergence of limited memory BFGS method (Liu and Nocedal, 1989). Exploring optimal step size selection presents another open direction (Nocedal and Wright, 2006). Despite deriving from a different perspective, it is satisfying that the steplength for our inverse Jacobian update in Eq.(11) reveals that used for the first version of STEM as a special case Varadhan and Roland (2008). Nonetheless, exploring the practical and theoretical merits of alternatives may reap further advantages.

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6. Appendix

6.1. Proof of Theorem 1

Let $\mathbb{R}^{p\times p}$ denote linear space of real matrices of order $p \times p$. Recall that $\|A\|_M := \|MAM\|_F$ is a matrix norm of matrix A for any matrix M, $\|\cdot\|_F$ is the Frobenius norm, and $\|\cdot\|$ denotes a vector norm or its induced operator norm.

Proof. The proof argues that if $\boldsymbol{x}_0 \in D$, then $\boldsymbol{x}_1$ also lies in D using the inequality in Eq.(15). Additionally, it is shown that the distance of $\boldsymbol{x}_1$ from $\boldsymbol{x}^*$ is less than or equal to some rth fraction of the distance of $\boldsymbol{x}_0$ from $\boldsymbol{x}^*$. By induction, we prove that $\boldsymbol{x}_i \in D$ for all $i \geq 1$, and eventually converge to $\boldsymbol{x}^*$ with r rate of convergence.

To this end, we upper bound the norm of the Jacobian and inverse Jacobian matrices at $\boldsymbol{x}^*$ as $\|dG(\boldsymbol{x}^*)\| \leq \sigma$ and $\|dG(\boldsymbol{x}^*)^{-1}\| \leq \gamma$. For any $r \in (0,1)$, we can choose $\epsilon(r) = \epsilon$ and $\delta(r) = \delta$ such that

$$[2\alpha_1\delta + \alpha_2]\frac{\epsilon^d}{1-r^d} \leq \delta \tag{17}$$

$$2\sigma\delta\eta + (\gamma + 2\eta\delta)K\epsilon^d \leq r\,. \tag{18}$$

If necessary, we may further restrict ϵ and δ such that $(\boldsymbol{x}, H) \in N$ whenever $\|\boldsymbol{x} - \boldsymbol{x}^*\| < \epsilon$ and $\|H - dG(\boldsymbol{x}^*)^{-1}\|_M < 2\delta$. Now suppose $\|\boldsymbol{x}_0 - \boldsymbol{x}^*\| < \epsilon$ and $\|H_0 - dG(\boldsymbol{x}^*)^{-1}\|_M < \delta$. Then $\|H_0 - dG(\boldsymbol{x}^*)^{-1}\| < \eta\delta < 2\eta\delta$ by the equivalence of norms in finite-dimensional vector spaces. From Eq.(18), $2\sigma\delta\eta \leq 2r$, and therefore the Banach lemma gives,

$$\|H_0^{-1}\| \leq \frac{\sigma}{1-r}\,.$$

Now, we will show that if $\boldsymbol{x}_0 \in D$, then $\boldsymbol{x}_1$ also lies in D. For this purpose, we add and subtract $H_0 dG(\boldsymbol{x}^*)(\boldsymbol{x}_0 - \boldsymbol{x}^*)$ and add the null term $H_0 G(\boldsymbol{x}^*)$ to the known update formulation for $\boldsymbol{x}_1$ giving

$$\begin{aligned}\boldsymbol{x}_1 - \boldsymbol{x}^* &= \boldsymbol{x}_0 - H_0 G(\boldsymbol{x}_0) - \boldsymbol{x}^* \\ &= -H_0\left[G(\boldsymbol{x}_0) - G(\boldsymbol{x}^*) - dG(\boldsymbol{x}^*)(\boldsymbol{x}_0 - \boldsymbol{x}^*)\right] + \left[I_p - H_0 dG(\boldsymbol{x}^*)\right](\boldsymbol{x}_0 - \boldsymbol{x}^*)\,.\end{aligned}$$

Using the fact that $\|I_p - H_0 dG(\boldsymbol{x}^*)\| = \|dG(\boldsymbol{x}^*)(H_0 - dG(\boldsymbol{x}^*)^{-1})\| \leq \|dG(\boldsymbol{x}^*)\|\|H_0 - dG(\boldsymbol{x}^*)^{-1}\| \leq \sigma(2\delta\eta)$ and Inequality (13),

$$\|\boldsymbol{x}_1 - \boldsymbol{x}^*\| \leq \|H_0\|K\epsilon^d\|\boldsymbol{x}_0 - \boldsymbol{x}^*\| + 2\sigma\delta\eta\|\boldsymbol{x}_0 - \boldsymbol{x}^*\| \quad = \Big[\|H_0\|K\epsilon^d + 2\sigma\epsilon\delta\eta\Big]\,\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|\,.$$

