# Adaptive Gradient Sampling Algorithms for Nonconvex Nonsmooth Optimization

**Frank E. Curtis**, Lehigh University

joint work with

**Xiaocun Que**, Lehigh University

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# Outline

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# Context

Much research today is focused on solving structured optimization problems

- structure often means convex
- seeking sparsity, low matrix rank, low total variation, etc.

This talk focuses on solving unstructured problems

- problems may be nonconvex
- general-purpose algorithms are needed

# Context

Much research today is focused on solving structured optimization problems

- structure often means convex
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This talk focuses on solving unstructured problems

- problems may be nonconvex
- general-purpose algorithms are needed

We propose stochastic methods for deterministic optimization

- No gradient info? e.g., simulation-based optimization
- Only some gradient info? e.g., machine learning
- Only some subdifferential info? e.g., (un)structured nonsmooth optimization

Good theory, computational flexibility, etc.

# Background

Quasi-Newton methods, e.g., BFGS

- general-purpose for smooth optimization
- "first-order" method, i.e., gradients only
- superlinear convergence

} Broyden (1970)
Fletcher (1970)
Goldfarb (1970)
Shanno (1970)

- good performance on nonsmooth problems
- . . . but little in terms of convergence guarantees

} Lemaréchal (1981)
Lukšan & Vlček (1999, 2001)
Lewis & Overton (2013)

Gradient sampling (GS)

- general-purpose for nonsmooth optimization
- "first-order" method
- global convergence guarantees (w.p.1)
- good performance in practice
- . . . but expensive! $\mathcal{O}(n)$ gradients per iteration

} Burke, Lewis, & Overton (2005)
Kiwiel (2007)

## Contributions

New general-purpose methods for nonconvex nonsmooth optimization

- adaptive sampling, $\Omega(1)$ gradients per iteration
- Hessian approximation strategies
- convergence guarantees (w.p.1)
- dramatically reduced per-iteration & overall cost

} Curtis & Que (2013)

- BFGS-based strategy
- adaptive sampling, $\mathcal{O}(1)$ gradients per iteration
- convergence guarantees (w.p.1)
- further empirical improvements
- `BFGS-GS` software (C++)

} Curtis & Que (2015)

# Outline

# Problem formulation

Consider optimization problems of the form:

$$\boxed{\min_{x \in \mathbb{R}^n} \; f(x)}$$

## Assumption 1

*The objective function $f$ is*

- *locally Lipschitz in $\mathbb{R}^n$*
- *continuously differentiable in an open, dense subset $\mathcal{D}$ of $\mathbb{R}^n$*

A point $x$ is stationary if

$$0 \in \partial f(x) := \bigcap_{\epsilon > 0} \operatorname{cl}\operatorname{conv} \nabla f(\mathbb{B}_\epsilon(x) \cap \mathcal{D}).$$

A point $x$ is $\epsilon$-stationary if

$$0 \in \partial_\epsilon f(x) := \operatorname{cl}\operatorname{conv} \partial f(\mathbb{B}_\epsilon(x)).$$

# GS idea

At $x_k$, let $x_{k0} := x_k$ and sample $\{x_{k1}, \ldots, x_{kp}\} \subset \mathbb{B}_{\epsilon_k}(x_k) \cap \mathcal{D}$, yielding:

$$\begin{array}{lllllllll} X_k & := & \{ & x_{k0}, & x_{k1}, & \cdots, & x_{kp} & \} & \text{(sample points)} \\ G_k & := & [ & g_{k0} & g_{k1} & \cdots & g_{kp} & ] & \text{(sample gradients)} \end{array}$$

The $\epsilon_k$-subdifferential is approximated by the convex hull of sampled gradients:

$$\begin{aligned} \partial_{\epsilon_k} f(x_k) &= \operatorname{cl} \operatorname{conv} \partial f(\mathbb{B}_{\epsilon_k}(x_k)) \\ &\approx \operatorname{conv}\{g_{k0}, g_{k1}, \ldots, g_{kp}\} \end{aligned}$$

Define the projection of the origin onto the convex hull of sampled gradients:

$$\boxed{g_k := \operatorname{Proj}(0 | \operatorname{conv}\{g_{k0}, g_{k1}, \ldots, g_{kp}\})}$$

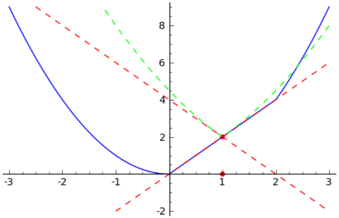
The vector $d_k = -g_k$ is an approximate $\epsilon_k$-steepest descent step.

