$R$-Linear Convergence of Limited Memory Steepest Descent

Frank E. Curtis, Lehigh University

joint work with

Wei Guo, Lehigh University

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Outline

Introduction

Limited Memory Steepest Descent (LMSD)

*R*-Linear Convergence of LMSD

Numerical Demonstrations

Summary
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Introduction

Limited Memory Steepest Descent (LMSD)

$R$-Linear Convergence of LMSD

Numerical Demonstrations

Summary
Consider the unconstrained optimization problem

$$\min_{x \in \mathbb{R}^n} f(x), \text{ where } f : \mathbb{R}^n \to \mathbb{R} \text{ is } C^1.$$ 

Let us focus exclusively on a steepest descent framework:

**Algorithm SD  Steepest Descent**

**Require:** $x_1 \in \mathbb{R}^n$

1: for $k \in \mathbb{N}$ do 
2: Compute $g_k \leftarrow \nabla f(x_k)$
3: Choose $\alpha_k \in (0, \infty)$
4: Set $x_{k+1} \leftarrow x_k - \alpha_k g_k$
5: end for

All that remains to be determined are the stepsizes $\{\alpha_k\}$. 

$R$-Linear Convergence of Limited Memory Steepest Descent
Minimizing strongly convex quadratics

Suppose \( f(x) = \frac{1}{2} x^T A x - b^T x \), where \( A \) has eigenvalues \( \lambda_n \geq \cdots \geq \lambda_1 > 0 \).

Convergence (rate) of the algorithm depends on choices for \( \{\alpha_k\} \).
Suppose $f(x) = \frac{1}{2} x^T A x - b^T x$, where $A$ has eigenvalues $\lambda_n \geq \cdots \geq \lambda_1 > 0$.

Choosing $\alpha_k \leftarrow 1/\lambda_n$ leads to $Q$-linear convergence with constant $(1 - \lambda_1/\lambda_n)$. 

![Diagram showing eigenvalue distribution with 0, 1/\lambda_n, 1/\lambda_1 markers.](image)
Minimizing strongly convex quadratics

Suppose $f(x) = \frac{1}{2} x^T A x - b^T x$, where $A$ has eigenvalues $\lambda_n \geq \cdots \geq \lambda_1 > 0$.

...but certain “components” of the gradient vanish in a larger range.
Minimizing strongly convex quadratics

Suppose $f(x) = \frac{1}{2} x^T A x - b^T x$, where $A$ has eigenvalues $\lambda_n \geq \cdots \geq \lambda_1 > 0$.

Goal: Allow large stepsizes, shrink range (automatically) to catch entire gradient.
Consider Fletcher’s limited memory steepest descent (LMSD) method.

- Extends the Barzilai-Borwein (BB) “two-point stepsize strategy”.
- BB methods known to have $R$-linear convergence rate; Dai and Liao (2002).
- We prove that LMSD also attains $R$-linear convergence.

Although proved convergence rate is not necessarily better than that for BB, one can see reasons for improved empirical performance.
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**Decomposition**

\[
\begin{align*}
\min_{x \in \mathbb{R}^n} f(x), \quad \text{where} \quad f(x) &= \frac{1}{2} x^T A x - b^T x \\
\end{align*}
\]

Let \( A \) have the eigendecomposition \( A = Q \Lambda Q^T \), where

\[
Q = \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix} \quad \text{is orthogonal}
\]

and \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \) with \( \lambda_n \geq \cdots \geq \lambda_1 > 0 \).
Decomposition

\[
\min_{x \in \mathbb{R}^n} f(x), \quad \text{where} \quad f(x) = \frac{1}{2} x^T Ax - b^T x
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Let \( A \) have the eigendecomposition \( A = Q\Lambda Q^T \), where

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and \( \Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n) \) with \( \lambda_n \geq \cdots \geq \lambda_1 > 0 \).

