Hessian Initialization Strategies for \(\ell\)-BFGS Solving Non-linear Inverse Problems

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Abstract. \(\ell\)-BFGS is the state-of-the-art optimization method for many large scale inverse problems. It has a small memory footprint and achieves superlinear convergence. The method approximates Hessian based on an initial approximation and an update rule that models current local curvature information. The initial approximation greatly affects the scaling of a search direction and the overall convergence of the method.

We propose a novel, simple, and effective way to initialize the Hessian. Typically, the objective function is a sum of a data-fidelity term and a regularizer. Often, the Hessian of the data-fidelity is computationally challenging, but the regularizer’s Hessian is easy to compute. We replace the Hessian of the data-fidelity with a scalar and keep the Hessian of the regularizer to initialize the Hessian approximation at every iteration. The scalar satisfies the secant equation in the sense of ordinary and total least squares and geometric mean regression.

Our new strategy not only leads to faster convergence, but the quality of the numerical solutions is generally superior to simple scaling based strategies. Specifically, the proposed schemes based on ordinary least squares formulation and geometric mean regression outperform the state-of-the-art schemes.

The implementation of our strategy requires only a small change of a standard \(\ell\)-BFGS code. Our experiments on convex quadratic problems and non-convex image registration problems confirm the effectiveness of the proposed approach.

Keywords: inverse problem, optimization, quasi-newton, \(\ell\)-BFGS, Hessian initialization.

1 Introduction

Many real-life problems fit the framework of an inverse problem. Fluorescence optical tomography [17], ultrasound tomography [2], and photoacoustic tomography [18] are just a few non-invasive imaging techniques that image a human body’s internal structure by solving inverse problems.

Inverse problems are typically ill-posed in nature [8]. The solution may not be unique and unstable with variations in the data due to unavoidable factors such
as physical noise. Regularizing the problem with prior information, we obtain a solution by minimizing an objective function

$$J : \mathbb{R}^n \to \mathbb{R}, \quad J(x) = D(x) + S(x),$$

where $D$ denotes a data-fitting term and $S$ a regularizer. For many non-linear problems, the objective function is non-convex, and the main limitation is computationally demanding operations. Hence, an efficient optimization method to be designed that requires fewer evaluations of an objective function, its gradient and Hessian, and more occasional calls to a linear solver.

Numerous optimization schemes exist to solve these problems. Still, schemes that do not require more than first-order information are generally preferable. Hessian computation is usually expensive.

Steepest-descent (SD) and quasi-newton methods are the most popular first-order methods. SD converges only linearly; hence super-linear convergent quasi-Newton methods such as Gauss-Newton (GN) schemes or the Broyden-class are preferable. The quasi-Newton method’s key idea is to replace Hessian with an approximation that models the local curvature information. It leads to not only faster convergence but as well higher solution accuracy than simple gradient descent methods; see, e.g. [17,9] and references therein.

The Hessian approximation in the GN method is based on linearizing a function that involves a matrix-vector product with a Jacobian matrix. For applications such as optical tomography [17], the Jacobians are generally dense, and hence per iteration costs can be very high. Therefore, Broyden-class methods are preferred in practice. The most popular member is the limited-memory version of BFGS scheme ($\ell$-BFGS) for large scale inverse problems; see its application to recent work in ultrasound tomography [2] and image registration [11].

The Broyden-class works with approximations of the Hessian that are based on an initial approximation and an update rule that is typically based on current curvature information derived from a secant equation [15, Chapter 2] for Hessian $B$,

$$B' p = y \quad \text{or, for the inverse of } B, \quad p = H' y. \quad (1)$$

Based on an initial choice $H_0$, BFGS-schemes update the current approximation $H = H_k$ using a constrained and weighted least squares fit,

$$H_{k+1} \in \arg\min \{ |M - H_k|_F, \; M = M^\top, \; My_k = p_k \},$$

where a weighted Frobenius-norm $|A|_F^2 = \text{trace}(W AW^\top)$ is used. If the weight matrix satisfies secant equation $WP = y$, one obtains a unique and scale-invariant solution for $H_{k+1}$ as a rank two update of the $H_k$,

$$H_{k+1} = V_k^\top H_k V_k + \alpha_k p_k p_k^\top, \quad \text{with } \alpha_k := (y_k^\top p_k)^{-1}, \; V_k := I - \alpha y_k p_k^\top. \quad (2)$$