But $\|H_0\| \leq \|H_0 - dG(\boldsymbol{x}^*)^{-1}\| + \|dG(\boldsymbol{x}^*)^{-1}\| \leq 2\eta\delta + \gamma$. Therefore,

$$\|\boldsymbol{x}_1 - \boldsymbol{x}^*\| \leq [(2\eta\delta + \gamma)K\epsilon^d + 2\sigma\epsilon\delta\eta]\|\boldsymbol{x}_0 - \boldsymbol{x}^*\| \leq r\|\boldsymbol{x}_0 - \boldsymbol{x}^*\|$$

using the inequality in Eq.(18), and hence $\boldsymbol{x}_1 \in D$. The rest of the proof proceeds by induction. Assume that $\|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M < 2\delta$, which implies $H_k \in N_2$ and $\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\| \leq r\|\boldsymbol{x}_k - \boldsymbol{x}^*\|$ for $k = 0, 1, \ldots, m-1$. Now since $\boldsymbol{x}_k \in N_1 \subseteq S$, we have $\|F(\boldsymbol{x}_k) - \boldsymbol{x}^*\|^d \leq \tau^d\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^d$ by the local convergence of the MM algorithm in S. It follows from the inequality in Eq.(15) that

$$\begin{aligned}\|H_{k+1} - dG(\boldsymbol{x}^*)^{-1}\|_M - \|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M &\leq \alpha_1\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^d\|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M + \alpha_2\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^d \\ &\leq \alpha_1(r^{kd}\epsilon^d)(2\delta) + \alpha_2 r^{kd}\epsilon^d\,.\end{aligned}$$

Therefore, from the inequality in Eq.(17), we have

$$\|H_m - dG(\boldsymbol{x}^*)^{-1}\|_M \leq \|H_0 - dG(\boldsymbol{x}^*)^{-1}\|_M + (2\alpha_1\delta + \alpha_2)\frac{\epsilon^d}{1-r^d} \leq 2\delta\,.$$

In this way, the induction step is completed by following the same proof as the case for $m = 1$. In particular, since $\|H_m - dG(\boldsymbol{x}^*)^{-1}\| \leq 2\eta\delta$, the Banach lemma implies that

$$\|H_m^{-1}\| \leq \frac{\sigma}{1-r}\,.$$

6.2. *Proof of Theorem 2*

In order to show that our algorithm satisfies (15) for meeting the conditions of Theorem 1, we write (11) as

$$\bar{E} = E\left[I_p - \frac{M^{-1}\boldsymbol{v}(M\boldsymbol{v})^T}{\|\boldsymbol{v}\|^2}\right] + \frac{M(\boldsymbol{u} - dG(\boldsymbol{x}^*)^{-1}v)(M\boldsymbol{v})^T}{\|\boldsymbol{v}\|^2}, \tag{19}$$

where $\bar{E} = M(\bar{H} - dG(\boldsymbol{x}^*)^{-1})M$ and $E = M(H - dG(\boldsymbol{x}^*)^{-1})M$. Eq.(19) will allow us to derive the relationship between $\|H - dG(\boldsymbol{x}^*)^{-1}\|_M$ and $\|\bar{H} - dG(\boldsymbol{x}^*)^{-1}\|_M$ satisfying the inequality in (15). For this purpose, we present the following technical lemma with four important inequalities satisfied by our algorithm. Since our update formulation falls in the classical line of thought, we inherit the following properties directly from the analysis presented by Broyden et al. (1973), so the proofs have been omitted. Nonetheless, the results have been included for the sake of completion for Theorem 2.