Let \( g := \nabla f \). For any \( x \in \mathbb{R}^n \), the gradient of \( f \) at \( x \) can be expressed as

\[
g(x) = \sum_{i=1}^{n} d_i q_i, \quad \text{where} \quad d_i \in \mathbb{R} \quad \text{for all} \quad i \in [n] := \{1, \ldots, n\}.
\]
Recursion

Let $g := \nabla f$. For any $x \in \mathbb{R}^n$, the gradient of $f$ at $x$ can be expressed as

$$g(x) = \sum_{i=1}^{n} d_i q_i, \quad \text{where} \quad d_i \in \mathbb{R} \quad \text{for all} \quad i \in [n] := \{1, \ldots, n\}. \quad (1)$$
Recursion

Let $g := \nabla f$. For any $x \in \mathbb{R}^n$, the gradient of $f$ at $x$ can be expressed as

$$g(x) = \sum_{i=1}^{n} d_i q_i,$$

where $d_i \in \mathbb{R}$ for all $i \in [n] := \{1, \ldots, n\}$. \hfill (1)

If $x^+ \leftarrow x - \alpha g(x)$, then the weights satisfy the recursive property:

$$d_i^+ = (1 - \alpha \lambda_i) d_i \quad \text{for all} \quad i \in [n].$$
Recursion

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Proof (Sketch).

Since $g(x) = Ax - b$,

$$x^+ = x - \alpha g(x)$$

$$Ax^+ = Ax - \alpha g(x)$$

$$g(x^+) = (I - \alpha A)g(x)$$

$$g(x^+) = (I - \alpha Q \Lambda Q^T)g(x),$$

then decompose according to (1).
Recursion

Let \( g := \nabla f \). For any \( x \in \mathbb{R}^n \), the gradient of \( f \) at \( x \) can be expressed as

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g(x) = \sum_{i=1}^{n} d_i q_i, \quad \text{where} \quad d_i \in \mathbb{R} \quad \text{for all} \quad i \in [n] := \{1, \ldots, n\}. \quad (1)
\]

If \( x^+ \leftarrow x - \alpha g(x) \), then the weights satisfy the recursive property:

\[
d_i^+ = (1 - \alpha \lambda_i) d_i \quad \text{for all} \quad i \in [n].
\]

Proof (Sketch). Since \( g(x) = Ax - b \),

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\begin{align*}
x^+ &= x - \alpha g(x) \\
Ax^+ &= Ax - \alpha g(x) \\
g(x^+) &= (I - \alpha A)g(x) \\
g(x^+) &= (I - \alpha Q \Lambda Q^T)g(x),
\end{align*}
\]

then decompose according to (1).

Idea: Choose stepsizes as reciprocals of (estimates of) eigenvalues of \( A \).
Fletcher (2012):

- Repeated cycles (or “sweeps”) of $m$ iterations.
- At start of $(k+1)$st cycle, suppose one has the $k$th cycle values in $G_k := [g_{k,1}, \ldots, g_{k,m}]$ corresponding to $\{x_{k,1}, \ldots, x_{k,m}\}$.
- Iterate displacements lie in Krylov sequence initiated from $g_{k,1}$. 

LMSD method: Main idea
Fletcher (2012):

- Repeated cycles (or “sweeps”) of \( m \) iterations.
- At start of \((k+1)\)st cycle, suppose one has the \( k \)th cycle values in

\[
G_k := \begin{bmatrix} g_{k,1} & \cdots & g_{k,m} \end{bmatrix} \text{ corresponding to } \{x_{k,1}, \ldots, x_{k,m}\}.
\]

- Iterate displacements lie in Krylov sequence initiated from \( g_{k,1} \).
- Performing a QR decomposition to obtain

\[
G_k = Q_k R_k,
\]

one obtains \( m \) eigenvalue estimates (Ritz values) as eigenvalues of

\[
(T_k \leftarrow Q_k^T A Q_k,
\]

which are contained in the spectrum of \( A \) in an optimal sense (more later).
- One can also obtain these estimates more cheaply and with less storage...
LMSD method: Efficient eigenvalue estimation

