Derivative-Free Optimization of Noisy Functions via Quasi-Newton Methods

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Discussion

1. The BFGS method continues to surprise
2. One of the best methods for nonsmooth optimization (Lewis-Overton)
3. Leading approach for (deterministic) DFO derivative-free optimization
4. This talk: Very good method for the minimization of noisy functions

We had not fully recognized the power and generality of quasi-Newton updating until we tried to find alternatives!

Subject of this talk:

1. Black-box noisy functions
2. No known structure
3. Not the finite sum loss functions arising in machine learning, where cheap approximate gradients are available

Outline

Problem 1: $\min f(x)$ f smooth but derivatives not available: DFO

1. f contains no noise
2. Scalability, Parallelism
3. Robustness

Problem 2: $\min f(x;\xi)$ $f(\cdot;\xi)$ smooth

$$\min f(x) = \phi(x) + \epsilon(x) \qquad f(x) = \phi(x)(1+\epsilon(x))$$

- Propose method build upon classical quasi-Newton updating using finite-difference gradients
- Estimate good finite-difference interval h
- Use noise estimation techniques (More'-Wild)
- Deal with noise adaptively
- Can solve problems with thousands of variables
- Novel convergence results – to neighborhood of solution (Richard Byrd)

DFO: Derivative free deterministic optimization (no noise)

$$\min f(x) \qquad f \text{ is smooth}$$

- Direct search/pattern search methods: not scalable
- Much better idea:
  - Interpolation based models with trust regions (Powell, Conn, Scheinberg,…)

$$\min \quad m(x) = x^T Bx + g^T x \quad \text{s.t.} \quad \| x \|_2 \leq \Delta$$

1. Need *(n+1)(n+2)/2* function values to define quadratic model by pure interpolation
2. Can use O(*n*) points and assume minimum norm change in the Hessian
3. Arithmetic costs high: n^4 ← *scalability*
4. Placement of interpolation points is important
5. Correcting the model may require many function evaluations
6. Parallelizable? ←

Why not simply BFGS with finite difference gradients?

$$x_{k+1} = x_k - \alpha_k H_k \nabla f(x_k)$$

$$\frac{\partial f(x)}{\partial x_i} \approx \frac{f(x + he_i) - f(x)}{h}$$

- Invest significant effort in estimation of gradient
- Delegate construction of model to BFGS
- Interpolating gradients
- Modest linear algebra costs *O(n)* for L-BFGS
- Placement of sample points on an orthogonal set
- BFGS is an overwriting process: no inconsistencies or ill conditioning *with* Armijo-Wolfe line search
- Gradient evaluation parallelizes easily

Why now?

- Perception that n function evaluations per step is too high
- Derivative-free literature rarely compares with FD – quasi-Newton
- Already used extensively: fminunc MATLAB
- Black-box competition and KNITRO

Some numerical results

Compare:

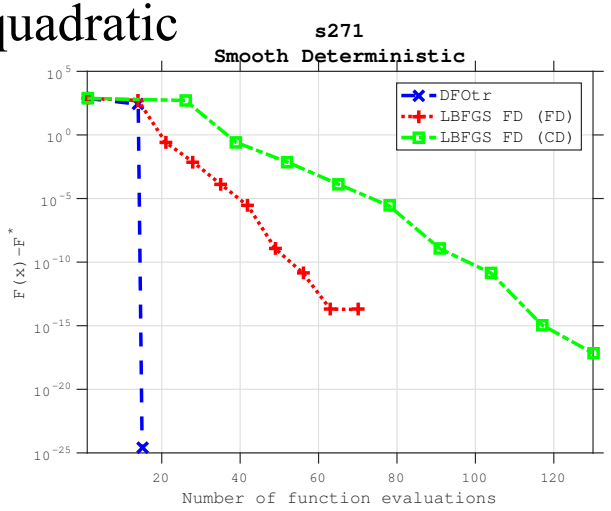
Model based trust region code DFOtr by Conn, Scheinberg, Vicente

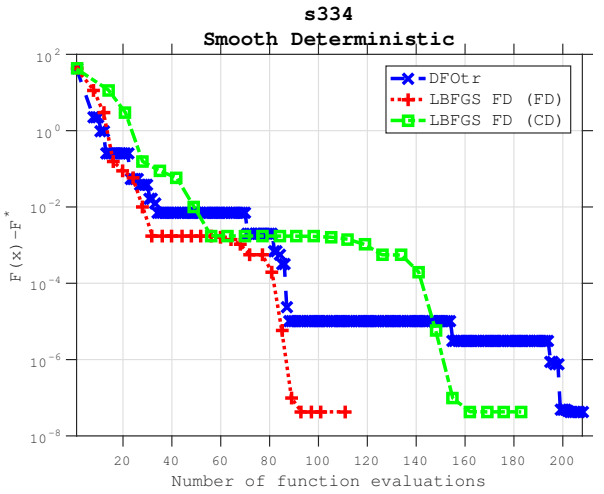
vs FD-L-BFGS with forward and central differences

