Weighted Trust-Region Methods

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US & Mexico Workshop on Optimization and its Applications

January 9 -13th, 2023
Outline

Problem formulation

Method

Numerical Experiments

Conclusions
Problem Formulation

Nonlinear unconstrained optimization

$$\text{minimize } f(x) \quad x \in \mathbb{R}^n$$

where $$f : \mathbb{R}^n \to \mathbb{R}$$. 
Problem Formulation

Nonlinear unconstrained optimization

\[
\begin{align*}
\text{minimize} \quad & f(x) \\
\text{subject to} \quad & x \in \mathbb{R}^n
\end{align*}
\]

where \( f : \mathbb{R}^n \rightarrow \mathbb{R} \).

Assumptions:

- \( f \) is twice continuously differentiable
- Gradients \( \nabla f(x) \) are available
- Second derivatives are unavailable
Trust-Region Step

Iterates are updated in a trust-region method: \( x_{k+1} = x_k + s_k \)
Trust-Region Step

Iterates are updated in a trust-region method: $x_{k+1} = x_k + s_k$

A quadratic subproblem defines a step:

$$\arg\min_{\|s\| \leq \Delta_k} s^T g_k + \frac{1}{2} s^T B_k s$$

$$0 < \Delta_k \text{ (radius)}, \quad g_k = \nabla f(x_k), \quad B_k \text{ (symmetric } n \times n)$$
Trust-Region Step

Iterates are updated in a trust-region method: \( \mathbf{x}_{k+1} = \mathbf{x}_k + \mathbf{s}_k \)

A quadratic subproblem defines a step:

\[
\arg\min_{\mathbf{s}} \frac{1}{2} \mathbf{s}^\top \mathbf{B}_k \mathbf{s} + \mathbf{s}^\top \mathbf{g}_k \quad \text{s.t.} \quad \|\mathbf{s}\| \leq \Delta_k
\]

\( \mathbf{0} < \Delta_k \) (radius), \( \mathbf{g}_k = \nabla f(\mathbf{x}_k) \), \( \mathbf{B}_k \) (symmetric \( n \times n \))

Typical norms are the two-norm or infinity-norm.
Typical subproblem norms

\[ \| s \|_2 \leq \Delta_k \]

\[ \| s \|_\infty \leq \Delta_k \]

Computing the trust-region step is normally challenging.
Related Work

For efficiency, often approximate solutions to the trust-region subproblem are effective, with a family of methods:

[Moré and Sorenson, ’81]: Sequence of Cholesky factorizations

[Steihaug, ’83]: Truncated conjugate-gradient

[Gertz, ’04]: Infinity norm trust-region quasi-Newton

[Nocedal and Wright, ’06]: Dogleg method
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[Nocedal and Wright, ’06]: Dogleg method

Even these methods can be computationally intensive for large problems, or not applicable to indefinite subproblems.
Suppose a stable symmetric indefinite factorization is obtained

\[ B_k = L_k D_k L_k^T, \]

\( L_k \) is lower triangular with normalized columns, \( D_k \) is diagonal.
Method

Suppose a stable symmetric indefinite factorization is obtained

\[ B_k = L_k D_k L_k^\top, \]

where \( L_k \) is lower triangular with \textit{normalized columns}, \( D_k \) is diagonal.

\textbf{Properties:}

- \( D_k \) and \( B_k \) share the same inertia
- Solves with the factorization are efficient
- Effective rank-1 updates to the factorization
Use the factorization for a change of variable: \( \mathbf{v} = L_k^\top \mathbf{s} \) and

\[
\mathbf{s}^\top B_k \mathbf{s} = \mathbf{s}^\top L_k D_k L_k^\top \mathbf{s} = \mathbf{v}^\top D_k \mathbf{v}
\]

A diagonal Hessian in the new variables.
Use the factorization for a change of variable: \( v = L_k^T s \) and
\[
\begin{align*}
  s^T B_k s &= s^T L_k D_k L_k^T s = v^T D_k v \\
\end{align*}
\]

A diagonal Hessian in the new variables.

Consider the weighted norm
\[
\| v \| = \| L_k^T s \| \leq \Delta_k
\]
Use the factorization for a change of variable: $\mathbf{v} = L_k^T \mathbf{s}$ and

$$s^T B_k s = s^T L_k D_k L_k^T s = v^T D_k v$$

A diagonal Hessian in the new variables.

