Merging Trust-Region and Limited Memory Technologies for Large-Scale Nonlinear Optimization

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Outline

1. Introduction.
    - General format of large-scale nonlinear optimization problem.
    - Main difficulties.
2. Large-scale unconstrained problem.
    - Description of the algorithm.
    - Numerical Algebra.
    - Numerical Results.
3. Active-set Trust-region Algorithm(ASTRAL) for bounded constrained problems.
    - Description of the algorithm.
    - Numerical Algebra.
    - Numerical Results.

Problem Format

$$\begin{array}{ll} \min & f(x) \\ \text{s.t.} & l \leq x \leq u \end{array}$$

Assumptions:

1. $f : \mathbb{R}^n \to \mathbb{R}$ is smooth, but difficult to evaluate.
   high dimensional integration
   simulation
   systems of PDE/ODE's
   multiple levels of optimization

2. $-\infty \leq l_i \leq u_i \leq \infty$

3. n is large. ($n \geq 1000$, e.g. $n = 2^{19}$ for imaging applications).

Computational Costs

(1) Dominant Costs: function and gradient evaluations.

Jorge Moré and Nick Gould
No test sets now available for *hard* to evaluate functions.

(2) Numerical linear algebra.

A very significant concern due to dimensionality.
But, due to *expensive* functions, we want to exploit all data as fully as possible.

Computational Costs

(1) Dominant Costs: function and gradient evaluations.

line-search vs trust-region

(2) Numerical linear algebra.

matrix multiplies vs equation solves

The Unconstrained Problem

Objective: $\min f(x)$

Algorithm: $x^{k+1} = x^k + s^k$

Notation: $g^k = \nabla f(x^k), \quad B_k \approx \nabla^2 f(x^k)^{-1}, \quad H_k \approx \nabla^2 f(x^k)$

- Line-Search: $s^k = -\lambda_k B_k d^k$

  λ_k a stepsize (weak or strong Wolfe conditions).
  Requires repeated function and gradient evaluations.

- Trust-Region: s^k solves

$$\begin{array}{ll} \min & (g^k)^T s + \frac{1}{2} s^T H_k s \\ \text{s.t.} & \|s\| \le \Delta_k \end{array}$$

Hessian Approximations

Scalar Secant Equation:

$$H_k = \frac{\nabla f(x^k) - \nabla f(x^{k-1})}{x^k - x^{k-1}}$$

Matrix Secant Equation:

$$H_k(x^k - x^{k-1}) = \nabla f(x^k) - \nabla f(x^{k-1})$$

n linear equations in $\frac{n(n+1)}{2}$ unknowns

BFGS Update:

H_0 sym. and positive definite $\Rightarrow H_k$ sym. and positive definite

$$H_{k+1} = H_k - \frac{H_k s^k {s^k}^T H_k}{{s^k}^T H_k s^k} + \frac{y^k {y^k}^T}{{s^k}^T y^k} \qquad \text{whenever } {s^k}^T y^k > 0$$

$$= H_k - [y^k \;\; H_k s^k] \begin{pmatrix} -{s^k}^T y^k & 0 \\ 0 & {s^k}^T H_k s^k \end{pmatrix}^{-1} [y^k \;\; H_k s^k]^T$$

where

$$s^k = x^{k+1} - x^k \quad \text{and} \quad y^k = g^{k+1} - g^k.$$

Compact m-Step Representation

Nocedal, Byrd and Schnabel (1994)

$$H_{k+m} \;=\; H_k - [Y \;\; H_k S] \begin{pmatrix} -D & L^T \\ L & {s^k}^T H_k s^k \end{pmatrix}^{-1} [Y \;\; H_k S]^T$$

where

$$S = [s^k, \cdots, s^{k+m-1}], \qquad Y = [y^k, \cdots, y^{k+m-1}],$$

and

$$S^T Y = L + D + R$$

with L strictly lower triangular,
D diagonal, and
R strictly upper triangular.

Limited Memory BFGS Updating

$$H = \lambda I - \Psi\Gamma^{-1}\Psi^T.$$

where

$$\lambda = \frac{{y^k}^T y^k}{{s^k}^T y}, \qquad \Psi = [Y,\ \lambda S], \qquad \Gamma = \begin{bmatrix} -D & L^T \\ L & \lambda S^T S \end{bmatrix}_{2m\times 2m},$$

$$S^T Y = L + D + R$$

$$S = [s^{k_1}, \cdots, s^{k_m}], \qquad Y = [y^{k_1}, \cdots, y^{k_m}]$$

Typically, $m = 5$.
λ-scaling – an approximate Rayleigh quotient
Oren-Spedicato (1976), Phua-Shanno (1980), Barzilai-Borwein (1988).

