Nonsmooth, Nonconvex Optimization
Algorithms and Examples

Michael L. Overton
Courant Institute of Mathematical Sciences
New York University

Convex and Nonsmooth Optimization Class, Spring 2020, Lecture 13

Based on my research work with
Jim Burke (Washington), Adrian Lewis (Cornell) and others

Introduction

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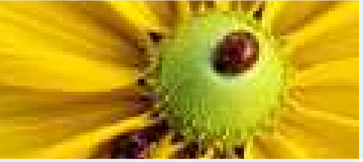
What happens if we simply use gradient descent (steepest descent) with a standard line search?



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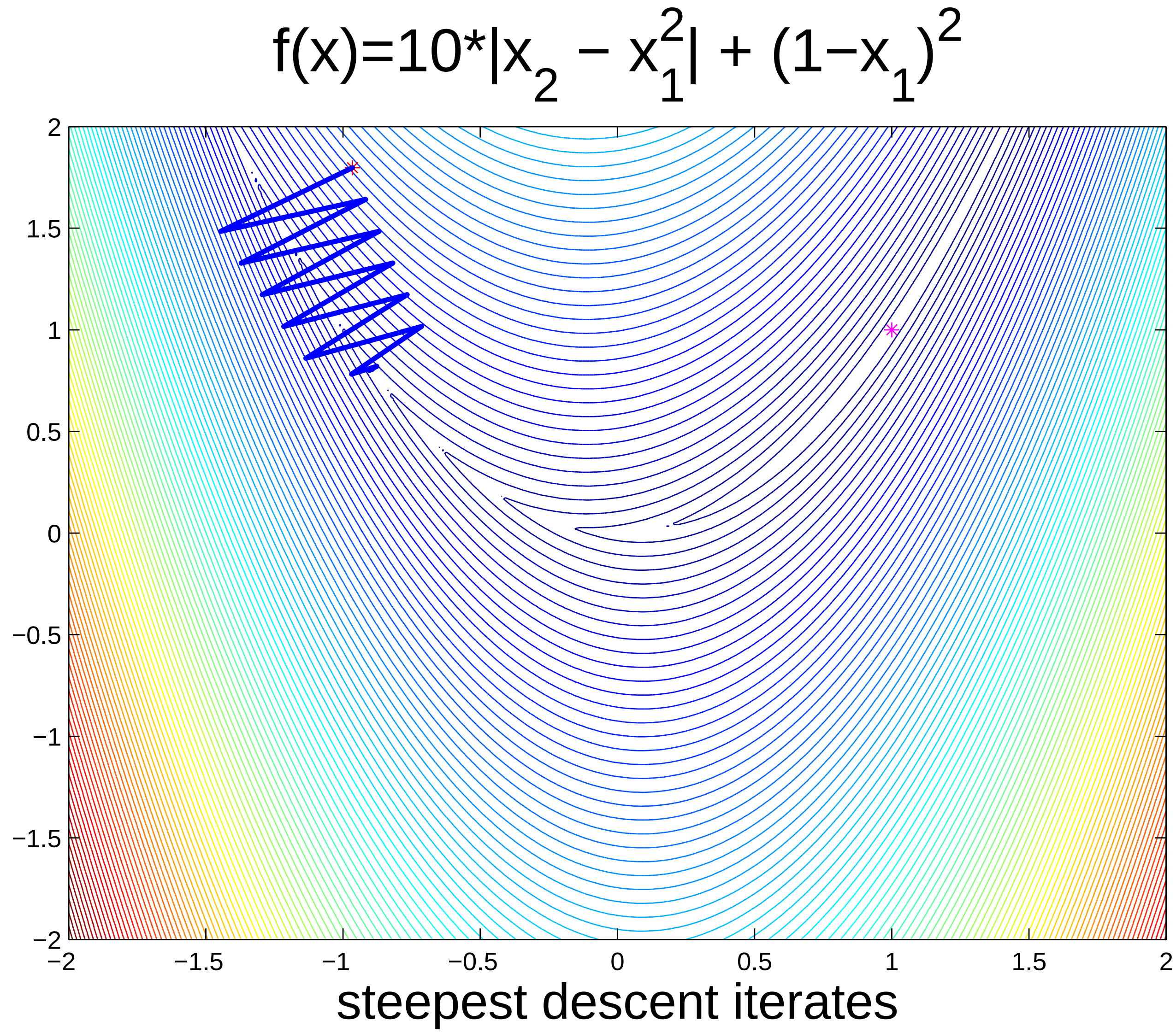