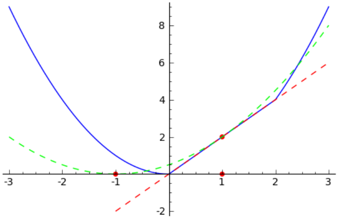
# GS step computation

Alternatively, one can view $d_k$ as the minimizer of a piecewise quadratic model:

$$\max_{(z,d)\in\mathbb{R}\times\mathbb{R}^n} \; z + \tfrac{1}{2}\|d\|_2^2 \quad \text{s.t. } f(x_k)e + G_k^T d \le ze \qquad \underbrace{\Leftrightarrow}_{\text{primal/dual}} \qquad \max_{y\in\mathbb{R}^{p+1}} \; f(x_k) - \tfrac{1}{2}\|G_k y\|_2^2 \quad \text{s.t. } e^T y = 1,\; y \ge 0$$

Figure: Sampling yielding a small/zero step (left) vs. nonzero step (right)



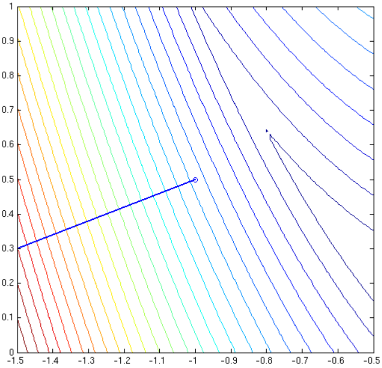



# GS illustration

Example: nonsmooth Rosenbrock

$$\min_{x \in \mathbb{R}^2} \; 10|x_{(2)} - x_{(1)}^2| + (1 - x_{(1)})^2 \;\; \text{at } x_k = (-1, \tfrac{1}{2})$$

Figure: Without gradient sampling (left) and with gradient sampling (right)



# GS algorithm

**Algorithm 1** Gradient Sampling (GS) Algorithm

**Require:**

initial point $x_0 \in \mathbb{R}^n$, initial sampling radius $\epsilon_0 > 0$

sufficient decrease tolerance $\eta_\alpha \in (0,1)$, stationarity tolerance $\eta_\epsilon > 0$

backtracking constant $\gamma_\alpha \in (0,1)$, sampling decrease constant $\gamma_\epsilon \in (0,1)$

sample size $p \geq n+1$

**procedure** GS

  **for** $k = 0, 1, 2, \ldots$ **do**

    sample $p$ points $\{x_{k1}, \ldots, x_{kp}\} \subset \mathbb{B}_{\epsilon_k}(x_k) \cap \mathcal{D}$

    compute $d_k = -g_k$ via

$$\boxed{g_k := \text{Proj}(0 \,|\, \text{conv}\{g_{k0}, g_{k1}, \ldots, g_{kp}\})}$$

    set $\alpha_k$ as the largest element of $\{\gamma_\alpha^0, \gamma_\alpha^1, \gamma_\alpha^2, \ldots\}$ such that

$$f(x_k + \alpha_k d_k) \leq f(x_k) - \eta_\alpha \alpha_k \|d_k\|_2^2$$

    set $x_{k+1} \leftarrow x_k + \alpha_k d_k$ (or perturb to ensure $x_{k+1} \in \mathcal{D}$)

    if $\|d_k\|_2 \leq \eta_\epsilon \epsilon_k$, then set $\epsilon_{k+1} \leftarrow \gamma_\epsilon \epsilon_k$; else, set $\epsilon_{k+1} \leftarrow \epsilon_k$

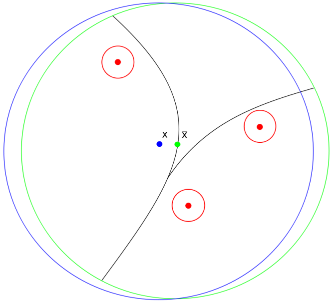
# GS global convergence

## Theorem 2

*If Assumption 1 holds, then w.p.1 either*

- $\{f(x_k)\} \to -\infty$, *or*
- *every cluster point of* $\{x_k\}$ *is stationary for* $f$

**Proof idea**: At $x_k$, either a direction of sufficient descent is produced or




$\exists\{y_{ki}\}_{i=1,\ldots,p}$ and $\delta > 0$ such that $\mathrm{Proj}(0|\{\nabla f(y_{ki} + O(\delta))\}) \approx \mathrm{Proj}(0|\partial_{\epsilon_k} f(\bar{x}))$