The Trust-Region Subproblem

$$\begin{array}{ll} \min & (g^k)^T s + \frac{1}{2} s^T H_k s \\ \text{s.t.} & \|s\| \leq \Delta_k \end{array}$$

Apply Newton's method to find $\mu > 0$ so that

$$\phi(\mu) = 0$$

where

$$\phi(\mu) = \frac{1}{\Delta_k} - \frac{1}{\|s(\mu)\|} \qquad \text{and} \qquad s(\mu) = -(\mu I + H_k)^{-1} g^k \ .$$

$$\mu_+ = \mu - \frac{\phi(\mu)}{\phi'(\mu)}, \quad \text{where} \quad \phi'(\mu) = -\frac{g^T(\mu I + H)^{-3} g}{\|s(\mu)\|^3}.$$

(Our implementation avoids the *hard case*.)

Powers of $(\mu I + H)^{-1}$

$$(\mu I + H)^{-1} = \frac{1}{\tau}[I + \Psi(\tau\Gamma - \Psi^T\Psi)^{-1}\Psi^T]$$

$$(\mu I + H)^{-2} =$$

$$\frac{1}{\tau^2}[I + \Psi(\tau\Gamma - \Psi^T\Psi)^{-1}\Psi^T + \tau\Psi(\tau\Gamma - \Psi^T\Psi)^{-1}\Gamma(\tau\Gamma - \Psi^T\Psi)^{-1}\Psi^T],$$

where $\tau = \mu + \lambda$.

Triangular Factorization of $\tau\Gamma - \Psi^T\Psi$

Set

$$\hat{D} = (\mu + \lambda)D + Y^T Y, \quad \hat{W} = \lambda\mu S^T S, \quad \text{and} \quad \hat{L} = \mu L - \lambda(R + D).$$

Compute Cholesky factorizations

$$\begin{array}{rcl} \hat{D} & = & M M^T \\ \hat{W} + \hat{L}\hat{D}^{-1}\hat{L}^T & = & J J^T \end{array}$$

Then

$$\tau\Gamma - \Psi^T\Psi = \begin{bmatrix} M & 0 \\ -\hat{L}M^{-T} & J \end{bmatrix} \begin{bmatrix} -M^T & M^{-1}\hat{L}^T \\ 0 & J^T \end{bmatrix}.$$

The trust-region Newton iteration occurs entirely in dimension $2m$.
Cost $\approx O(mn)$ assuming $m^3 << n$.

Numerical Results

TEST SET: 24 problems from MINPACK-2 set, $2500 \leq n \leq 160,000$.

Termination Criteria:

$$f_{\text{best}} \sim \text{ best known function value.}$$

1. $|f^k - f_{\text{best}}| / \max(1, |f_{\text{best}}|) \leq \epsilon$.

2. $\text{nf} \geq 1000$.

Performance Profile: (Dolen and Moré 2001)

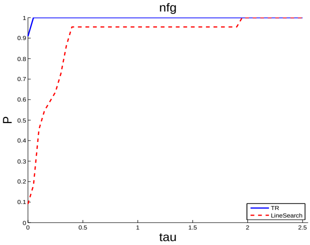
Given a problem set $\mathcal{P}$,

$$
\begin{aligned}
t_{i,s_j} &= \text{nfg(CPU time) of solving prob i by alg } s_j \\
r_{i,s_j} &= \frac{t_{i,s_j}}{\min_j t_{i,s_j}}.
\end{aligned}
$$

Set

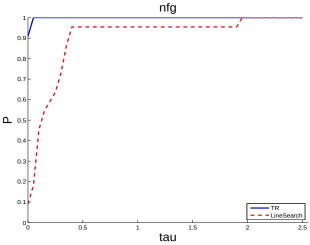
$$\rho_{s_j}(\tau) = \frac{1}{n_p}|\{i \in \mathcal{P} : r_{i,s_j} \leq \tau\}|.$$

Comparison of number of the function and gradient evaluations

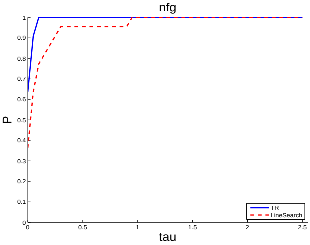


(a) relative accuracy 10^{-5}

Comparison of number of the function and gradient evaluations

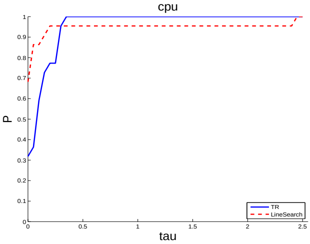


(c) relative accuracy 10^{-5}

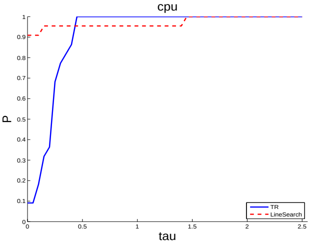


(d) relative accuracy 10^{-3}

Comparison of CPU time



(e) relative accuracy 10^{-5}



(f) relative accuracy 10^{-3}

More Implementation Details

Initialization: $x^0,\ g^0 = \nabla f(x^0),\ H_0 \succeq 0,\ 0 < \kappa < 1,\ 0 < \sigma < 1.$