LEMMA 2. *Let $M \in \mathbb{R}^{p\times p}$ be a non-singular symmetric matrix such that*

$$\|M\boldsymbol{c} - M^{-1}\boldsymbol{d}\| \leq \beta\|M^{-1}\boldsymbol{d}\| \tag{20}$$

for some $\beta \in [0, 1/3]$ and vectors $\boldsymbol{c}$ and $\boldsymbol{d}$ in $\mathbb{R}^p$ with $\boldsymbol{d} \neq \boldsymbol{0}$. Then using E and $\bar{E}$ as defined earlier,

(a) $(1-\beta)\|M^{-1}\boldsymbol{d}\|^2 \leq \boldsymbol{c}^T\boldsymbol{d} \leq (1+\beta)\|M^{-1}\boldsymbol{d}\|^2\,.$

(b) $E\left[I - \dfrac{(M^{-1}\boldsymbol{d}(M^{-1}\boldsymbol{d})^T}{\boldsymbol{c}^T\boldsymbol{d}}\right] \leq \sqrt{1-\alpha\theta^2}\|E\|_F\,.$

(c) $\left\|E\left[I - \dfrac{M^{-1}\boldsymbol{d}(M\boldsymbol{c})^T}{\boldsymbol{c}^T\boldsymbol{d}}\right]\right\|_F \leq \left[\sqrt{1-\alpha\theta^2} + (1-\beta)^{-1}\dfrac{\|M\boldsymbol{c} - M^{-1}\boldsymbol{d}\|}{\|M^{-1}\boldsymbol{d}\|}\right]\|E\|_F\,,$
where

$$\alpha = \frac{1-2\beta}{1-\beta^2} \in [3/8, 1]$$

and

$$\theta = \frac{\|EM^{-1}\boldsymbol{d}\|}{\|E\|_F\|M^{-1}\boldsymbol{d}\|} \in [0,1]\,.$$

Moreover, for any $\boldsymbol{a} \in \mathbb{R}^p$,

$$\text{(d)} \quad \left\| \frac{(\boldsymbol{a} - dG(\boldsymbol{x}^*)^{-1}\boldsymbol{d})(M\boldsymbol{c})^T}{\boldsymbol{c}^T\boldsymbol{d}} \right\|_F \leq 2\frac{\|\boldsymbol{a} - dG(\boldsymbol{x}^*)^{-1}\boldsymbol{d}\|}{\|M^{-1}\boldsymbol{d}\|}\,.$$

In the following proof, we will use results from the above lemma with $\boldsymbol{c} = \boldsymbol{v}$, $\boldsymbol{d} = \boldsymbol{v}$, and result (d) particularly for $\boldsymbol{a} = \boldsymbol{u}$. We are now ready to show that the conditions of Theorem 1 are satisfied by our update formula. This allows us to construct the exact neighborhood for each $r \in (0,1)$ wherein our algorithm converges to the stationary point with rate r.

Proof (Theorem 2). Firstly, we construct the neighborhoods N_1 and N_2 wherein our the updates in (2) and (11) are well-defined. Define $N_2 = \{H \in \mathbb{R}^{p\times p} : \|dG(\boldsymbol{x}^*)\|\|H - dG(\boldsymbol{x}^*)^{-1}\| < 1/2\}$ such that each $H \in N_2$ is non-singular, and there exists a constant $\nu > 0$ such that $\|H\| \leq \nu$ for all $H \in N_2$. Using Lemma 1, we we also choose ϵ and ρ such that $\max\{\|\bar{\boldsymbol{x}} - \boldsymbol{x}^*\|^d, \|\boldsymbol{x} - \boldsymbol{x}^*\|^d\} \leq \epsilon$ implies that (14) holds. In particular, if $\|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \epsilon$ and $H \in N_2$, then $\boldsymbol{x} \in D$ and

$$(1/\rho)\|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \|G(\boldsymbol{x})\| \leq \rho\|\boldsymbol{x} - \boldsymbol{x}^*\|\,.$$

As a consequence of applying the inequality above on Eq.(2), we have

$$\|\boldsymbol{s}\| \leq \|H\|\|G(\boldsymbol{x})\| \leq \rho\|H\|\|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \rho\nu\|\boldsymbol{x} - \boldsymbol{x}^*\|\,.$$

Now define N_1 as the set of all $\boldsymbol{x} \in \mathbb{R}^p$ such that

$$\|\boldsymbol{x} - \boldsymbol{x}^*\| < \min\{\epsilon/2, \epsilon/(2\rho), \epsilon/(2\rho\nu)\}$$

where $\rho\epsilon < (3\mu_2)^{-1/d}$. Now if $\boldsymbol{x} \in N_1$ then

$$\|\boldsymbol{s}\| \leq \rho\nu\|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \epsilon/2 \qquad \text{and} \qquad \|F(\boldsymbol{x}) - \boldsymbol{x}\| \leq \rho\|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \epsilon/2\,. \tag{21}$$