# GS illustration

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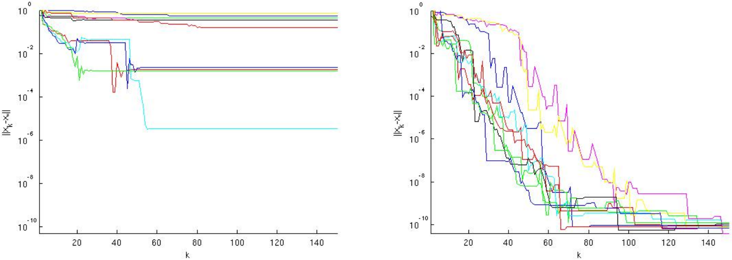
Figure: Without gradient sampling (left) and with gradient sampling (right)



# GS issues

Practical limitations:

- $p \geq n + 1$ gradient evaluations per iteration
- subproblems distinct; solved from scratch
- "steepest descent" method

# GS issues AGS solutions

Practical limitations:

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- subproblems distinct; solved from scratch
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Adaptive GS: Curtis & Que (2013)

- adaptive sampling: Kiwiel (2010)
- $\Theta(1)$ gradients per iteration
- maintain sample points within $\epsilon$-ball
- warm/hot-started subproblem solves
- quasi-Newton or over-estimation "Hessian" approximations ($W_k = H_k^{-1}$)

$$\max_{(z,d)\in\mathbb{R}\times\mathbb{R}^n} \; z + \tfrac{1}{2}\|d\|_{H_k}^2 \quad \text{s.t. } f(x_k)e + G_k^T d \leq ze \qquad \Leftrightarrow \qquad \max_{y\in\mathbb{R}^{p+1}} \; f(x_k) - \tfrac{1}{2}\|G_k y\|_{W_k}^2 \quad \text{s.t. } e^T y = 1,\; y \geq 0$$

# Outline

# Motivation

Why merge BFGS and GS?

BFGS:

- fast, cheap
- no automatic stationarity condition
- limited convergence guarantees
- . . . difficult to obtain as Hessians "blow up"

GS:

- expensive
- automatic stationarity condition
- convergence guarantees w.p.1

Idea: BFGS iteration, employing GS only when it appears needed

# Search direction computation

At $x_k$, given an inverse Hessian approximation $W_k \succ 0$:

$$\boxed{d_k \leftarrow -W_k g_k}$$

On the other hand, if we have

$$\begin{array}{lcllll} X_k & := & \{ & x_{k0}, & x_{k1}, & \cdots, & x_{kp_k} & \} & \text{(sample points)} \\ G_k & := & [ & g_{k0} & g_{k1} & \cdots & g_{kp_k} & ] & \text{(sample gradients)} \end{array}$$

and a Hessian approximation $H_k$ or inverse approximation $W_k$, then:

$$\boxed{\begin{aligned} \max_{z,d}\ & z + \tfrac{1}{2}\|d\|^2_{H_k} \\ \text{s.t. } & f(x_k)e + G_k^T d \le ze \end{aligned}} \quad \Leftrightarrow \quad \boxed{\begin{aligned} \max_{y}\ & f(x_k) - \tfrac{1}{2}\|G_k y\|^2_{W_k} \\ \text{s.t. } & e^T y = 1,\ y \ge 0 \end{aligned}}$$

With $p_k = 0$, we recover the BFGS step $d_k \leftarrow -W_k g_k$

# Line search and iterate update

In a BFGS method, to avoid damping or skipping, the line search would ideally yield a step size satisfying the Wolfe conditions

- Forward/backtracking line search to satisfy the Wolfe conditions

$$f(x_k) - f(x_k + \alpha_k d_k) > \underline{\eta}\alpha_k \|d_k\|^2_{H_k} \qquad // \ \underline{\eta} \in (0,1)$$

$$v^T d_k \geq \overline{\eta}\nabla f(x_k)^T d_k, \text{ where } v \in \partial f(x_k + \alpha d_k) \qquad // \ \overline{\eta} \in (\underline{\eta}, 1)$$

- Curvature condition is abandoned after finite number of forward/backtracks (Motivation: Finite termination if $f_k(\alpha) := f(x_k + \alpha d_k) - f(x_k)$ is weakly lower semismooth: Lewis, Overton (2012); Mifflin (1977); Lemaréchal (1981))
- Line search abandoned ($\alpha_k \leftarrow 0$) if unsuccessful after finite number of forward/backtracks and sample size is not sufficiently large ($p_k \geq n+1$)