Storing the \( k \)th cycle reciprocal stepsizes in

\[
J_k \leftarrow \begin{bmatrix}
\alpha_{k,1}^{-1} \\
-\alpha_{k,1}^{-1} & \ddots \\
& \ddots & \ddots \\
& & -\alpha_{k,m}^{-1} & \alpha_{k,m}^{-1} \\
& & & -\alpha_{k,m}^{-1}
\end{bmatrix},
\]

one finds that by computing the (partially extended) Cholesky factorization

\[
G_k^T \begin{bmatrix} G_k & g_{k,m+1} \end{bmatrix} = R_k^T \begin{bmatrix} R_k & r_k \end{bmatrix},
\]

one has

\[
T_k \leftarrow \begin{bmatrix} R_k & r_k \end{bmatrix} J_k R_k^{-1}.
\]

Long story short: One can obtain Ritz values (and stepsizes) in \( \sim \frac{1}{2} m^2 n \) flops

- ... and this is done only once every \( m \) steps.
- Hence, costs \( \mathcal{O}(mn) \) per iteration, like limited memory quasi-Newton.
Algorithm LMSD  Limited Memory Steepest Descent

Require: \( x_{1,1} \in \mathbb{R}^n \), \( m \in \mathbb{N} \), and \( \epsilon \in \mathbb{R}_+ \)
1: Choose stepsizes \( \{\alpha_{1,j}\}_{j \in [m]} \subset \mathbb{R}_+ \)
2: Compute \( g_{1,1} \leftarrow \nabla f(x_{1,1}) \)
3: if \( \|g_{1,1}\| \leq \epsilon \), then return \( x_{1,1} \)
4: for \( k \in \mathbb{N} \) do
5: \hspace{1em} for \( j \in [m] \) do
6: \hspace{2em} Set \( x_{k,j+1} \leftarrow x_{k,j} - \alpha_{k,j} g_{k,j} \)
7: \hspace{2em} Compute \( g_{k,j+1} \leftarrow \nabla f(x_{k,j+1}) \)
8: \hspace{2em} if \( \|g_{k,j+1}\| \leq \epsilon \), then return \( x_{k,j+1} \)
9: \hspace{1em} end for
10: Set \( x_{k+1,1} \leftarrow x_{k,m+1} \) and \( g_{k+1,1} \leftarrow g_{k,m+1} \)
11: Set \( G_k \) and \( J_k \)
12: Compute \( (R_k, r_k) \), then compute \( T_k \)
13: Compute \( \{\theta_{k,j}\}_{j \in [m]} \subset \mathbb{R}_+ \) as the eigenvalues of \( T_k \)
14: Compute \( \{\alpha_{k+1,j}\}_{j \in [m]} \leftarrow \{\theta_{k,j}^{-1}\}_{j \in [m]} \subset \mathbb{R}_+ \)
15: end for

(Note: There is also a version using harmonic Ritz values.)
Known convergence properties

BB methods ($m = 1$):
- $R$-superlinear when $n = 2$; Barzilai and Borwein (1988)
- Convergent for any $n$ from any starting point; Raydan (1993)
- $R$-linear for any $n$; Dai and Liao (2002)

LMSD methods ($m \geq 1$):
- Convergent for any $n$ from any starting point; Fletcher (2012)
- Prior to our work: Convergence rate not yet analyzed.
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\textit{R-Linear Convergence of LMSD}

Numerical Demonstrations

Summary
Basic Assumptions

Assumption 1

(i) Algorithm LMSD is run with $\epsilon = 0$ and $g_{k,j} \neq 0$ for all $(k, j) \in \mathbb{N} \times [m]$.

(ii) For all $k \in \mathbb{N}$, the matrix $G_k$ has linearly independent columns. Further, there exists $\rho \in [1, \infty)$ such that, for all $k \in \mathbb{N}$,

$$\|R_k^{-1}\| \leq \rho\|g_{k,1}\|^{-1}. \tag{2}$$

To justify (2), note that when $m = 1$, one has

$$Q_k R_k = G_k = g_{k,1} \quad \text{where} \quad Q_k = g_{k,1}/\|g_{k,1}\| \quad \text{and} \quad R_k = \|g_{k,1}\|.$$

Hence, (2) holds with $\rho = 1$. 
**Lemma 2**

*For all $k \in \mathbb{N}$, the eigenvalues of $T_k$ satisfy*

$$\theta_{k,j} \in [\lambda_{m+1-j}, \lambda_{n+1-j}] \subseteq [\lambda_1, \lambda_n] \text{ for all } j \in [m].$$

Recall...