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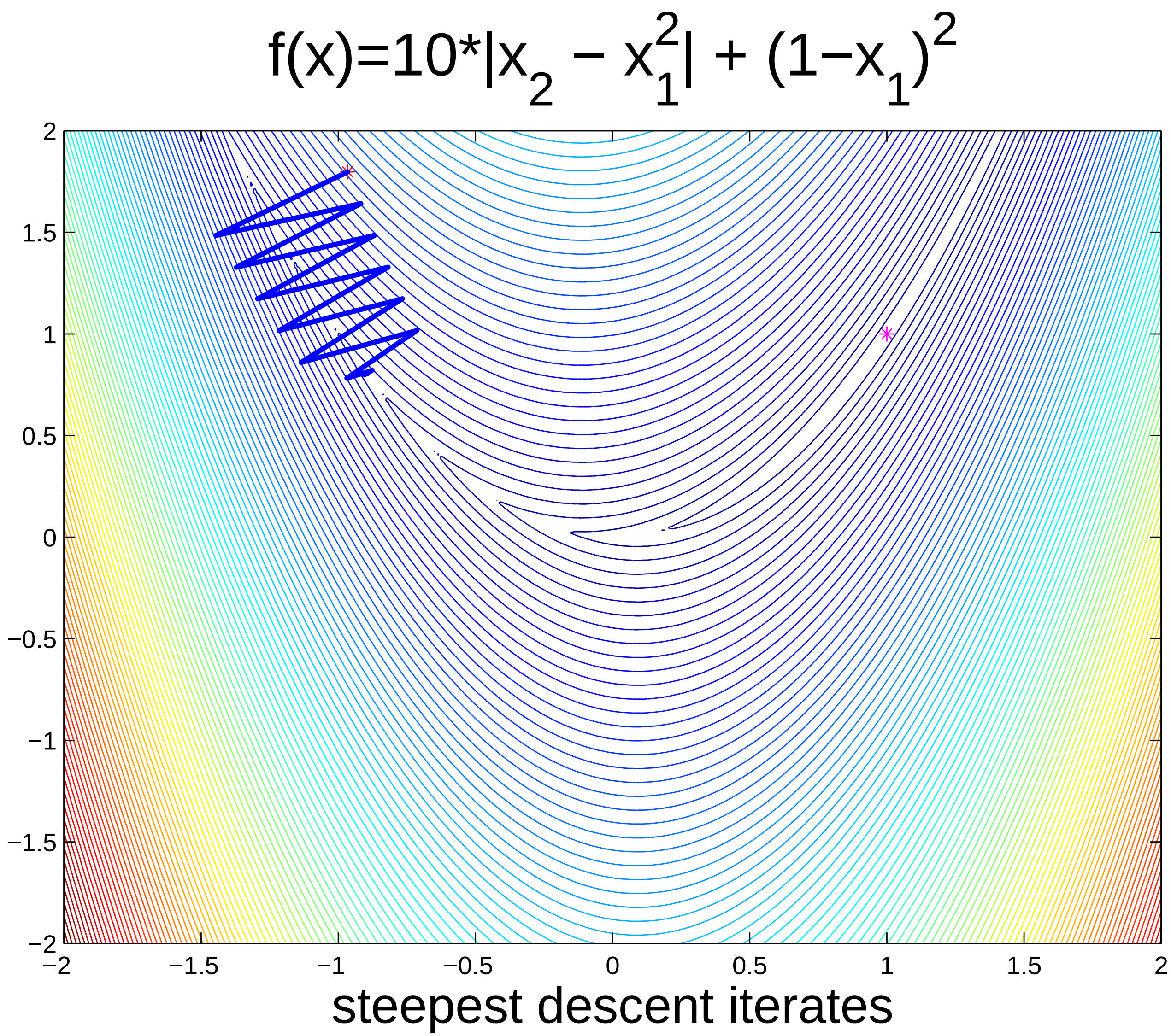

On this example, iterates invariably converge to a nonstationary point

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Failure can be avoided by using sufficiently short steplengths (N.Z. Shor, 1970s), but this is slow.

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- the Armijo condition holds for sufficiently small t as long as f is continuous
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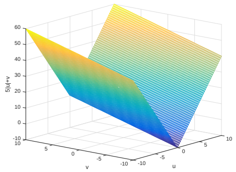
Searching for "Armijo-Wolfe" on the web, we found Melissa Armijo-Wolfe's LinkedIn page!

Failure of Gradient Method: Simple Convex Example

Let $f(x) = a|x_1| + x_2$, with $a \geq 1$. Although f is unbounded below, it is bounded below along any direction $d = -\nabla f(x)$.



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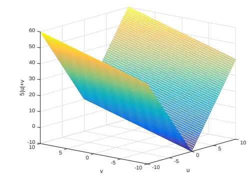


Theorem. Let $x^{(0)}$ satisfy $x_1^{(0)} \neq 0$ and define $x^{(k)} \in \mathbb{R}^2$ by

$$x^{(k+1)} = x^{(k)} + t_k d^{(k)} \text{ where } d^{(k)} = -\nabla f(x^{(k)})$$