If necessary, perturb $x_k + \alpha_k d_k$ to find $x_{k+1} \in \mathcal{D}$ satisfying

$$f(x_k) - f(x_{k+1}) > \underline{\eta}\alpha_k \|d_k\|^2_{H_k}$$

$$\nabla f(x_{k+1})^T d_k \geq \overline{\eta}\nabla f(x_k)^T d_k$$

$$\|x_k + \alpha_k d_k - x_{k+1}\|_2 \leq \min\{\alpha_k, \epsilon_k\}\|d_k\|_2$$

# Sample radius update

Reduce the sampling radius (i.e., choose $\epsilon_{k+1} \leftarrow \gamma_\epsilon \epsilon_k$) if

$$\|d_k\|_{H_k}^2 \leq \eta_\epsilon \epsilon_k \qquad // \ \eta_\epsilon > 0$$

$$\|d_k\|_{H_k}^2 \geq \underline{\xi} \epsilon_k \|d_k\|_2 \qquad // \ \underline{\xi} \in (0,1)$$

$$\alpha_k > 0$$

# Sample point generation

At $x_k$, suppose we had

$$\begin{array}{lllllll} X_k & := & \{ & x_{k0}, & x_{k1}, & \cdots, & x_{kp_k} & \} & \text{(sample points)} \\ G_k & := & [ & g_{k0} & g_{k1} & \cdots & g_{kp_k} & ] & \text{(sample gradients)} \end{array}$$

If curvature is bounded and step-size sufficiently large in that

$$\begin{aligned} \underline{\xi}\epsilon_k\|d_k\|_2^2 \leq \|d_k\|_{H_k}^2 \leq \overline{\xi}\epsilon_k^{-1}\|d_k\|_2^2 \quad & // \; 0 < \underline{\xi} < \overline{\xi} \\ \underline{\alpha} \leq \alpha_k \quad & // \; 0 < \underline{\alpha} \end{aligned}$$

then erase sample set (i.e., $X_{k+1} \leftarrow \{x_{k+1}\}$ and $p_{k+1} \leftarrow 0$); else,

- discard gradients outside of radius $\epsilon_{k+1}$ about $x_{k+1}$
- maintain sample points within radius; warm/hot-starting
- sample $\Theta(1)$ new gradient(s)
- discard "old gradients" so $p_{k+1} \leq n + 1$

Overall,

$$X_{k+1} \leftarrow (X_k \cap \mathbb{B}_{\epsilon_{k+1}}(x_{k+1})) \cup \{x_{k+1}\} \cup \overline{X}_{k+1}$$

where $\overline{X}_{k+1} \subset \mathbb{B}_{\epsilon_{k+1}}(x_{k+1}) \cap \mathcal{D}$

# Quasi-Newton updating

If curvature is bounded and step-size sufficiently large in that

$$\underline{\xi}\epsilon_k\|d_k\|_2^2 \leq \|d_k\|_{H_k}^2 \leq \overline{\xi}\epsilon_k^{-1}\|d_k\|_2^2 \quad // \ 0 < \underline{\xi} < \overline{\xi}$$
$$\underline{\alpha} \leq \alpha_k \quad // \ 0 < \underline{\alpha}$$

then standard BFGS update; else, L-BFGS update with pairs satisfying

$$\max\{\|s_j\|_2^2, \|y_j\|_2^2\} \leq \sigma \quad // \ \sigma > 0$$
$$s_j^T y_j \geq \gamma \quad // \ \gamma > 0$$

## Theorem 3

*Initializing $H_{k+1} \leftarrow \mu_k I \succ 0$, after $m$ updates we have for any $d \in \mathbb{R}^n$ that*

$$\left(\frac{2^m}{\mu_k}\left(1+\frac{\sigma^2}{\gamma^2}\right)^m + \frac{\sigma}{\gamma}\left(\frac{2^m\left(1+\frac{\sigma^2}{\gamma^2}\right)^m - 1}{2\left(1+\frac{\sigma^2}{\gamma^2}\right)-1}\right)\right)^{-1}\|d\|_2^2 \leq \|d\|_{H_{k+1}}^2 \leq \left(\mu_k + \frac{m\sigma}{\gamma}\right)\|d\|_2^2$$