For large-scale problems, a limited-memory version of BFGS ($\ell$-BFGS) is used [12]. In $\ell$-BFGS, at most the last $\ell$ pairs are used. More precisely, only pairs
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\((y_j, p_j)\) with \(k_\ell := \max\{1, k - \ell - 1\} \leq j \leq k\) are used. Formally, \(H_{k+1} = M_{k+1}\) results from the modified recursion

\[M_{j+1} := V_j^T M_j V_j + \alpha_j p_j p_j^T, \quad j = k_\ell, \ldots, k.\] (3)

The convergence depends on the quality of Hessian approximation which generally can not be controlled. It has been observed numerically that a “good” initial guess of the Hessian greatly affects the scaling of a search direction and convergence of the overall scheme \([5,7,13,1]\). Note that ℓ-BFGS-method allows to re-initialize Hessian at every iteration. This opportunity provides a window to rescale the search direction and infuse more information in the scheme.

The state-of-the-art strategy initialize the Hessian (or its inverse) with a scaled identity matrix

\[H_k^0 = \tau_k I.\]

The scalar \(\tau_k\) is computed at each iteration to satisfy the secant equation \((1)\) in a ordinary least square sense following the Oren–Luenberger scaling strategy \([16]\). This results in two choices for scaling factor \(\tau_k\), i.e.,

\[\tau_k^{LSy} = (y^T p)/(y^T y) \quad \text{and} \quad \tau_k^{LSp} = (p^T p)/(y^T p).\] (4)

In practice, it has been observed that the factor \(\tau_k^{LSy}\) ensures a well-scaled search direction and as a result, most of the iterations accept a steplengt of one \([7]\).

In this paper, we suggest to improve the quality of the initial Hessian approximation by including computationally manageable parts from the regularizer. More precisely, we suggest to use

\[B_k^0 = \tau_k I + \nabla^2 S,\]

where \(\nabla^2 S\) denotes the Hessian of a not necessarily quadratic regularizer. We derive four options for scaling factor \(\tau_k\) based on ordinary and total-least squares formulations, and geometric mean regression.

Our work is motivated by ideas in image registration \([14,9]\) and molecular energy minimization \([10]\). In \([14,9]\), the Hessian is initialized by a positive-definite matrix \(B_0 = \tau I + A\), where \(A\) is the Hessian of a quadratic regularizer and constant. The parameter \(\tau > 0\) is chosen manually. In \([9]\), it is reported that this strategy outperforms the simple scaling approach. In \([10]\), the proposed strategy is similar to ours but requires expensive incomplete Cholesky factorization at each iteration to ensure positive-definiteness of Hessian approximation. Moreover, the value for \(\tau\) is heuristically defined. But, in this paper, we show that it satisfies secant equation in a sense of geometric mean regression.

We assume the regularization part to be computationally manageable. Typical examples include \(L_2\)-norm based Tikhonov regularizers \([14,8]\), smooth total-variation norm \([19]\), or, more generally, quadratic forms of derivative based regularization. Here, \(R(x) = \|Bx\|_{L_2}\) and \(B\) is a linear differential operator. Non-quadratic forms such as the hyperelastic regularizer \([3]\) also fit into this class.

Our new strategy is easy to integrate into an ℓ-BFGS code. Only the Hessian initialization routine needs to be changed, all other parts remain unchanged.
In this paper, we also demonstrate on various test cases that the proposed approach achieves fast convergence and improves the solution accuracy compared to the standard scaling based approaches. Our test cases include convex quadratic problems and non-convex image registration problems with both, quadratic and non-quadratic regularization. Due to the page limitation, the theoretical investigation will be a part of the extended version of this paper.

In Sec. 2, we derive four scaling factors for the proposed initialization strategy and present a practical algorithm. We report the numerical experiments with results in Sec. 3. In Sec. 4, we conclude our findings.