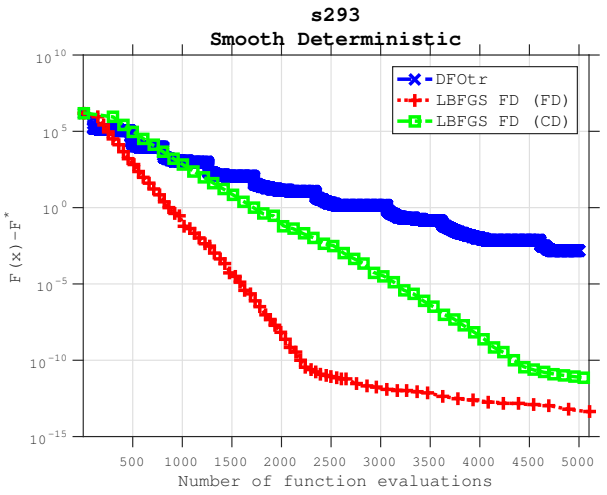
Plot function decrease vs total number of function evaluations

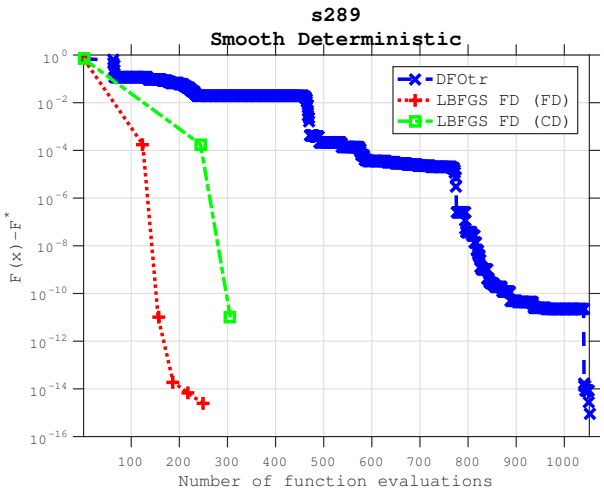
Comparison: function decrease vs total # of function evaluations

quadratic









Conclusion: DFO without noise

Finite difference BFGS is a real competitor of DFO method based on function evaluations
Can solve problems with thousands of variables

… but really nothing new.

Optimization of Noisy Functions

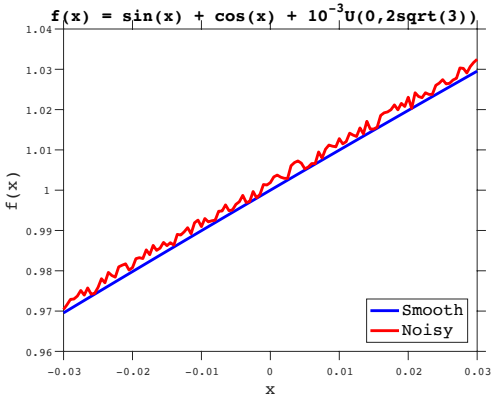
$$\min f(x;\xi) \quad \text{where} \quad f(\cdot;\xi) \text{ is smooth}$$