# BFGS-GS method

**Algorithm 2** BFGS Gradient Sampling (BFGS-GS) Algorithm

**Require:**

```
initial point x_0 ∈ R^n, initial sampling radius ϵ_0 > 0, initial W_0 ≻ 0
procedure BFGS-GS
    for k = 0, 1, 2, ... do
        compute y_k from (dual) subproblem QP
        compute d_k = −W_k G_k y_k
        forward/backtrack Armijo/Wolfe line search to obtain α_k
        perturb (if necessary) to obtain x_{k+1} ∈ D
        set sampling radius ϵ_{k+1} ≤ ϵ_k
        set sample set X_{k+1}
        set (L-)BFGS inverse Hessian approximation W_{k+1}
```

## Theorem 4

*If Assumption 1 holds, then w.p.1 either*

- $\{f(x_k)\} \to -\infty$, *or*
- *every cluster point of* $\{x_k\}$ *is stationary for* $f$

# BFGS-GS

Implemented in C++

- implemented QP solver, adapted from Kiwiel (1985)
- 26 test problems, 10 random initial points each

Comparisons with:

- `HANSO-BFGS`: BFGS method, Overton et al.
- `HANSO-DEFAULT`: BFGS then GS, Overton et al.
- `LMBM`: limited memory bundle method, Haarala et al.

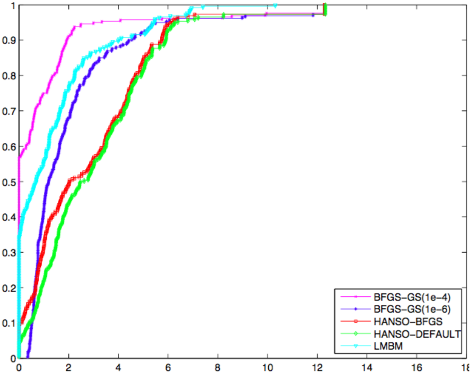
Termination flags:

(1) stationarity tolerance satisfied
(2) maximum iteration limit reached
(3) other

| flag | BFGS-GS($10^{-4}$) | BFGS-GS($10^{-6}$) | HANSO-BFGS | HANSO-DEFAULT | LMBM |
|---|---|---|---|---|---|
| (1) | 253 | 229 | 68 | 68 | 20 |
| (2) | 7 | 31 | 31 | 19 | 0 |
| (3) | 0 | 0 | 161 | 173 | 240 |

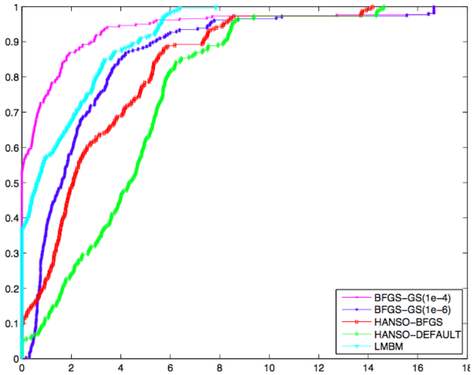
# Performance profile: Iterations

Figure: Performance profile for iterations



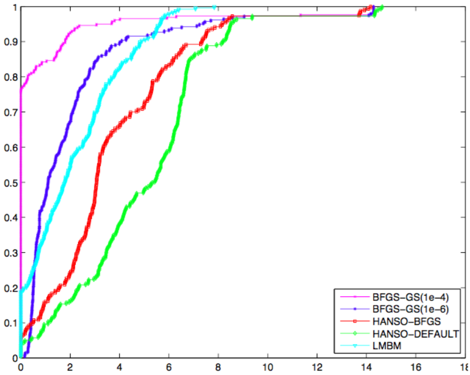
# Performance profile: Function evaluations

Figure: Performance profile for function evaluations



# Performance profile: Gradient evaluations

Figure: Performance profile for gradient evaluations




Overall, to obtain solutions of similar quality (see paper):

- BFGS-GS$(10^{-4})$ more efficient than LMBM
- BFGS-GS$(10^{-6})$ at least competitive with HANSO-BFGS and HANSO

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# Contributions

New general-purpose methods for nonconvex nonsmooth optimization

- adaptive sampling, $\Theta(1)$ gradients per iteration
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- convergence guarantees (w.p.1)
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- convergence guarantees (w.p.1)
- further empirical improvements
- `BFGS-GS` software (C++)

} Curtis & Que (2015)

⋆ F. E. Curtis and X. Que.
An Adaptive Gradient Sampling Algorithm for Nonsmooth Optimization.
*Optimization Methods and Software*, 28(6):1302–1324, 2013.

⋆ F. E. Curtis and X. Que.
A Quasi-Newton Algorithm for Nonconvex, Nonsmooth Optimization with Global Convergence Guarantees.
*Mathematical Programming Computation*, DOI: 10.1007/s12532-015-0086-2, 2015.