2 Proposed Hessian Initialization Strategy and Algorithm

As common for inverse problems, we assume that the objective function $J$ is a sum of a data fitting term $D$ and a regularizer $S$. Hence

$$\nabla^2 J = \nabla^2 D + \nabla^2 S,$$

(5)

where $A_k := \nabla^2 S(x_k)$ is symmetric positive semidefinite (SPSD). We assume that $A_k$ is “easy”, i.e. has low memory requirements and $A_k x = b$ can be solved efficiently. Problems may occur from the data fitting part $\nabla^2 D(x_k)$, which might be computationally complex and potentially ill-conditioned.

In the proposed strategy, we suggest to approximate $\nabla^2 D(x_k) \approx \tau_k I$, where $\tau_k$ is a tuning parameter to be determined. Hence

$$B_0^k = \tau_k I + A_k.$$  

(6)

The role of $B_0^k$ is to mimic the Hessian at least for the current update. In this regard, we aim to satisfy the secant equation (1) in some least squares sense, where now

$$y = B_0^k p = \tau_k p + A_k p \iff \tau_k p - z = 0, \quad z := y - A_k p.$$  

(7)

Since $B_0^k$ is required to be symmetric positive definite (SPD), we have $\tau_k \geq \tau_{\min} := \varepsilon - \mu_{\min}$, where $\varepsilon > 0$ is a small tolerance, typically $\varepsilon = 10^{-6}$ and $\mu_{\min}$ is the smallest eigenvalue of $A_k$. This adds a constraint to the least squares problems. First we summarize the ordinary least square approach; cf. Lem. 1.

We removed subscript $k$ for clarity.

Lemma 1. Let $p, z \in \mathbb{R}^n$ with $p^T z \neq 0$ and $\tau_{\min} \in \mathbb{R}$. Then

$$\tau_{Dp} := \max\{(p^T z)/(p^T p), \tau_{\min}\} \text{ and } \tau_{Dz} := \max\{(z^T z)/(p^T z), \tau_{\min}\}$$

are optimal scaling parameters resulting from a minimization of $|\xi u - v|$ subject to $\xi \geq \tau_{\min}$, where $(u,v) = (p,z)$ for $(Dp)$ and $(u,v) = (z,p)$ for $(Dz)$.

Moreover, it holds $|\tau_{Dp}| \leq |\tau_{Dz}|$.

Proof. For $(Dp)$: the unique minimizer $\xi$ of the unconstrained problem follows from the basic calculus. If $\xi < \tau_{\min}$, the minimum is attained on the boundary. For $(Dz)$: the result follows from rescaling. The inequality follows the Cauchy-Schwarz-inequality $|p^T z|^2 \leq (p^T p)(z^T z)$.
The above choices have a preference either for the $p$ or $z$ direction. A total least squares approach can be used for an unbiased approach; cf. Lem. 2.

**Lemma 2.** Let $p, z \in \mathbb{R}^n$ with $\delta := p^T z \neq 0$, $\tau_{\text{min}} \in \mathbb{R}$. Then

$$\tau^{Du} := \max\{|z|^2 - \lambda|/\delta, \tau_{\text{min}}\}, \quad \lambda = (|p|^2 + |z|^2 - \sqrt{(|p|^2 - |z|^2)^2 + 4\delta^2})/2,$$

is an optimal scaling parameter from the rescaling of minimizer $\eta = [\eta_1, \eta_2]$ of the total least squares formulation $|\eta_1 p - \eta_2 z|$ subject to $|\eta| = 1$. With $\tau^{dp}$ and $\tau^{dz}$ as in Lem. 1, it holds $|\tau^{dp}| \leq |\tau^{Du}| \leq |\tau^{Dz}|$.

**Proof.** We have the necessary condition of first order $(U^T U - \mu I)\eta = 0$ subject to $|\eta| = 1$, where $U = [p, -z]$ and $\mu$ denotes the Lagrange-multiplier. This indicates that $\mu$ is the smallest eigenvalue of the symmetric 2-by-2 matrix $U^T U$ with diagonal elements $|p|^2$ and $|z|^2$ and off diagonal $-\delta$. Hence, $\mu = \lambda$ and $\eta := v/|v|$ is a normalized version of the associated eigenvector $v = (\delta, |p|^2 - \lambda)$. The value for $\tau^{Du}$ follows from proper scaling.