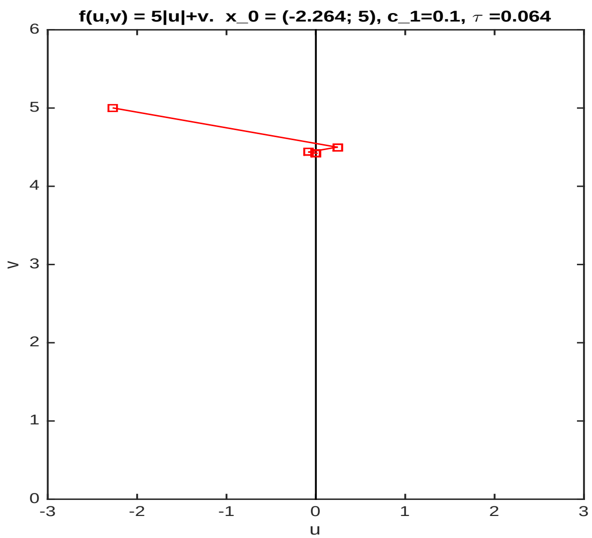
and t_k is *any* steplength satisfying the Armijo and Wolfe conditions with Armijo parameter c_1. If

$$c_1(a^2 + 1) > 1$$

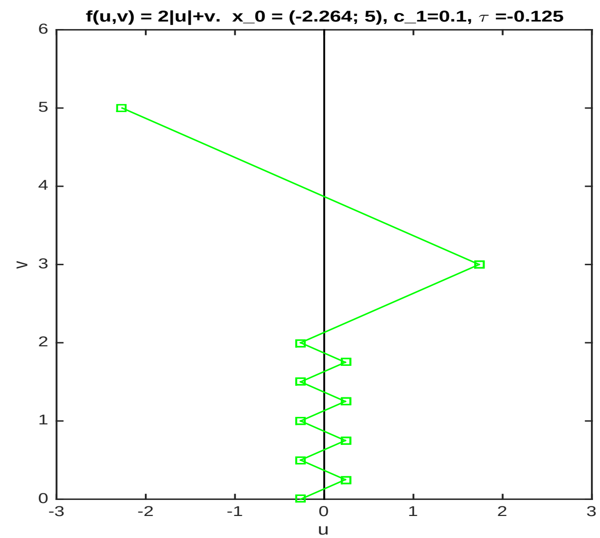
then $x^{(k)}$ converges to $\bar{x}$ with $\bar{x}_1 = 0$, even though f is unbounded below.

Azam Asl and M.L.O., 2017

Illustration of Failure and Success



$$a = 5, c_1 = 0.1$$
$$x^{(k)} \to \bar{x}$$



$$a = 2, c_1 = 0.1$$
$$f(x^{(k)}) \downarrow -\infty$$

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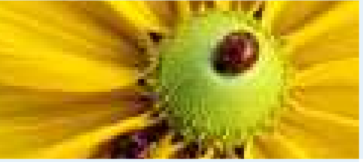

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- BFGS: traditional workhorse for smooth optimization, works amazingly well for nonsmooth optimization too, but very limited convergence theory

Gradient Sampling

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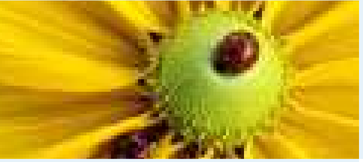

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J.V. Burke, A.S. Lewis and M.L.O., SIOPT, 2005.

[1] Needed in theory, but typically not in practice.