Consider the weighted norm

$$\|\mathbf{v}\| = \|L_k^T \mathbf{s}\| \leq \Delta_k$$

The trust-region subproblem simplifies this way.
Use the factorization for a change of variable: \( \mathbf{v} = L_k^\top \mathbf{s} \) and

\[
\mathbf{s}^\top B_k \mathbf{s} = \mathbf{s}^\top L_k D_k L_k^\top \mathbf{s} = \mathbf{v}^\top D_k \mathbf{v}
\]

A diagonal Hessian in the new variables.

Consider the weighted norm

\[
\|\mathbf{v}\| = \|L_k^\top \mathbf{s}\| \leq \Delta_k
\]

The trust-region subproblem simplifies this way.

Note: \( \mathbf{s}^\top \mathbf{g}_k = \mathbf{v}^\top L_k^{-1} \mathbf{g}_k \)
Method

The weighted trust-region subproblem (WTR)

\[
\min_{\|L_k^T s\| \leq \Delta_k} s^T g_k + \frac{1}{2} s^T B_k s = \min_{\|v\| \leq \Delta_k} v^T L_k^{-1} g_k + \frac{1}{2} v^T D_k v
\]
Method

The weighted trust-region subproblem (WTR)

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\min_{\|L_k^\top s\| \leq \Delta_k} s^\top g_k + \frac{1}{2} s^\top B_k s = \min_{\|v\| \leq \Delta_k} v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v
\]

Properties:

- The solution \( v_k \) to (WTR) can be found straightforwardly
- The step from a triangular solve \( s_k = L_k^{-\top} v_k \)
The weighted trust-region subproblem (WTR)

\[
\begin{align*}
\min_{\|L_k^T s\| \leq \Delta_k} & \quad s^T g_k + \frac{1}{2} s^T B_k s \\
& = \min_{\|v\| \leq \Delta_k} v^T L_k^{-1} g_k + \frac{1}{2} v^T D_k v
\end{align*}
\]

Properties:

- The solution \( v_k \) to (WTR) can be found straightforwardly
- The step from a triangular solve \( s_k = L_k^{-T} v_k \)

Different weighted norms are possible, e.g. \( \|L_k^T s\|_2 \) or \( \|L_k^T s\|_\infty \)
Weighted Subproblems: WTR

\[ \| L_k^T s \|_2 \leq \Delta_k \]

\[ \| L_k^T s \|_\infty \leq \Delta_k \]

Computing the weighted trust-region step \( L^T s_k = v_k \) is less challenging.
Solve the trust-region subproblem

\[
\text{minimize } v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v.
\]

\[
\|v\|_2 \leq \Delta_k
\]
Weighted L2 norm

Solve the trust-region subproblem

\[
\text{minimize } \left\| L_k^{-1} g_k + \frac{1}{2} v L_k^{-1} D_k v \right\|_2 \leq \Delta_k
\]

Find a pair \((v_k, \sigma_k)\) that satisfies the optimality conditions:

\[
\sigma_k \geq 0,
\]

\[
(D_k + \sigma_k I) \geq 0, \quad (D_k + \sigma_k I) v_k = -L_k^{-1} g_k, \quad \sigma_k(\|v_k\|_2 - \Delta_k) = 0
\]
Weighted L2 norm

Solve the trust-region subproblem

\[
\text{minimize } \|v\|_2^2 \leq \Delta_k \quad v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v.
\]

Find a pair \((v_k, \sigma_k)\) that satisfies the optimality conditions:

\[
\sigma_k \geq 0, \\
(D_k + \sigma_k I) \succeq 0, \quad (D_k + \sigma_k I)v_k = -L_k^{-1} g_k, \quad \sigma_k(\|v_k\|_2 - \Delta_k) = 0
\]

A 1D Newton iteration can efficiently determine \(\sigma_k\) and \(v_k\), since \(D_k\) is diagonal.
Weighted L2 norm

Solve the trust-region subproblem

\[
\minimize \quad v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v.
\]

\[
\|v\|_2 \leq \Delta_k
\]

Find a pair \((v_k, \sigma_k)\) that satisfies the optimality conditions:

\[
\sigma_k \geq 0,
\]

\[
(D_k + \sigma_k I) \succeq 0, \quad (D_k + \sigma_k I)v_k = -L_k^{-1} g_k, \quad \sigma_k (\|v_k\|_2 - \Delta_k) = 0
\]

A 1D Newton iteration can efficiently determine \(\sigma_k\) and \(v_k\), since \(D_k\) is diagonal.