To show the inequality, we use the relationship $|(z^2 - \lambda|/\delta = \delta/(|p|^2 - \lambda)$ derived from $\det(U^T U - \mu I) = 0$. Since $U^T U$ is SPSD, we know $\lambda \geq 0$. Hence, the inequalities $|(z^2 - \lambda)/|\delta| \leq |z|^2/|\delta|$ and $|\delta/|p|^2 \leq |\delta/(|p|^2 - \lambda)$ satisfies. It leads to $|\tau^{dp}| \leq |\tau^{Du}| \leq |\tau^{Dz}|$ following the definition of $\tau^{dp}$, $\tau^{dz}$, and $\tau^{Du}$.

Geometric mean regression is another unbiased approach; see [6] for details. The optimal scaling parameter is defined as the geometric mean of scaling parameters obtained from ordinary least squares problems in Lem. 1, i.e.,

$$\tau^{GM} = \max\{|\tau^{dp}\tau^{dz}\}^{1/2}, \tau_{\text{min}}\} = \max\{|(z^2/|p|^2|^{1/2}, \tau_{\text{min}}\} \quad (8)$$

and follows $|\tau^{dp}| \leq \tau^{GM} \leq |\tau^{Dz}|$.

**Remarks on scaling parameters:** Note that, the tuning of parameter $\tau$ changes both the angle and length of search direction, whereas the simple scaling based schemes $\tau^{ly}$ and $\tau^{lp}$ majorly changes the length of the search direction.

To achieve fast convergence, we aim to reduce the number of iterations and the line-search steps at every iteration. For that, we seek a search direction that is closer to the Newton direction and take fewer iterations to convergence. Furthermore, we seek well-scaled search directions that satisfy steplength equal to one and avoid any line-search steps for reducing the total run-time.

For a simple quadratic problem, we observe that the search directions with the proposed choices for $\tau$ behave almost in a similar fashion with respect to the Newton direction. Hence, all options are practically equivalent.

But, in practice, we observe that the length of a search direction is inversely proportional to the value of $\tau$ for our schemes. Hence, a small $\tau$ leads to a long step. Although it is desirable, but an overestimated length leads to many line-search steps. On the other hand, with a large $\tau$, we take small steps and, as results, require many iterations for convergence; see results in Sec. 3. These facts suggest an optimal scaling factor, but the exact criterion are so far unknown to us. Nevertheless, we provide four choices for $\tau$ covering a wide range and describe their inter-relationship in Lem. 2 and (8).
Algorithm 1: Standard $\ell$-BFGS algorithm with the proposed Hessian initialization strategy

1. Initialize a starting guess $x_0$, integer $\ell > 0$, and $\varepsilon > 0$;
2. $k \leftarrow 0$;
3. repeat
   4. Compute $B^0_k$ following steps in Algo. 2;
   5. Compute search direction $d_k \leftarrow -H_k \nabla J(x_k)$ using $B^0_k$ in the two-step recursive algorithm based on (3); see details in [12];
   6. Compute $x_{k+1} \leftarrow x_k + \alpha_k d_k$ where $\alpha_k$ is obtained with a line-search algorithm;
   7. if $k > \ell$ then
      8. Discard the vector pair $\{p_{k-\ell}, y_{k-\ell}\}$ from the storage;
   9. end
10. Compute and save $p_k \leftarrow x_{k+1} - x_k$ and $y_k = \nabla J(x_{k+1}) - \nabla J(x_k)$;
11. $k \leftarrow k + 1$;
12. until convergence;

Algorithm 2: Secant equation based Hessian initialization strategies

1. Compute $A_k$, Hessian of regularizer at $x_k$;
2. Set $\tau_{\text{min}} \leftarrow \varepsilon$;
3. if first iteration ($k = 0$) then
   4. Set $\tau_k \leftarrow \tau_{\text{min}}$;
   5. else
      6. Compute $z_k \leftarrow y_k - A_k p_k$;
      7. Set $\tau_k$ to either $\tau_k^{\text{DP}}, \tau_k^{\text{DU}}, \tau_k^{\text{Dz}},$ or $\tau_k^{\text{GM}}$;
   8. end
9. Initialize $B^0_k \leftarrow \tau_k I + A_k$;

Practical algorithm: Now, we are ready to present pseudo code for the standard $\ell$-BFGS algorithm with the proposed Hessian initialization strategies where we motivate to initialize Hessian $B^0_k$ at every iteration with (6); see Algo. 1 [15]. In the standard $\ell$-BFGS code, we only need to change the Hessian initialization routine; see Line 4 in Algo. 1 with a few lines of code described in Algo. 2.