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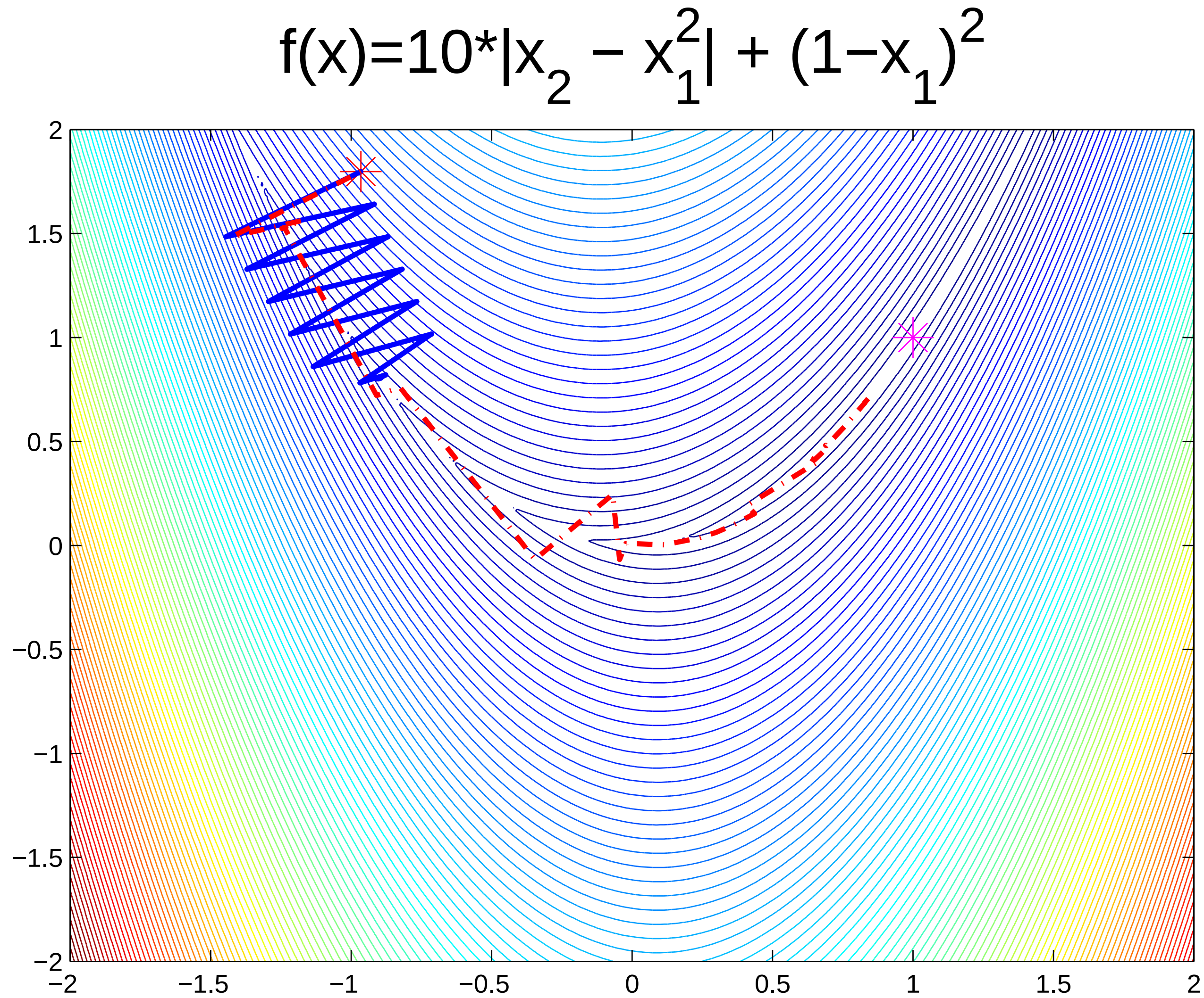

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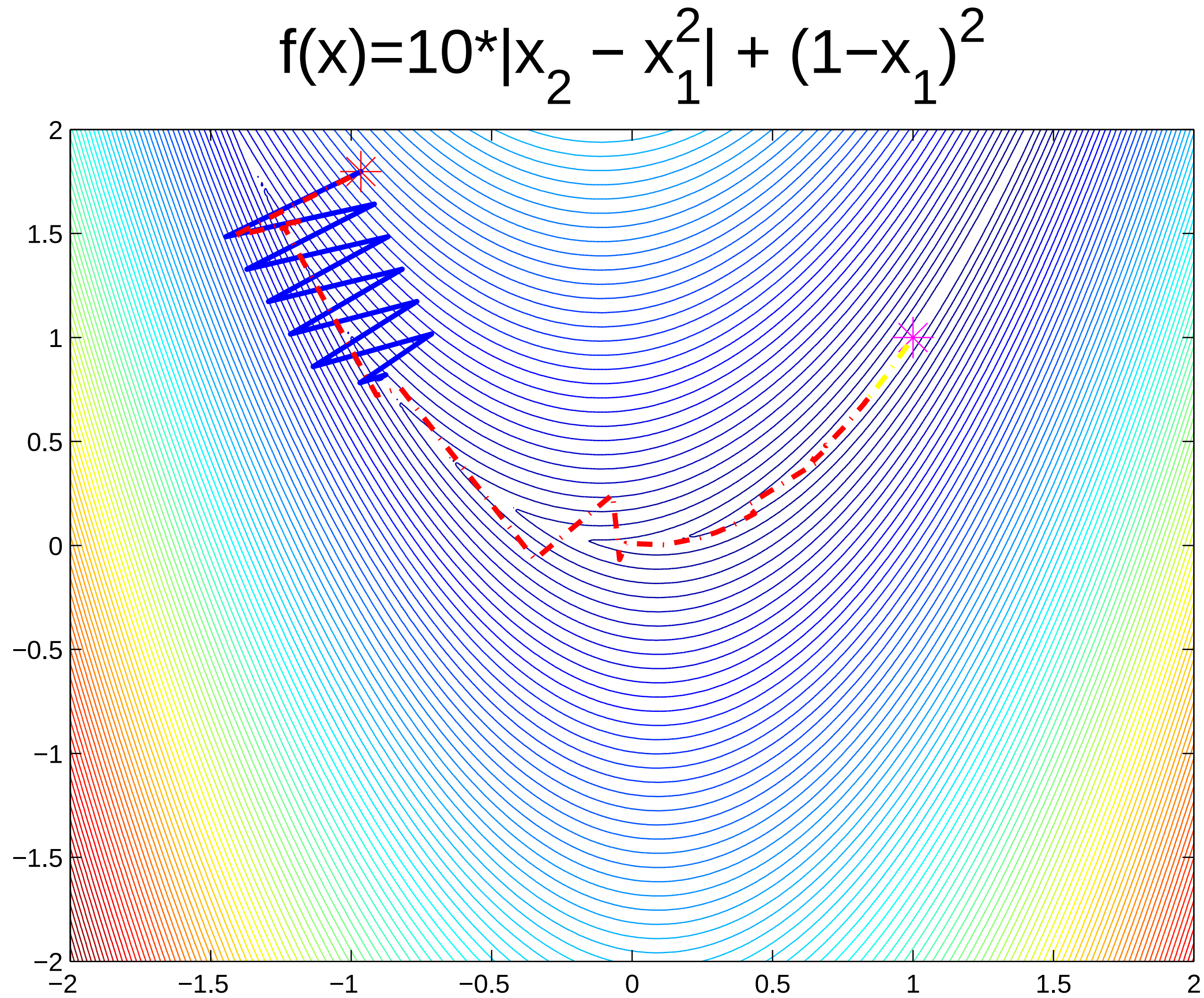