Iteration:

1. Set $\bar{s} = -H_k^{-1} g^k$ and $r(\bar{s}) = \frac{f(x^k+\bar{s})-f(x^k)}{q(\bar{s})}$. (98% acceptance)

2. WHILE $r(\bar{s}) < \kappa$

   a. Let $\delta = \sigma \|\bar{s}\|$.

   b. Solve

$$\begin{array}{ll} \min & q(s) = s^T g^k + \frac{1}{2} s^T H_k s \\ \text{s.t.} & \qquad ||s|| \le \delta. \end{array}$$

   c. Compute $r(\bar{s}) = \frac{f(x^k+\bar{s})-f(x^k)}{q(\bar{s})}$.

   END WHILE

3. Set $x^{k+1} = x^k + \bar{s}$. Update H_{k+1}.

Minimization with bounded constraints

$$(\mathcal{P}) \qquad \min \qquad f(x)$$
$$l \le x \le u.$$

Active-set Trust-region Algorithm (ASTRAL).

We use an ℓ^∞ trust-region to conform with the constraint geometry.

$$\Omega = \{x \mid l \le x \le u\}, \quad \mathbb{B}_\infty = \{x \mid \|x\|_\infty \le 1\}$$

and

$$\Omega_k = \Omega \cap (x_k + \Delta_k \mathbb{B}_\infty) = \left\{x \,\middle|\, l^k \le x \le u^k \right\}.$$

Binding Constraints

Active Constraints

$$A(x) = \{i \mid x_i = l_i \text{ or } x_i = u_i\}$$

Binding Constraints

$$\mathcal{B}(x) = \left\{ i \;\middle|\; \begin{array}{c} x_i = l_i \text{ and } (\nabla f(x))_i > 0, \\ \text{or } x_i = u_i \text{ and } (\nabla f(x))_i < 0 \end{array} \right\}$$

Non-Binding Constraints

$$\mathcal{B}^c(x) = \{1, 2, \ldots, n\} \setminus \mathcal{B}(x), \qquad \nu(x) = |\mathcal{B}^c(x)|.$$

$\Phi(x)$ is an $n \times \nu(x)$ matrix whose columns are those of the identity matrix corresponding to the non-binding constraints $\mathcal{B}^c(x)$.

Active-set Trust-region Algorithm

1. Identify $\mathcal{B}(x^k)$ and set $\Phi_k = \Phi(x^k)$.

2. Set $\quad \tilde{H}_k = \Phi_k^T H_k \Phi_k, \quad \tilde{g}^k = \Phi_k^T g^k, \quad \tilde{l}^k = \Phi_k^T l^k,$ and $\tilde{u}^k = \Phi_k^T u^k$.

3. Solve trust-region subproblem

$$\begin{array}{ll} \min & \frac{1}{2} s^T \tilde{H}_k s + \tilde{g}^k s \\ \text{subject to} & \tilde{l}^k \leq s \leq \tilde{u}^k \end{array}$$

4. Form the ratio $r = \frac{f(x^k) - f(x^k + \bar{s})}{q_k(\bar{s})}$ and update.

Trust Region Sub-Probroblem Reduction

Let $\quad w = s - \tilde{l}^k, h = \tilde{u}^k - \tilde{l}^k.$

$$\begin{array}{ll} \min & \frac{1}{2}s^T\tilde{H}_k s + \tilde{g}^k s \\ \text{s.t.} & \tilde{l}^k \le s \le \tilde{u}^k \end{array} \equiv \begin{array}{ll} \min & \frac{1}{2}w^T\tilde{H}w + k^T w \\ \text{s.t.} & 0 \le w \le h. \end{array}.$$

Since $\tilde{H} = \Phi^T H \Phi$ is positive definite, this QP is convex.

We solve using an interior point algorithm.

$$W = \operatorname{diag}(w)$$

Interior Point Newton Equations

$$\begin{aligned}
p &= z - v - k - t\,U^{-1}e + U^{-1}V\,h + t\,W^{-1}e \\
r &= (\tilde{H} + U^{-1}V + W^{-1}Z)^{-1}p, \\
\Delta w &= -w + r \\
\Delta u &= -w + h - u - \Delta w, \\
\Delta v &= t\,U^{-1}e - v - U^{-1}V\,\Delta s, \\
\Delta z &= -W^{-1}Z\,\Delta w + t\,W^{-1}e - z.
\end{aligned}$$

$t =$ homotopy parameter.