To initialize $B^0_k$, we start with setting $\tau_{\text{min}}$, computing the Hessian of regularizer, and evaluating $z_k$. The parameter $\tau_k$ can be set with either $\tau_k^{\text{DP}}, \tau_k^{\text{DU}}, \tau_k^{\text{Dz}},$ or $\tau_k^{\text{GM}}$.

In the first iteration, we can not compute $z_k$ due to the lack of information on the required iterates. Hence, initially, we set $\tau = \varepsilon$ in our experiments. Other initialization options, e.g., based on the norm of a gradient [15], are also possible.

Recall that the parameter $\tau_k$ should be greater than $\tau_{\text{min}} = \varepsilon - \mu_{\text{min}}(A_k)$ to ensure the positive-definiteness of Hessian $B^0_k$. To determine $\tau_{\text{min}}$, we need the smallest eigenvalue of $A_k$ that could be computationally expensive operation for large scale problems. Hence, we avoid the eigenvalue computation in practice and set $\tau_{\text{min}} = \varepsilon = 10^{-6}$ in our experiments.
Table 1. Optimization methods used for evaluations. $A_k$ be the Hessian of regularizer.

| No. | Optimization methods | Hessian initialization | References |
|-----|----------------------|-----------------------|------------|
| 1.  | Steepest descent (SD) | $H_k^0 = \tau_k I$   | see [15]   |
| 2.  | $\ell$-BFGS          | $H_k^0 = \tau_k I$   | $\tau_k = I, \tau_k^{LSy}, \text{or} \tau_k^{LSp}$; see [14] |
| 3.  | $\ell$-BFGS (FAIR scheme) | $B_k^0 = \tau I + A_k$ | $\tau$ is set manually; see [14] |
| 4.  | $\ell$-BFGS (proposed) | $B_k^0 = \tau_k I + A_k$ | $\tau_k = \tau_k^{DP}, \tau_k^{Dz}, \tau_k^{Du}, \text{or} \tau_k^{GM}$; see Lem. 1, Lem. 2, and (8) |
| 5.  | Gauss-Newton (GN)    | -                     | see [15]   |

3 Numerical Experiments and Results

We report on the performance of the proposed Hessian initialization strategies for typical inverse problems: a) **Strictly convex quadratic problems**: This class is chosen to validate the convergence properties of the proposed strategy numerically. b) **Non-convex image registration problems**: This class is chosen to show the effectiveness of the proposed strategy on a few challenging real-world problems.

We investigate in total eight Hessian initialization strategies for $\ell$-BFGS method; see Tab. 1 for details. Along with $\ell$-BFGS, we also report results with Gauss-Newton (GN) and steepest descent (SD) method. GN is a widely used method in the field of image registration. GN may achieve quadratic convergence close to the solution. Even though, GN may converge to a local optimal point in a few iterations, but for large scale problems, per iteration cost for GN could be very high due to additional matrix-vector products with Jacobian; see run-time for GN in Tab. 4 for image registration problems. On the other hand, SD follows a linear and $\ell$-BFGS a superlinear convergence.

Note that, the methods Dp, Du, Dz, GM, FAIR, and GN solve a linear system at each iteration to compute the search direction. For that, we use Jacobi preconditioned conjugate gradient (PCG) method. Moreover, the associated system matrices are not stored, rather matrix-vector product has been computed directly. We run PCG until the relative residual is less than $10^{-6}$ or the maximum iterations reach to 100. The iteration count is set to low with the purpose of reducing extra computational time at each iteration due to the linear solver.

The Hessian initialization in the FAIR [14] is similar to ours. But, they set manually the parameter $\tau = 10^{-3}c$, where $c$ is the first diagonal element of $A$.

We use Armijo backtracking line-search algorithm to estimate the step-size. As noted in [15], if curvature condition is not satisfied at any iteration, we skip the Hessian update. For stopping criteria, we follow [14] p. 78 and set $\varepsilon_J = 10^{-5}$, $\varepsilon_W = 10^{-1}$, and $\varepsilon_G = 10^{-2}$. For $\ell$-BFGS, we use the standard choice $\ell = 5$.