$$\min f(x) = \phi(x) + \epsilon(x) \qquad f(x) = \phi(x)(1+\epsilon(x))$$

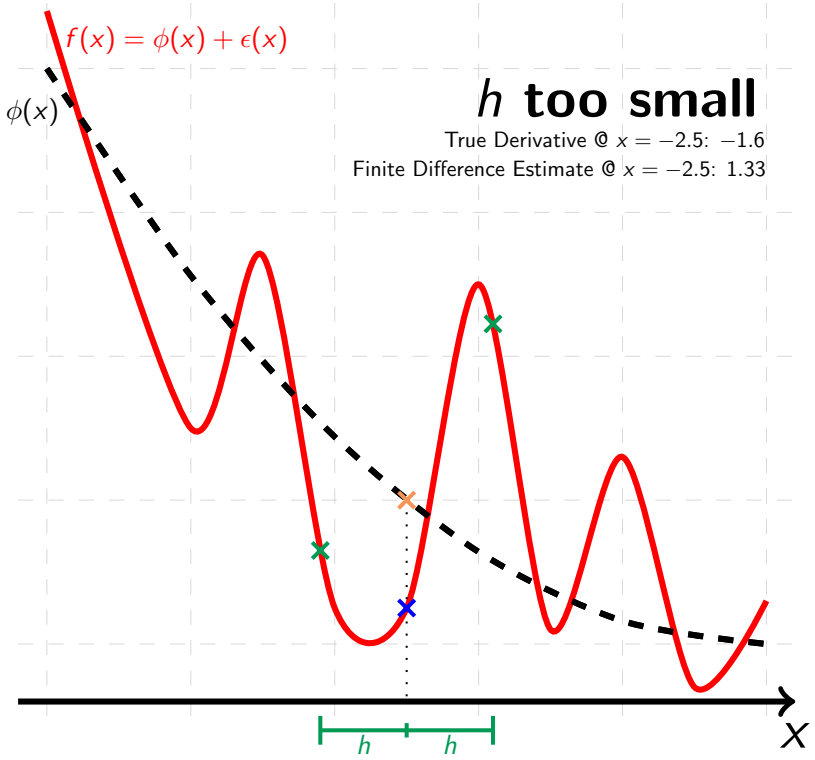
Focus on additive noise

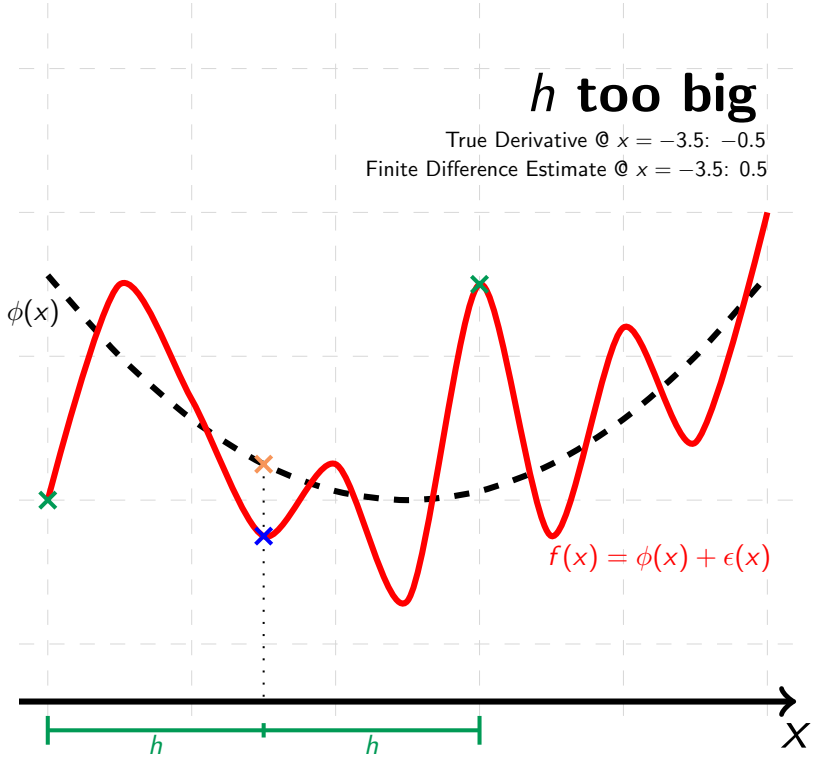
Finite-difference BFGS should not work!

1. Difference of noisy functions dangerous
2. Just one bad update once in a while: disastrous
3. Not done to the best of our knowledge



Finite Differences – Noisy Functions





A Practible Algorithm

$$\min f(x) = \phi(x) + \epsilon(x) \qquad f(x) = \phi(x)(1 + \epsilon(x))$$

Outline of adaptive finite-difference BFGS method

1. Estimate noise $\epsilon(x)$ at every iteration -- More'-Wild
2. Estimate h
3. Compute finite difference gradient
4. Perform line search (?!)
5. Corrective Procedure when case line search fails
   - (need to modify line search)
   - Re-estimate noise level

Will require very few extra f evaluations/iteration – even none

Noise estimation

More'-Wild (2011)

$$\min f(x) = \phi(x) + \epsilon(x)$$

Noise level: $\sigma = [var(\epsilon(x))]^{1/2}$

Noise estimate: ϵ_f

At x choose a random direction v

evaluate f at $q+1$ equally spaced points $x + i\beta v, \quad i = 0,...,q$

Compute function differences:

$$\Delta^0 f(x) = f(x)$$

$$\Delta^{j+1} f(x) = \Delta^j [\Delta f(x)] = \Delta^j [f(x+\beta)] - \Delta^j [f(x)]]$$