$(\tilde{H} + U^{-1}V + W^{-1}Z)^{-1}$

$$\tilde{H} = \Phi^T H \Phi = \Phi^T(\lambda I - \Psi\Gamma^{-1}\Psi^T)\Phi$$

$$(\tilde{H} + U^{-1}V + W^{-1}Z)^{-1}$$
$$=$$
$$G^{-1} + G^{-1}(\Phi^T\Psi)\left[\Gamma - (\Phi^T\Psi)^T G^{-1}(\Phi^T\Psi)\right]^{-1}(\Phi^T\Psi)^T G^{-1}$$

where

$$G = \lambda I + U^{-1}V + W^{-1}Z.$$

Triangular Factorization

Write

$$\Gamma - (\Phi_k^T \Psi)^T G^{-1} (\Phi_k^T \Psi) = \begin{bmatrix} -\hat{D} & \hat{L}^T \\ \hat{L} & \hat{W} \end{bmatrix}.$$

Compute Cholesky factors

$$\hat{D} = MM^T \quad \text{and} \quad \hat{W} + \hat{L}\hat{D}^{-1}\hat{L}^T = JJ^T.$$

Then

$$\Gamma - (\Phi_k^T \Psi)^T G^{-1} (\Phi_k^T \Psi) = \begin{bmatrix} M & 0 \\ -\hat{L}M^{-T} & J \end{bmatrix} \begin{bmatrix} -M^T & M^{-1}\hat{L}^T \\ 0 & J^T \end{bmatrix}.$$

Numerical Results

TEST SET: 23 problems from CUTEr set. $n \geq 1000$.

21 problems have dimension ≥ 10000.

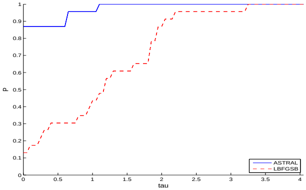
Termination Criteria: $f_{\text{best}} =$ best known function value.

1. $|f^k - f_{\text{best}}| / \max(1, |f_{\text{best}}|) \leq \epsilon$.

2. nf ≥ 1000.

Comparison of nfg between L-BFGS-B and ASTRAL

L-BFGS-B: Nocedal-Zhu-Byrd-Liu (1997)



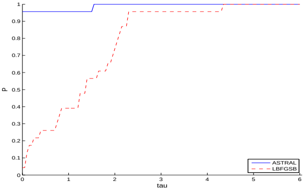


Figure 1a   Figure 1b

Figure 1a. Performance profiles, sum of the function and gradient evaluations, relative accuracy 10^{-5}. Figure 1b. Performance profiles, sum of the function and gradient evaluations, relative accuracy 10^{-3}.

Comparison of CPU time

Note that the average cost of each function evaluation in our test set is 0.002s, and the average cost of each gradient evaluation is 0.008s.

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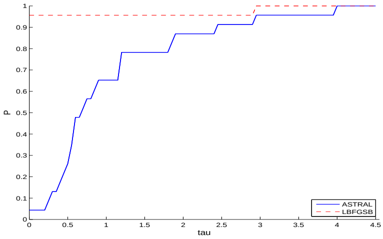

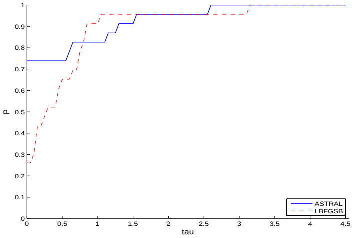

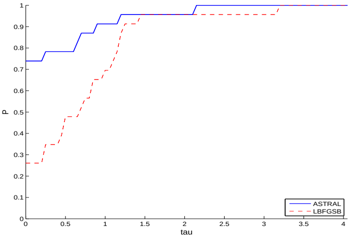

cpu(f) = 0.02s, cpu(g) = 0.08s

cpu(f) = 0.04s, cpu(g) = 0.16s

Thank You

Reference.

1. Limited Memory BFGS Updating in a Trust–Region Framework for Unconstrained Optimization, with James V. Burke, and Andreas Wiegmann.

2. ASTRAL: An Active Set l_∞-Trust-Region Algorithm for Box Constrained Optimization, with James V. Burke.

Literature Review:

Hager and Zhang(2006)

Zhang and Hager(2004)

Gilbert and Nocedal(1992)

Liu and Nocedal(1989)

Nash(1984)

Previous Work

- Hager and Zhang(2006)
- Birgin and Martínez(SPG, 2001, 2002)
- Lin and Moré(TRON, 1999)
- Coleman and Li(1994, 1996)
- Byrd, Lu, Norcedal, and Zhu(l-bfgsb, 1995, 1998)
- Conn, Gould, and Toint(1988)