We essentially prove that...

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**Introduction**

LMSD Method

*R-Linear Convergence*

Numerics

Summary
Worst-case “blow-up” of weights over a cycle

Lemma 3

For each \((k, j, i) \in \mathbb{N} \times [m] \times [n]\):

\[
|d_{k,j+1,i}| \leq \delta_{j,i} |d_{k,j,i}| \quad \text{where} \quad \delta_{j,i} := \max \left\{ \left| 1 - \frac{\lambda_i}{\lambda_{m+1-j}} \right|, \left| 1 - \frac{\lambda_i}{\lambda_{n+1-j}} \right| \right\}.
\]

Hence, for each \((k, j, i) \in \mathbb{N} \times [m] \times [n]\):

\[
|d_{k+1,j,i}| \leq \Delta_i |d_{k,j,i}| \quad \text{where} \quad \Delta_i := \prod_{j=1}^{m} \delta_{j,i}.
\]

Furthermore, for each \((k, j, p) \in \mathbb{N} \times [m] \times [n]\):

\[
\sqrt{\sum_{i=1}^{p} d_{k,j+1,i}^2} \leq \hat{\delta}_{j,p} \sqrt{\sum_{i=1}^{p} d_{k,j,i}^2} \quad \text{where} \quad \hat{\delta}_{j,p} := \max_{i \in [p]} \delta_{j,i},
\]

while, for each \((k, j) \in \mathbb{N} \times [m]\):

\[
\|g_{k+1,j}\| \leq \Delta \|g_{k,j}\| \quad \text{where} \quad \Delta := \max_{i \in [n]} \Delta_i.
\]
Q-linear convergence of weight $i = 1$

Lemma 4

If $\Delta_1 = 0$, then $d_{1+\hat{k},\hat{j},1} = 0$ for all $(\hat{k}, \hat{j}) \in \mathbb{N} \times [m]$. Otherwise, if $\Delta_1 > 0$, then:

(i) for $(k, j) \in \mathbb{N} \times [m]$ with $d_{k,j,1} = 0$, it follows that $d_{k+\hat{k},\hat{j},1} = 0$ for all $(\hat{k}, \hat{j}) \in \mathbb{N} \times [m]$;

(ii) for $(k, j) \in \mathbb{N} \times [m]$ with $|d_{k,j,1}| > 0$ and any $\epsilon_1 \in (0, 1)$, it follows that

$$\frac{|d_{k+\hat{k},\hat{j},1}|}{|d_{k,j,1}|} \leq \epsilon_1 \quad \text{for all } \hat{k} \geq 1 + \left\lceil \frac{\log \epsilon_1}{\log \Delta_1} \right\rceil \quad \text{and } \hat{j} \in [m].$$
Lemma 5

For all \((k, j) \in \mathbb{N} \times [m]\), let \(q_{k,j} \in \mathbb{R}^m\) denote the unit eigenvector corresponding to the eigenvalue \(\theta_{k,j}\) of \(T_k\), i.e., that with \(T_k q_{k,j} = \theta_{k,j} q_{k,j}\) and \(\|q_{k,j}\| = 1\). Then, defining

\[
D_k := \begin{bmatrix}
d_{k,1,1} & \cdots & d_{k,m,1} \\
\vdots & \ddots & \vdots \\
d_{k,1,n} & \cdots & d_{k,m,n}
\end{bmatrix} \quad \text{and} \quad c_{k,j} := D_k R_k^{-1} q_{k,j},
\]

it follows that, with the diagonal matrix of eigenvalues (namely, \(\Lambda = Q^T A Q\)),

\[
\theta_{k,j} = c_{k,j}^T \Lambda c_{k,j} \quad \text{and} \quad c_{k,j}^T c_{k,j} = 1.
\]
“If first $p$ weights small, then bound for weight $p + 1$...”