Run-time and solution accuracy are our main criteria to evaluate the performance of optimization methods.
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Table 2. Optimization results for quadratic problem with eight Hessian initialization strategies (S). Iteration counts and average line-searches (LS) per iteration are mentioned for weakly ($\alpha = 10^{-5}$), mildly ($\alpha = 10^{-3}$), and strongly ($\alpha = 10^{-1}$) regularized problems with $\ell = 1, 5, 10, \infty$.

|          | $\alpha = 10^{-5}$ |          | $\alpha = 10^{-3}$ |          | $\alpha = 10^{-1}$ |
|----------|--------------------|----------|--------------------|----------|--------------------|
|          | S./$\ell$           | 1 5 10 10 | S./$\ell$           | 1 5 10 10 | S./$\ell$           | 1 5 10 10 |
| Id       | 5000 3858 3893 171 | 5000 754 628 128 | 567 137 97 47 |
| LSp      | 4108 908 383 37   | 539 145 65 28  | 79 37 31 23 |
| LSy      | 2705 1460 870 90  | 558 230 115 39 | 69 39 30 23 |
| FAIR     | 5000 869 389 18   | 168 93 31 15  | 18 7 7 7   |
| Dp       | 4400 817 262 30   | 565 79 47 20  | 23 12 10 10|
| Dz       | 3716 1128 633 84  | 564 228 163 50 | 49 27 19 17|
| Du       | 5000 760 274 30   | 578 88 36 20  | 23 11 10 10|
| GM       | 2880 588 269 61   | 356 125 56 30 | 30 13 11 11|
|          | avg. LS per iter.  |          |                    |          |                    |
| Id       | 1.00 1.00 1.00 1.00| 1.00 1.00 1.00 1.00| 1.00 1.00 1.00 1.00|
| LSp      | 2.73 7.05 8.13 1.16| 2.43 3.78 3.08 1.18| 1.76 1.62 1.48 1.43|
| LSy      | 1.15 1.10 1.11 1.00| 1.15 1.15 1.17 1.00| 1.07 1.05 1.10 1.04|
| FAIR     | 14.74 12.92 12.04 5.56| 8.08 6.41 3.74 2.67| 2.11 1.43 1.43 1.43|
| Dp       | 2.68 6.64 6.86 1.80| 2.32 3.62 2.79 1.65| 1.35 1.17 1.20 1.20|
| Dz       | 1.15 1.10 1.11 1.18| 1.10 1.06 1.09 1.18| 1.04 1.07 1.11 1.12|
| Du       | 2.71 6.49 7.55 1.80| 2.38 3.10 2.58 1.65| 1.26 1.27 1.20 1.20|
| GM       | 1.77 3.04 3.54 1.28| 1.63 1.88 1.89 1.33| 1.10 1.15 1.18 1.18|

3.1 Quadratic problem

We minimize a strictly convex quadratic function $0.5(x - c)^{\top}(D + \alpha R)(x - c)$ that has the unique minimizer at $x^* = c \in \mathbb{R}^n$ with $D$ and $R$ be a symmetric and positive-definite matrix and $\alpha > 0$. In experiments, $D$ is a diagonal matrix with exponentially decaying eigenvalues, i.e., $D_{ii} = \exp(-i)$. It is a highly ill-conditioned matrix with condition number of order $10^6$ reflecting Hessian of a typical data-fidelity term in inverse problems. The regularization matrix $R$ be a well-known Laplacian matrix with zero boundary conditions. The regularization parameter $\alpha$ controls the ill-conditioning of the quadratic function. Here, we investigate weakly ($\alpha = 10^{-5}$), mildly ($\alpha = 10^{-3}$), and strongly ($\alpha = 10^{-1}$) regularized problems; see results in Tab. 2.

The iterations start with $x$ be a zero vector. The iterations stop when either the relative error $\|x - x^*\|/\|x^*\| \leq 10^{-5}$ or the iteration count reaches 5000.

As expected, the highly ill-conditioned problem, i.e., weakly regularized, requires many iterations for convergence. Especially, if the local curvature is not well-estimated; see results for $\ell = 1$ in Tab. 2. The iteration counts are decreasing with increasing regularization levels and with improving Hessian approximation that is increasing $\ell$. Note that this behavior is consistent across all Hessian initialization strategies taken into consideration in this work.