Obtain the step from a triangular solve \(s_k = L_k^{-\top} v_k\).
Solve the trust-region subproblem

\[
\text{minimize } \|v\|_{\infty} \leq \Delta_k \quad v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v.
\]
Weighted INF norm

Solve the trust-region subproblem

\[ \begin{align*}
\text{minimize} & \quad v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v \\
\text{subject to} & \quad \|v\|_\infty \leq \Delta_k
\end{align*} \]

Note: Since $D_k$ is diagonal the problem is separable
Weighted INF norm

Solve the trust-region subproblem

$$\min_{\|v\|_\infty \leq \Delta_k} \, v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v.$$  

Note: Since $D_k$ is diagonal the problem is separable

The **analytic solution**, when $D_k$ is positive definite is

$$(v_k)_i = \min(\Delta_k, \max(-\Delta_k, -(D_k^{-1} L_k^{-1} g_k)_i))$$
Weighted INF norm

Solve the trust-region subproblem

\[
\begin{align*}
\text{minimize} \quad & v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v \\
\text{subject to} \quad & \|v\|_\infty \leq \Delta_k
\end{align*}
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Weighted INF norm

Solve the trust-region subproblem

$$\minimize \ v^\top L_k^{-1} g_k + \frac{1}{2} v^\top D_k v.$$  
$$\|v\|_\infty \leq \Delta_k$$

Note: Since $D_k$ is diagonal the problem is separable

The analytic solution, when $D_k$ is positive definite is

$$(v_k)_i = \min(\Delta_k, \max(-\Delta_k, -(D_k^{-1} L_k^{-1} g_k)_i))$$

Obtain the step from a triangular solve $s_k = L_k^{-\top} v_k$.

(An analytic solution is also found when $D_k$ is indefinite)
Theoretical Bounds

Bounds of the weighted norms: $\|L_k^T s\|_2$ and $\|L_k^T s\|_\infty$
Theoretical Bounds

Bounds of the weighted norms: $\|L_k^T s\|_2$ and $\|L_k^T s\|_\infty$

Lower triangular matrix with normalized columns

\[
L_k^T = \begin{bmatrix}
l_{11} & l_{21} & l_{31} & l_{41} \\
l_{22} & l_{32} & l_{42} \\
l_{33} & l_{43} \\
1
\end{bmatrix}, \quad \text{diag}(L_k^T L_k) = I
\]
Theoretical Bounds

Bounds of the weighted norms: \( \|L_k^\top s\|_2 \) and \( \|L_k^\top s\|_\infty \)

Lower triangular matrix with normalized columns

\[
L_k^\top = \begin{bmatrix}
l_{11} & l_{21} & l_{31} & l_{41} \\
l_{22} & l_{32} & l_{42} & \\
l_{33} & l_{43} & \\
1 & \\
\end{bmatrix}, \quad \text{diag}(L_k^\top L_k) = I
\]

For \( \sigma_1 \) the smallest singular value of \( L_k \) then

\[
\sigma_1 \|s\|_2 \leq \|L_k^\top s\|_2 \leq \sqrt{n} \|s\|_2, \\
|s_n| \leq \|L_k^\top s\|_\infty \leq n \|s\|_\infty
\]
Implementation

The Hessian is estimated by a BFGS matrix.

\[
B_{k+1} = B_k - \frac{1}{\mathbf{s}_k^\top B_k \mathbf{s}_k} B_k \mathbf{s}_k \mathbf{s}_k^\top B_k + \frac{1}{\mathbf{s}_k^\top \mathbf{y}_k} \mathbf{y}_k \mathbf{y}_k^\top
\]

Here, \( \mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k \), \( \mathbf{y}_k = \mathbf{g}_{k+1} - \mathbf{g}_k \) and \( \mathbf{s}_k^\top \mathbf{y}_k > 0 \) ensures positive definiteness.
Implementation

The Hessian is estimated by a BFGS matrix.

\[
B_{k+1} = B_k - \frac{1}{s_k^T B_k s_k} B_k s_k s_k^T B_k + \frac{1}{s_k^T y_k} y_k y_k^T
\]

Here, \( s_k = x_{k+1} - x_k \), \( y_k = g_{k+1} - g_k \) and \( s_k^T y_k > 0 \) ensures positive definiteness.