If $N = ((N_1 \cap S) \times N_2) \cap N'$ and $(\boldsymbol{x}, H) \in N$, then $\boldsymbol{x}, \bar{\boldsymbol{x}}$, and $F(\boldsymbol{x})$ lie in D because using (21)

$$\|\bar{\boldsymbol{x}} - \boldsymbol{x}^*\| \leq \|\boldsymbol{s}\| + \|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \epsilon \quad \text{and} \quad \|F(\bar{\boldsymbol{x}}) - \boldsymbol{x}^*\| \leq \|F(\boldsymbol{x}) - \boldsymbol{x}\| + \|\boldsymbol{x} - \boldsymbol{x}^*\| \leq \epsilon\,.$$

Hence Inequality (14) shows that

$$\left(\frac{1}{\rho}\right)\|\boldsymbol{s}\| \le \|\boldsymbol{y}\| \le \rho\|\boldsymbol{s}\|\,, \tag{22a}$$

$$\left(\frac{1}{\rho}\right)\|\boldsymbol{u}\| \le \|\boldsymbol{v}\| \le \rho\|\boldsymbol{u}\|\,, \tag{22b}$$

and in particular

$$\mu_2\|\boldsymbol{y}\|^d \le \mu_2(\rho\epsilon)^d \le 1/3 \tag{23a}$$

$$\mu_2\|\boldsymbol{v}\|^d \le \mu_2(\rho\epsilon)^d \le 1/3\,. \tag{23b}$$

Thus $\boldsymbol{y} = 0$ if and only if $\boldsymbol{s} = 0$, which happens if and only if $\boldsymbol{x} = \boldsymbol{x}^*$. This shows that the update function in Eq.(2) and (11) is well-defined for all $(\boldsymbol{x}, H) \in N$. We now show that the update functions satisfy the conditions of Theorem 1. Since (16) and (23b) imply that (20) hold with $\beta = 1/3$, it follows from (16) and parts (c), (d) of Lemma 2 applied on (19) that

$$\|\bar{H} - dG(\boldsymbol{x}^*)^{-1}\|_M \le \left[\sqrt{1 - \frac{3}{8}\theta^2} + \frac{3}{2}\mu_2\|\boldsymbol{v}\|^d\right]\|H - dG(\boldsymbol{x}^*)^{-1}\|_M + \frac{2\|M\|\|\boldsymbol{u} - dG(\boldsymbol{x}^*)^{-1}\boldsymbol{v}\|}{\|M^{-1}\boldsymbol{v}\|}$$

where $\theta = \dfrac{\|M[H - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}\|}{\|H - dG(\boldsymbol{x}^*)^{-1}\|_M\|M^{-1}\boldsymbol{v}\|}$. But for any $\boldsymbol{x} \in N_1$,

$$\|\boldsymbol{u} - dG(\boldsymbol{x}^*)^{-1}\boldsymbol{v}\| \le K\|dG(\boldsymbol{x}^*)^{-1}\| \max\{\|F(\boldsymbol{x}) - \boldsymbol{x}^*\|^d, \|\boldsymbol{x} - \boldsymbol{x}^*\|^d\}\|\boldsymbol{u}\|\,.$$

Using Inequality (22b),

$$\|\bar{H} - dG(\boldsymbol{x}^*)^{-1}\|_M \le \sqrt{1 - \frac{3}{8}\theta^2}\|H - dG(\boldsymbol{x}^*)^{-1}\|_M + \max\{\|F(\boldsymbol{x}) - \boldsymbol{x}^*\|^d, \|\boldsymbol{x} - \boldsymbol{x}^*\|^d\}[\alpha_1\|H - dG(\boldsymbol{x}^*)^{-1}\|_M + \alpha_2] \tag{24}$$

where $\alpha_1 = \left(\frac{2}{3}\right)(2\rho)^d\mu_2$ and $\alpha_2 = 2\rho K\|M\|^2\|dG(\boldsymbol{x}^*)^{-1}\|$. This inequality now satisfies the assumptions of Theorem 1 and therefore, $\boldsymbol{x}_k$ converges locally to $\boldsymbol{x}^*$ as k increases.