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Key point: the convex hull of the set G generated by Gradient Sampling is a surrogate for $\partial^C f$.

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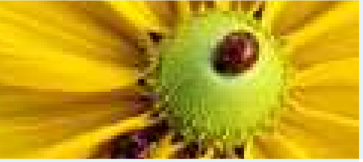
$$\nabla f(x) = 10\,\mathrm{sgn}\{x_2 - x_1^2\} \begin{bmatrix} -2x_1 \\ 1 \end{bmatrix} + \begin{bmatrix} -2(1 - x_1) \\ 0 \end{bmatrix}$$

so $\partial^C f(x) = \{\nabla f(x)\}$.



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so $\partial^C f(x) = \{\nabla f(x)\}$. For x with $x_2 = x_1^2$, there are two limiting gradients, namely

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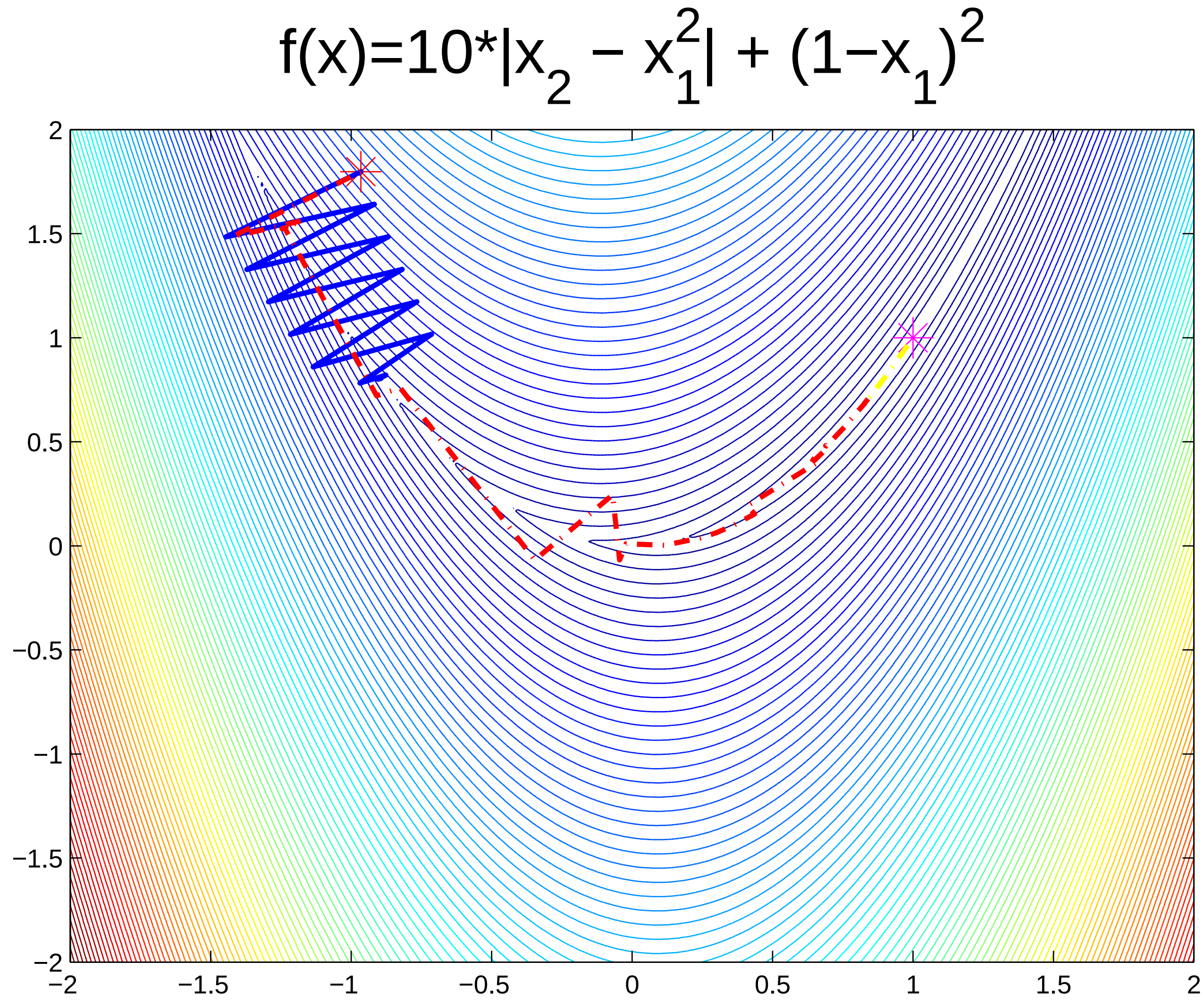
so $\partial^C f(x)$ consists of the convex hull of these two vectors. The unique x for which $0 \in \partial^C f(x)$ is $x = [1;\ 1]^T$, so this is the unique Clarke stationary point of f (it follows that it is the global minimizer).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Lemma. Let C be a compact convex set and $\|\cdot\| = \|\cdot\|_2$. Then