Identity initialized Hessian scheme converges very slow. But mostly, it satisfies step-length equal to one, which means it takes tiny steps at each iteration.
Table 3. Image registration test problems (TP) for the performance evaluation of optimization strategies. For TP-4, the initial TRE is not available (N.A.).

| TP | Dataset | Problem size | Data-Fidelity | Regularizer | Parameters | Initial TRE |
|----|---------|--------------|---------------|-------------|------------|-------------|
| 1  | Hand (2D) | 2 × 128 × 128 | SSD           | Curvature   | $\alpha = 1.5 \times 10^3$ | 1.04 (0.62) |
| 2  | Hand (2D) | 2 × 128 × 128 | MI            | Elastic     | $\alpha = 5 \times 10^{-3}$ | 1.04 (0.62) |
| 3  | Lung (3D) | 3 × 64 × 64 × 24 | NGF          | Curvature   | $\alpha = 10^2$     | 3.89 (2.78) |
| 4  | Disc-C (2D) | 2 × 16 × 16 | SSD           | Hyperelastic | $\alpha = (100, 20)$ | N.A. |

In most cases, the Hessian initialization schemes equipped with regularization require fewer iterations than the simple scaling based LSy and LSp schemes. In particular, the FAIR scheme takes the lowest iterations, but search-directions are badly scaled. Hence, line-searches (LS) per iteration are much higher than the other schemes. Moreover, LS steps highly depend on the regularization level.

But, for the proposed four schemes, the LS steps depend on the goodness of Hessian approximation, i.e., the value of $\ell$ rather than the regularization level. In practice, we generally work with a fixed $\ell$ and adjust the regularization level as per the need. Hence, the proposed scheme suits better for such a scenario. In particular, the Dz scheme generally take 1.15 LS steps per iteration and does not depend much on $\ell$. The Dp and Du schemes require higher LS steps than Dz whereas the GM between the Dp and the Dz. In terms of iterations, we observe an almost inverse relationship; e.g., the Dp and Du scheme take fewer iterations than Dz; follow the discussion in Sec. 2 for the underlying reason.

3.2 Image Registration

Now, we show effectiveness on four real-life large-scale problems from image registration. The registration problems are generally highly non-convex and ill-posed in nature; see [14] for details. Here, given a pair of images $T$ and $R$, the goal is to find a transformation field $\phi$ such that the transformed image $T(\phi)$ is similar to $R$, i.e., $T(\phi) \approx R$. To determine $\phi$, we solve an unconstrained optimization problem

$$J(\phi) = D(T(\phi), R) + \alpha S(\phi) \xrightarrow{\phi} \min$$

where $D$ measures the similarity between the transformed image $T(\phi)$ and $R$. The regularizer $S$ enforces smoothness in the field. Curvature, elastic, and hyperelastic are a few commonly used regularizers. The typical choices for similarity measures are the sum of squared difference (SSD), normalized gradient fields (NGF), and mutual information (MI).

Our four test problems (TP) represent a big class of registration models; see Tab. 3. The popular X-ray hand images are from [14], lung CT images from the well-known DIR dataset [11,4], and the academic Disc-C images from [3].

Note that our strategy works even when the Hessian of regularizer is available only partially. For that, we consider hyperelastic regularizer; see [3] for details.
Table 4. Optimization results for four image registration test problems (TP). The iteration counts (iter), the function evaluations (feval), the reduction in objective function $J(\phi)$, the average run-time in seconds, and the mean and standard deviation of TRE are reported. The gray-colored cell denotes the $\ell$-BFGS method that achieve either the smallest TRE (higher accuracy) or lowest run-time (faster convergence).