Proof (Proof of Corollary 2). To prove the Q-superlinear convergence, we use the Corollary 1 that guarantees the desired result if a subsequence of $\{H_k\}$ converges to

$dG(\boldsymbol{x}^*)^{-1}$. Define

$$\theta_k = \frac{\|M[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\|}{\|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M \|M^{-1}\boldsymbol{v}_k\|} .$$

Since $\sqrt{1-\alpha} < 1 - \alpha/2$, from Eq.(24) we get

$$\begin{aligned}\frac{3}{16}\theta_k^2 \|H - dG(\boldsymbol{x}^*)^{-1}\|_M &\leq \left[\|H - dG(\boldsymbol{x}^*)^{-1}\|_M - \|\bar{H} - dG(\boldsymbol{x}^*)^{-1}\|_M\right] \\ &\quad + \max\left\{\|F(\boldsymbol{x}) - \boldsymbol{x}^*\|^d, \|\boldsymbol{x} - \boldsymbol{x}^*\|^d\right\}[\alpha_1 \|H - dG(\boldsymbol{x}^*)^{-1}\|_M + \alpha_2] .\end{aligned} \tag{25}$$

If there is a subsequence $\{H_k\}$ such that it converges to $dG(\boldsymbol{x}^*)^{-1}$, then $\|H - dG(\boldsymbol{x}^*)^{-1}\|_M$ converges to zero and we are done by Corollary 1. Otherwise, $\|H - dG(\boldsymbol{x}^*)^{-1}\|_M$ is bounded by α but does not converge to zero. Now summation on Eq.(25) yields

$$\begin{aligned}\frac{3}{16}\sum_{k=1}^{\infty}\theta_k^2 \|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M &\leq \|H_0 - dG(\boldsymbol{x}^*)^{-1}\|_M - \|H_\infty - dG(\boldsymbol{x}^*)^{-1}\|_M \\ &\quad + [\alpha_1\alpha + \alpha_2]\epsilon^d \sum_{k=1}^{\infty} r^{(k-1)d} \\ &\leq 2\alpha + \frac{[\alpha_1\alpha + \alpha_2]\epsilon^d}{1 - r^d} < \infty .\end{aligned}$$

and since

$$\begin{aligned}\sum_{k=1}^{\infty}\theta_k^2 \|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M &= \sum_{k=1}^{\infty}\frac{\|M[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\|^2}{\|H_k - dG(\boldsymbol{x}^*)^{-1}\|_M \|M^{-1}\boldsymbol{v}_k\|^2} \\ &\geq \frac{1}{\alpha}\sum_{k=1}^{\infty}\frac{\|M[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\|^2}{\|M^{-1}\boldsymbol{v}_k\|^2} ,\end{aligned}$$

this forces the following limit to converge to zero.

$$\lim_{k\to\infty}\frac{\|[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\|}{\|\boldsymbol{v}_k\|} = 0 . \tag{26}$$

Using $H_k\boldsymbol{v}_k = H_kG(F(\boldsymbol{x}_k)) - H_kG(\boldsymbol{x}_k) = H_kG(F(\boldsymbol{x}_k)) + \boldsymbol{s}_k$, we can write

$$[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k = H_kG(F(\boldsymbol{x}_k)) - dG(\boldsymbol{x}^*)^{-1}[\boldsymbol{v}_k - dG(\boldsymbol{x}^*)s_k] .$$

At the end of the proof of Theorem 1, we prove that there exists $\upsilon > 0$ such that $\|H_k\| \leq \upsilon$. Using the above equation, Lemma 1, and the fact that $\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\| \leq \|\boldsymbol{x}_k - \boldsymbol{x}^*\|$, we get

$$\begin{aligned}
\|G(F(\boldsymbol{x}_k))\| &\leq \|H_k^{-1}\| \left[\|[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\| + \|dG(\boldsymbol{x}^*)^{-1}\|\|\boldsymbol{v}_k - dG(\boldsymbol{x}^*)\boldsymbol{s}_k\|\right] \\
&\leq v\big[\|[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\| + \|dG(\boldsymbol{x}^*)^{-1}\|K\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^d\|\boldsymbol{u}_k\| \\
&\qquad + \|dG(\boldsymbol{x}^*)^{-1}\|\|G'(\boldsymbol{x}^*)(\boldsymbol{s}_k - \boldsymbol{u}_k)\|\big] \\
&\leq v\big[\|[H_k - dG(\boldsymbol{x}^*)^{-1}]\boldsymbol{v}_k\| + \|dG(\boldsymbol{x}^*)^{-1}\|K\|\boldsymbol{x}_k - \boldsymbol{x}^*\|^d\|\boldsymbol{u}_k\| \\
&\qquad + \|dG(\boldsymbol{x}^*)^{-1}\|\|dG(\boldsymbol{x}^*)\|\|(\boldsymbol{x}_{k+1} - F(\boldsymbol{x}_k))\|\big] . \qquad (27)
\end{aligned}$$