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Gradient sampling: $C = \mathrm{conv}(G)$

$$= \mathrm{conv}(\{\nabla f(x), \nabla f(x + \epsilon u_1), \ldots, \nabla f(x + \epsilon u_m)\}).$$

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Quasi-Newton Methods

A Difficult Nonconvex Problem from Nesterov

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Quasi-Newton Methods

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Davidon was a well known active anti-war protester during the Vietnam War. In December 2013, it was revealed that he was the mastermind behind the break-in at the FBI office in Media, PA, on March 8, 1971, during the Muhammad Ali - Joe Frazier world heavyweight boxing championship.

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Davidon, Fletcher and Powell all died during 2013–2016.

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Pathological counterexamples to convergence in the smooth, nonconvex case are known to exist (Y.-H. Dai, 2002, 2013; W. Mascarenhas 2004), but it is widely accepted that the method works well in practice in the smooth, nonconvex case.

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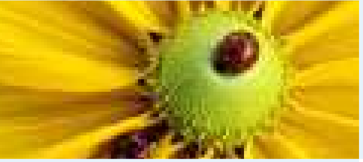

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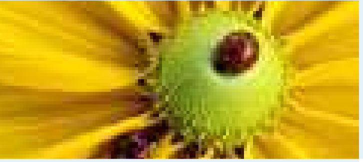

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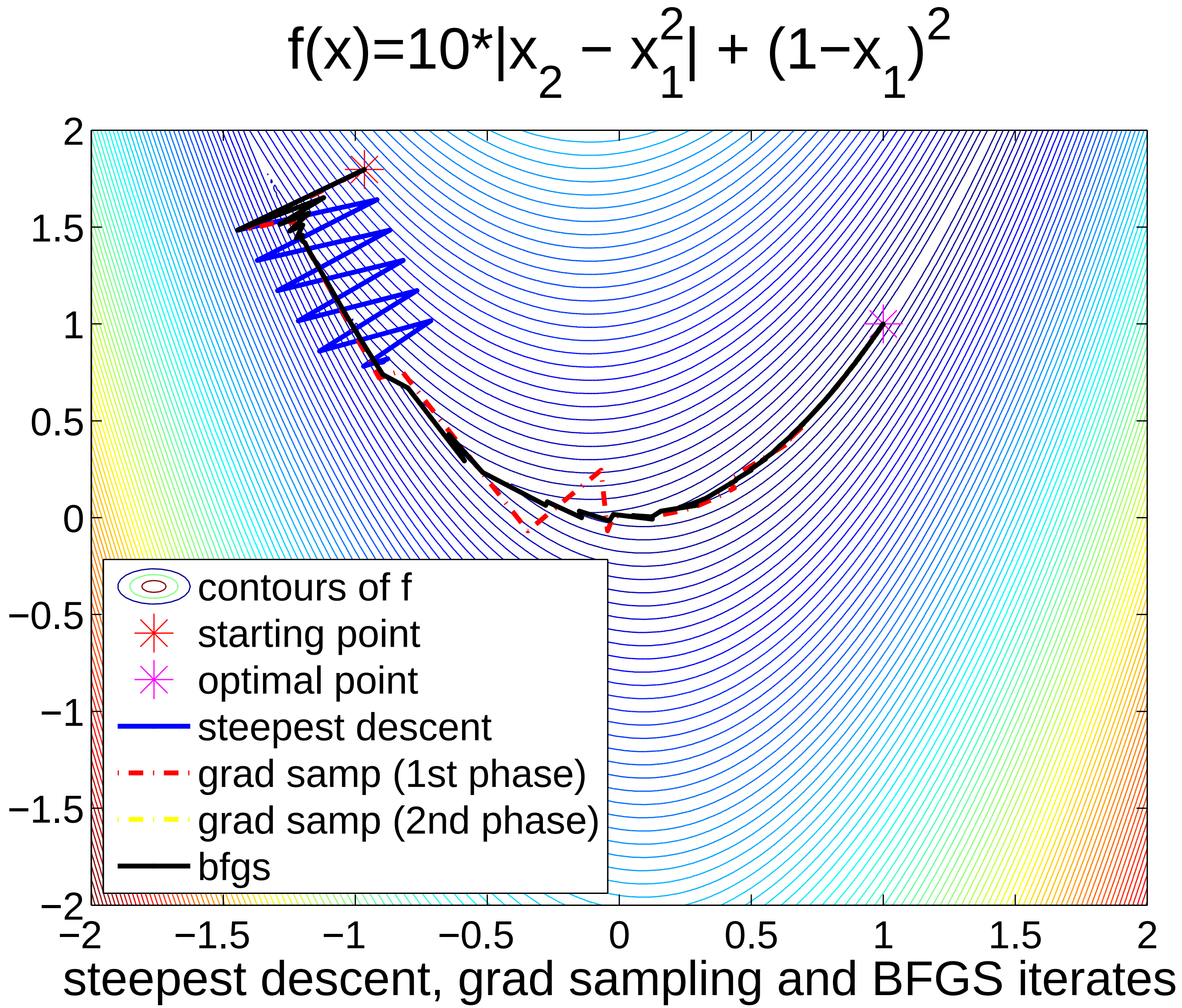
We have never seen convergence to non-stationary points that cannot be explained by numerical difficulties.