[Gill, Saunders et al., ’74]: Updates for the factorization

\[
L_{k+1} D_{k+1} L_{k+1}^T = L_k D_k L_k^T - [\text{rank-1}] + [\text{rank-1}]
\]
Implementation

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[Gill, Saunders et al., ’74]: Updates for the factorization

\[
L_{k+1} D_{k+1} L_{k+1}^T = L_k D_k L_k^T - [\text{rank-1}] + [\text{rank-1}]
\]

Other Hessian estimates (e.g., SR1) are possible.
Example: Rosenbrock 2D function
\[ f(x_0) = 8 \]
$f(x_0) = 8$
$f(x_1) = 1.58$
$f(x_2) = 1.02$
WTR-L2

\[ f(x_3) = 0.417 \]
$f(x_3) = 0.417$
WTR-L2

\[ f(x_4) = 0.318 \]
$f(x_4) = 0.318$
$f(x_5) = 0.0881$
$f(x_5) = 0.0881$
$f(x_7) = 0.00213$
$f(x_7) = 0.00213$
$f(x_8) = 7e^{-0.5}$
\[ f(x_8) = 7e - 05 \]
WTR-L2

\[ f(x_9) = 1.71e^{-07} \]
The function $f(x_9) = 1.71e^{-07}$ is depicted on a 2D plot with axes $x_1$ and $x_2$. The plot shows the contour lines and a shaded region indicating the function's behavior in a 2-dimensional space.
$f(x_9) = 1.71e - 07$
$f(x_{10}) = 9.28e - 10$
$f(x_{10}) = 9.28e - 10$
$f(x_{11}) = 1.86e - 15$
Additional Settings

A. If $d_n/d_1 \geq 10^{16}$ restart
   (conditioning)

B. Skip update if $s_k^T y_k < 0$
   If $\geq 20$ consecutive skips restart
   (definiteness)

C. If $\|g_k\| / \|g_{RST}\| \leq 10^{-2}$ and
   $\left( \frac{|\gamma_k|}{|\gamma_{RST}|} \geq 10 \text{ or } \frac{|\gamma_k|}{|\gamma_{RST}|} \leq 10^{-1} \right)$ restart
   (only for large problems, i.e., $n > 1000$)
   (scaling)

D. Initialization $\gamma_k I = B_0$ on restart $\gamma_k = \frac{\|g_k\|}{\alpha_k}$
   $\alpha_k$ is the step size of a line search after restart
Additional Settings

Count near:

If $\Delta_k \leq 10^{-4} \times \epsilon$ and

$$\|g_k\|_2 \leq 5 \times 10^{-8} \|g_0\|_2$$

or

$$|f_k| \leq 5 \times 10^{-11} |f_0|$$

or

$$\|g_k\|_2 \leq \sqrt{n} \times \epsilon$$

Parameters:

maxiter = 15000, $\epsilon = 10^{-4}$, optimal if $\|g_k\|_2 < \epsilon$
Additional Settings

Count near:

If $\Delta_k \leq 10^{-4} \times \epsilon$ and

$$\|g_k\|_2 \leq 5 \times 10^{-8} \|g_0\|_2$$

or

$$|f_k| \leq 5 \times 10^{-11} |f_0|$$

or

$$\|g_k\|_2 \leq \sqrt{n} \times \epsilon$$

Parameters:

$maxiter = 15000, \quad \epsilon = 10^{-4}, \quad \text{optimal if } \|g_k\|_2 < \epsilon$

Experiments on 250 CUTEst problems
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<th>Problem</th>
<th>(n)</th>
<th>Iter</th>
<th>(nF)</th>
<th>Time</th>
<th>Optimal</th>
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250 CUTEst Problems

Time

\[ \rho_s(\tau) \]

\[ \tau \]

-WTR INF
-WTR L2

WOA 23 | johannesbrust.com | 53 of 58
250 CUTEst Problems

Function Evaluations

\[ \rho_s(\tau) \]

- WTR INF
- WTR L2

\( \tau \)
Conclusions

- Symmetric indefinite factorization of the Hessian approximation
- Weighted L-2 and L-INF norms
- Effective subproblem solutions in the weighted norms
- Method can be robust for large class of problems

Future extension can be a trust-region line-search combination
References


References


Thank you
Extra: Line-search comparison

The graph shows the comparison of function evaluations for different line-search methods as a function of $\tau$. The blue line represents the WOLFE LS method, while the red line represents the WTR L2 method. The x-axis represents $\tau$, and the y-axis represents $\rho_s(\tau)$. The graph illustrates the performance of both methods across various $\tau$ values.
Extra: Line-search comparison

![Graph showing line-search comparison]

- **ρ_s(τ)**
- **Time**
- **WOA 23 | johannesbrust.com**

**Legend:**
- **WOLFE LS**
- **WTR L2**