A critical assumption is the condition that $\lim_{k\to\infty} \|\boldsymbol{x}_{k+1} - F(\boldsymbol{x}_k)\|/\|\boldsymbol{x}_k - \boldsymbol{x}^*\| = 0$. Since $\|\boldsymbol{u}_k\| \geq (1/\rho)\|\boldsymbol{v}_k\|$ and appealing to the limit in Eq.(26),

$$\lim_{k\to\infty} \frac{\|G(F(\boldsymbol{x}_k))\|}{\|\boldsymbol{u}_k\|} = 0.$$

Now using Eq.(14), we know that $\|F(\boldsymbol{x}_k) - \boldsymbol{x}^*\| \leq \rho\|G(F(\boldsymbol{x}_k))\|$ and $\|\boldsymbol{x}_k - \boldsymbol{x}^*\| \geq \|\boldsymbol{u}_k\|/\rho$. Therefore we have the string of inequalities

$$\frac{\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} \leq \frac{\|\boldsymbol{x}_{k+1} - F(\boldsymbol{x}_k)\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} + \frac{\|F(\boldsymbol{x}_k) - \boldsymbol{x}^*\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} \leq \frac{\|\boldsymbol{x}_{k+1} - F(\boldsymbol{x}_k)\|}{\|\boldsymbol{x}_k - \boldsymbol{x}^*\|} + \frac{\rho^2\|G(F(\boldsymbol{x}_k))\|}{\|\boldsymbol{u}_k\|} .$$

Q-superlinearity follows as the upperbound of $\|\boldsymbol{x}_{k+1} - \boldsymbol{x}^*\|/\|\boldsymbol{x}_k - \boldsymbol{x}^*\|$ goes to 0 as $k \to \infty$. This concludes the proof of Q-superlinearity of our quasi-Newton method for MM acceleration in a neighborhood of the limit point.

6.3. Examples

6.3.1. Truncated Beta Binomial

As discussed earlier in Example 4.2, we have the Lidwell and Sommerville (1951) dataset of cold incidences in households of size four. These holuseholds are classified as: (a) adults only, (b) adults and school children, (c) adults and infants, and (d) adults, school children, and infants. Only households with at least one cold incidence are reported, hence warranting the use of zero-truncated beta-binomial distribution to model the dataset.

We have already presented a comparative analysis of different MM acceleration methods for dataset subcategory (a) in Table 2. Using the same tolerance ϵ and starting points (π_0, α_0), we run the methods for the other three subcategories and present the unified

Table 5. The Lidwell and Somerville (1951) cold data on households of size 4 and corresponding MLEs under the truncated beta-binomial model.

Household	Number of cases				MLE	
	1	2	3	4	$\hat{\pi}$	$\hat{\alpha}$
(a)	15	5	2	2	0.0000	0.6151
(b)	12	6	7	6	0.1479	1.1593
(c)	10	9	2	7	0.0000	1.6499
(d)	26	15	3	9	0.0001	1.0594

results in Table 6. It is worth to note that while at least one SQUAREM methods fail to provide acceleration for each subcategory, BQN consistently accelerates over the slow MM algorithm.

Table 6. Truncated beta binomial: comparison of algorithms for the Lidwell and Somerville Data. The starting point is $(\pi, \alpha) = (0.5, 1)$, the stopping criterion is $\epsilon = 10^{-7}$, and the number of parameters is two.

Data	Algorithm	-ln L	Fevals	Iterations	Time (in sec)
(b)	MM	41.7286	5492	5492	0.026
	BQN, $q = 1$	41.7286	1012	507	0.036
	SqS1	41.7286	248	210	0.019
	SqS2	41.7286	1553	1148	0.106
	SqS3	41.7286	79	40	0.006
	ZAL, $q = 2$	41.7286	1136	1132	0.063
(c)	MM	37.3586	61843	61843	0.323
	BQN, $q = 1$	37.3589	1864	933	0.062
	SqS1	37.3587	1370	1345	0.122
	SqS2	37.3582	9649	8966	0.977
	SqS3	37.3582	145	73	0.010
	ZAL, $q = 2$	37.3582	28	24	0.004
(d)	MM	65.0423	25026	25026	0.132
	BQN, $q = 1$	65.0435	268	135	0.007
	SqS1	65.0413	1648	1622	0.136
	SqS2	65.0420	5727	5443	0.472
	SqS3	65.0402	97	49	0.007
	ZAL, $q = 2$	65.0402	25	21	0.003