(We express $\hat{\delta}_p \in [1, \infty)$ dependent only on $m$, $p$, and the spectrum of $A$.)

**Lemma 6 (simplified)**

For any $(k, p) \in \mathbb{N} \times [n - 1]$, if there exists $(\epsilon_p, K_p) \in (0, \frac{1}{2\delta_p \rho}) \times \mathbb{N}$ with

$$
\sum_{i=1}^{p} d_{k+\hat{k},1,i}^2 \leq \epsilon_p^2 \|g_{k,1}\|^2 \quad \text{for all } \hat{k} \geq K_p,
$$

then there exists $K_{p+1} \geq K_p$ dependent only on $\epsilon_p$, $\rho$, and the spectrum of $A$ with

$$
d_{k+K_{p+1},1,p+1}^2 \leq 4\hat{\delta}_p^2 \rho^2 \epsilon_p^2 \|g_{k,1}\|^2;
$$

**Proof (Key step).**

First $p$ elements of $c_{k+\hat{k},j}$ small enough such that

$$
\theta_{k+\hat{k},j} = \sum_{i=1}^{n} \lambda_i c_{k+\hat{k},j,i}^2 \geq \frac{3}{4} \lambda_{p+1} \quad \text{for } \hat{k} \geq K_p \quad \text{and } j \in [m].
$$
“If first \( p \) weights small, then bound for all first \( p + 1 \) weights...”

Lemma 7

For any \((k, p) \in \mathbb{N} \times [n - 1]\), if there exists \((\epsilon_p, K_p) \in (0, \frac{1}{2\delta_p \rho}) \times \mathbb{N}\) with

\[
\sum_{i=1}^{p} d_{k+\hat{k},1,i}^2 \leq \epsilon_p^2 \|g_{k,1}\|^2 \quad \text{for all } \hat{k} \geq K_p,
\]

then, with \(\epsilon_{p+1}^2 := (1 + 4 \max\{1, \Delta^4_{p+1}\} \delta_p^2 \rho^2) \epsilon_p^2\) and \(K_{p+1} \in \mathbb{N}\),

\[
\sum_{i=1}^{p+1} d_{k+\hat{k},1,i}^2 \leq \epsilon_{p+1}^2 \|g_{k,1}\|^2 \quad \text{for all } \hat{k} \geq K_{p+1}.
\]
Lemma 8

There exists $K \in \mathbb{N}$ dependent only on the spectrum of $A$ such that

$$\|g_{k+K,1}\| \leq \frac{1}{2} \|g_{k,1}\| \text{ for all } k \in \mathbb{N}.$$ 

Theorem 9

The sequence $\{\|g_{k,1}\|\}$ vanishes $R$-linearly in the sense that

$$\|g_{k,1}\| \leq c_1 c_2^k \|g_{1,1}\|,$$

where

$$c_1 := 2\Delta^{K-1} \text{ and } c_2 := 2^{-1/K} \in (0, 1).$$
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Numerical demonstrations with $n = 100$: $m = 1$ and $m = 5$

Figure: $\{\lambda_1, \ldots, \lambda_{100}\} \subset [1, 1.9]$
Numerical demonstrations with $n = 100$: $m = 1$ and $m = 5$

Figure: $\{\lambda_1, \ldots, \lambda_{100}\} \subset [1, 100]$
Numerical demonstrations with $n = 100$: $m = 1$ and $m = 5$

Figure: $\{\lambda_1, \ldots, \lambda_{100}\} \subset 5$ clusters, $m = 5$
Numerical demonstrations with $n = 100$: $m = 1$ and $m = 5$

Figure: $\{\lambda_1, \ldots, \lambda_{100}\} \subset 2$ clusters (low heavy), $m = 5$
Numerical demonstrations with $n = 100$: $m = 1$ and $m = 5$

Figure: $\{\lambda_1, \ldots, \lambda_{100}\} \subset 2$ clusters (high heavy), $m = 5$
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