| TP-1: Hand, SSD, Curvature | TP-2: Hand, MI, Elastic |
|---------------------------|-------------------------|
| **M.** | **iter** | **feval** | **$J(\phi)$** | **time (sec.)** | **TRE** | **mean (std.)** | **iter** | **feval** | **$J(\phi)$** | **time (sec.)** | **TRE** | **mean (std.)** |
| SD | 999 | 1600 | 86.27 | 23.31 | 1.04 (0.62) | 169 | 270 | 84.80 | 8.23 | 0.99 (0.63) |
| LSp | 1000 | 4157 | 28.07 | 40.46 | 0.67 (0.52) | 154 | 446 | 73.53 | 9.15 | 0.64 (0.37) |
| LSy | 1000 | 1029 | 24.48 | 20.44 | 0.52 (0.29) | 135 | 137 | 73.64 | 5.74 | 0.64 (0.36) |
| FAIR | 1000 | 1001 | 21.62 | 57.10 | 0.36 (0.18) | 170 | 171 | 72.78 | 12.27 | 0.56 (0.30) |
| Dp | 53 | 59 | 21.94 | 8.96 | 0.38 (0.17) | 43 | 67 | 72.76 | 7.63 | 0.58 (0.34) |
| Dz | 444 | 445 | 20.49 | 71.63 | 0.37 (0.16) | 72 | 94 | 72.84 | 6.73 | 0.58 (0.32) |
| Du | 444 | 445 | 20.49 | 71.79 | 0.37 (0.16) | 43 | 67 | 72.76 | 7.70 | 0.58 (0.34) |
| GM | 78 | 80 | 20.84 | 13.13 | 0.35 (0.17) | 64 | 66 | 72.77 | 8.83 | 0.57 (0.31) |
| GN | 18 | 19 | 28.45 | 4.58 | 0.69 (0.59) | 360 | 360 | 360 | 360 | 360 |

The ground truth transformation fields are not available for real-world problems. Hence, we compute the target registration error (TRE), defined as the Euclidean distance between the ground truth landmarks and the estimated landmarks after registration. To accumulate the TRE for each landmark position, we compute the mean and standard deviation (std.) of TRE. The regularization parameter is set to achieve the lowest TRE without foldings in the field.

The field $\phi$ is initialized with an identity map, i.e., $\phi_0(x) = x$ in all experiments. The open-source FAIR image registration toolbox [14] is the backbone of our implementations. We follow FAIR matrix-free approach.

In all the experiments, the regularization-equipped initialization schemes achieve higher accuracy than the simple scaling based approaches, i.e., LSp, LSy, and Id. Moreover, these simple scaling schemes converge to a higher value of the objective function; see TRE and reduction factor column in Tab. 4.

In terms of TRE, the FAIR scheme is almost similar to the proposed schemes, but it converges much slower than others; see the run-time column in Tab. 4. The proposed schemes are faster than others in all the experiments but TP-2.
Here, LSy converges faster but at the cost of lower accuracy. It is important to note that, even though the regularization-equipped schemes’ per-iteration cost is higher due to the linear solver, they converge faster. It is mainly because of the lower iteration counts, as also seen for quadratic problems; see Tab. 2.

Among the four proposed choices, the Dp and the GM turn out to be the best performing schemes. Although, we notice that the performance of a particular scheme greatly depends on the minimizing objective function at hand.

As expected, the steepest descent method is one of the slowest and inaccurate among all. The GN method generally needs fewer iterations, but the per-iteration cost is much higher due to the Jacobian computation; hence the run-time is high.

4 Conclusion

We have proposed a Hessian initialization strategy particularly suited for large-scale non-linear inverse problems. Typically, the objective function is the sum of a data-fidelity term and a regularizer. Often, the Hessian of the data-fidelity is computationally expensive. But not the Hessian of the regularizer.

We propose to replace the Hessian of the data-fidelity with a scalar and keep the Hessian of regularizer to initialize the Hessian approximation at every iteration. The scalar satisfies the well-known secant equation in the sense of ordinary and total least squares, and geometric mean regression. In total, we have proposed four choices for the scalar that leads to well-scaled search directions. We also established the inter-relationship between the derived scalars and discussed the consequences of a scalar choice on the convergence in terms of iteration counts and line-search steps. The implementation of our strategy requires only a small change of a standard ℓ-BFGS code.

Our experiments on highly non-convex image registration problems indicate that the proposed schemes converge faster and achieve higher accuracy than the simple scaling based approaches. The Dp, based on ordinary least squares, and GM, based on geometric mean regression, are best-performing schemes.

Under suitable assumptions, we can also show that the proposed parameters are the eigenvalue’s estimates of the Hessian of a data-fidelity term. The theoretical investigation will be a part of the extended version of this paper. Future work also addresses the application to inverse problems, e.g., ultrasound tomography [2], and optical tomography [18].

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