Compute finite diverence table:

$$T_{ij} = \Delta^j f(x + i\beta v)$$

$$1 < j < q \quad 0 < i < j - q$$

$$\sigma_j = \frac{\gamma_j}{q-1-j} \sum_{i=0}^{q-j} T_{i,j}^2 \qquad \gamma_j = \frac{(j!)^2}{(2j)!}$$

Noise estimation

More'-Wild (2011)

$$\min f(x) = \sin(x) + \cos(x) + 10^{-3}\mathrm{U}(0, 2\sqrt{3}) \qquad q = 6 \qquad \beta = 10^{-2}$$

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$	$\Delta^6 f$
$-3 \cdot 10^{-2}$	1.003	$7.54e-3$	$2.15e-3$	$1.87e-4$	$-5.87e-3$	$1.46e-2$	$-2.49e-2$
$-2 \cdot 10^{-2}$	1.011	$9.69e-3$	$2.33e-3$	$-5.68e-3$	$8.73e-3$	$-1.03e-3$	
-10^{-2}	1.021	$1.20e-2$	$-3.35e-3$	$3.05e-3$	$-1.61e-3$		
0	1.033	$8.67e-3$	$-2.96e-3$	$1.44e-3$			
10^{-2}	1.041	$8.38e-3$	$1.14e-3$				
$2 \cdot 10^{-2}$	1.050	$9.52e-3$					
$3 \cdot 10^{-2}$	1.059						
σ_k		$6.65e-3$	$8.69e-4$	$7.39e-4$	$7.34e-4$	$7.97e-4$	$8.20e-4$

High order differences of a smooth function tend to zero rapidly, while differences in noise are bounded away from zero. Changes in sign, useful.

Procedure is scale invariant!

Finite difference itervals

Once noise estimate ϵ_f has been chosen:

Forward difference: $h = 8^{1/4}(\frac{\epsilon_f}{\mu_2})^{1/2}$ $\mu_2 = \max_{x \in I} |f''(x)|$

Central difference: $h = 3^{1/3}(\frac{\epsilon_f}{\mu_3})^{1/3}$ $\mu_3 \approx |f'''(x)|$

Bad estimates of second and third derivatives can cause problems (not often)

Adaptive Finite Difference L-BFGS Method

Estimate noise ϵ_f

Compute h for forward or central differences [(4-8) function evaluations]

Compute g_k

While convergence test not satisfied:

$d = -H_k g_k$ [L-BFGS procedure]

$(x_+, f_+, flag) =$ LineSearch$(x_k, f_k, g_k, d_k, f_s)$

IF flag=1 [line search failed]

$(\mathrm{x}_+, f_+, h) =$ Recovery$(x_k, f_k, g_k, d_k, max_{iter})$

endif

$x_{k+1} = x_+, \; f_{k+1} = f_+$

Compute g_{k+1} [finite differences using h]

$s_k = x_{k+1} - x_k, \; y_k = g_{k+1} - g_k$

Discard (s_k, y_k) if $s_k^T y_k \le 0$

$k = k + 1$

endwhile

Line Search

BFGS method requires Armijo-Wolfe line search

$$f(x_k + \alpha d) \le f(x_k) + \alpha c_1 \nabla f(x_k) d \qquad \text{Armijo}$$

$$\nabla f(x_k + \alpha d)^T d \ge c_2 \nabla f(x_k)^T d \qquad \text{Wolfe}$$

Deterministic case: always possible if f is bounded below

- Can be problematic in the noisy case.
- Strategy: try to satisfy both but limit the number of attempts
- If first trial point (unit steplength) is not acceptable relax:

$$f(x_k + \alpha d) \le f(x_k) + \alpha c_1 \nabla f(x_k) d \; + 2\epsilon_f \qquad \text{relaxed Armijo}$$

Three outcomes: a) both satisfied; b) only Armijo; c) none

Corrective Procedure

Compute a new noise estimate $\overline{\epsilon}_f$ along search direction d_k

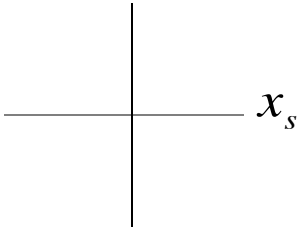
Compute corresponding $\overline{h}$

If $\hat{h} \neq h$ use new estimat $h \leftarrow \overline{h}$; return w.o. changing x_k

Else compute new iterate (various options):

small perturbation; stencil point

Finite difference Stencil (Kelley)



Some quotes

I believe that eventually the better methods will not use derivative approximations…
[Powell, 1972]

f is … somewhat noisy, which renders most methods based on finite differences of little or no use [X,X,X]. [Rios & Sahinidis, 2013]

END