Convergence rate of BFGS is typically linear (not superlinear) in the nonsmooth case.


$f(x)=10*|x_2 - x_1^2| + (1-x_1)^2$
contours of f
starting point
optimal point
steepest descent
grad samp (1st phase)
grad samp (2nd phase)
bfgs
steepest descent, grad sampling and BFGS iterates
2
1.5
1
0.5
0
−0.5
−1
−1.5
−2
−2
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0
0.5
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1.5
2

Example: Minimizing a Product of Eigenvalues

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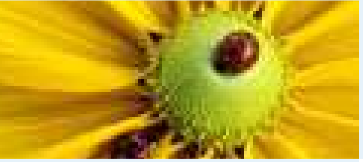

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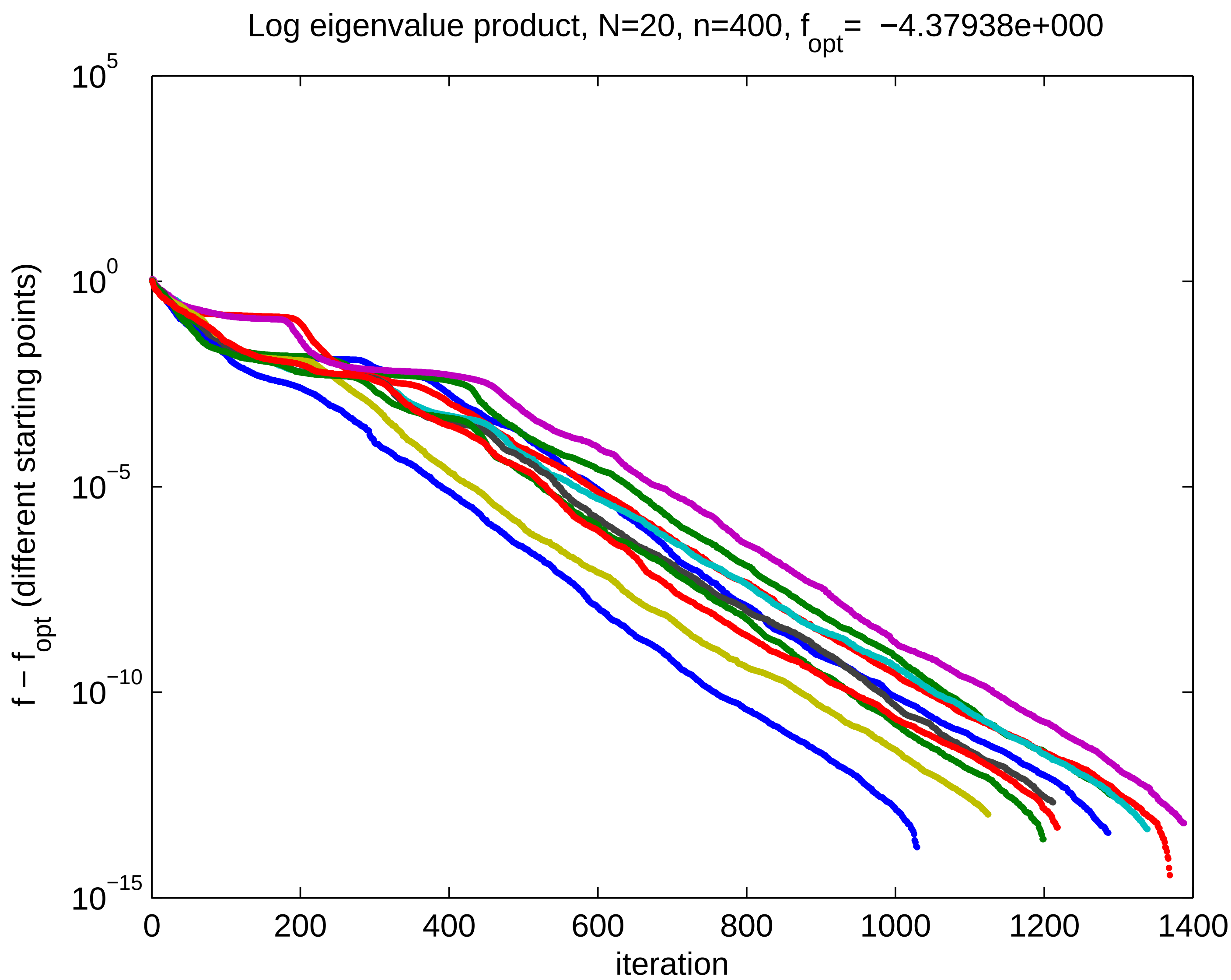
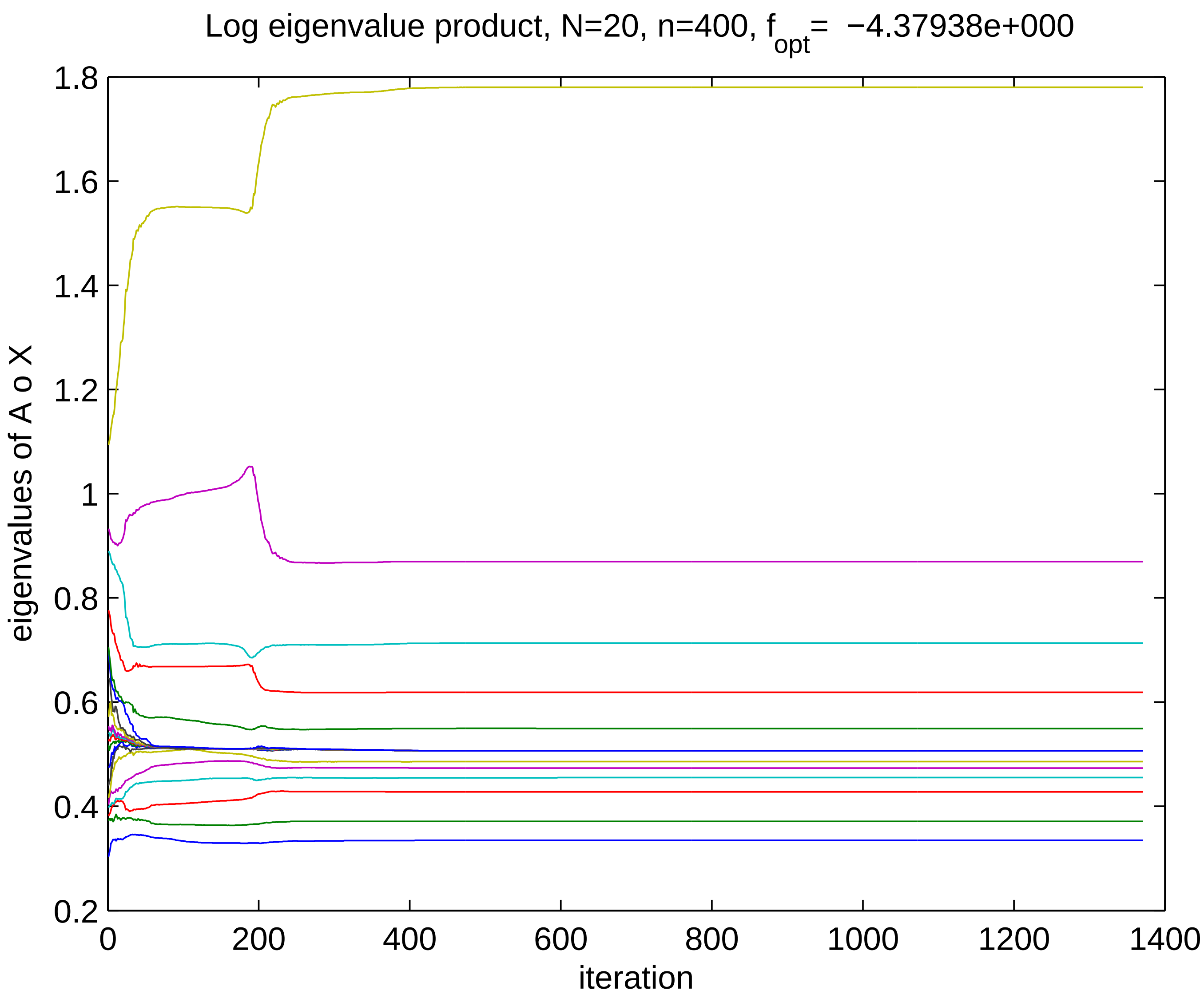
Application: entropy minimization in an environmental application (K.M. Anstreicher and J. Lee, 2004)

BFGS from 10 Randomly Generated Starting Points



$f - f_{\text{opt}}$, where f_{opt} is least value of f found over all runs

Evolution of Eigenvalues of $A \circ X$



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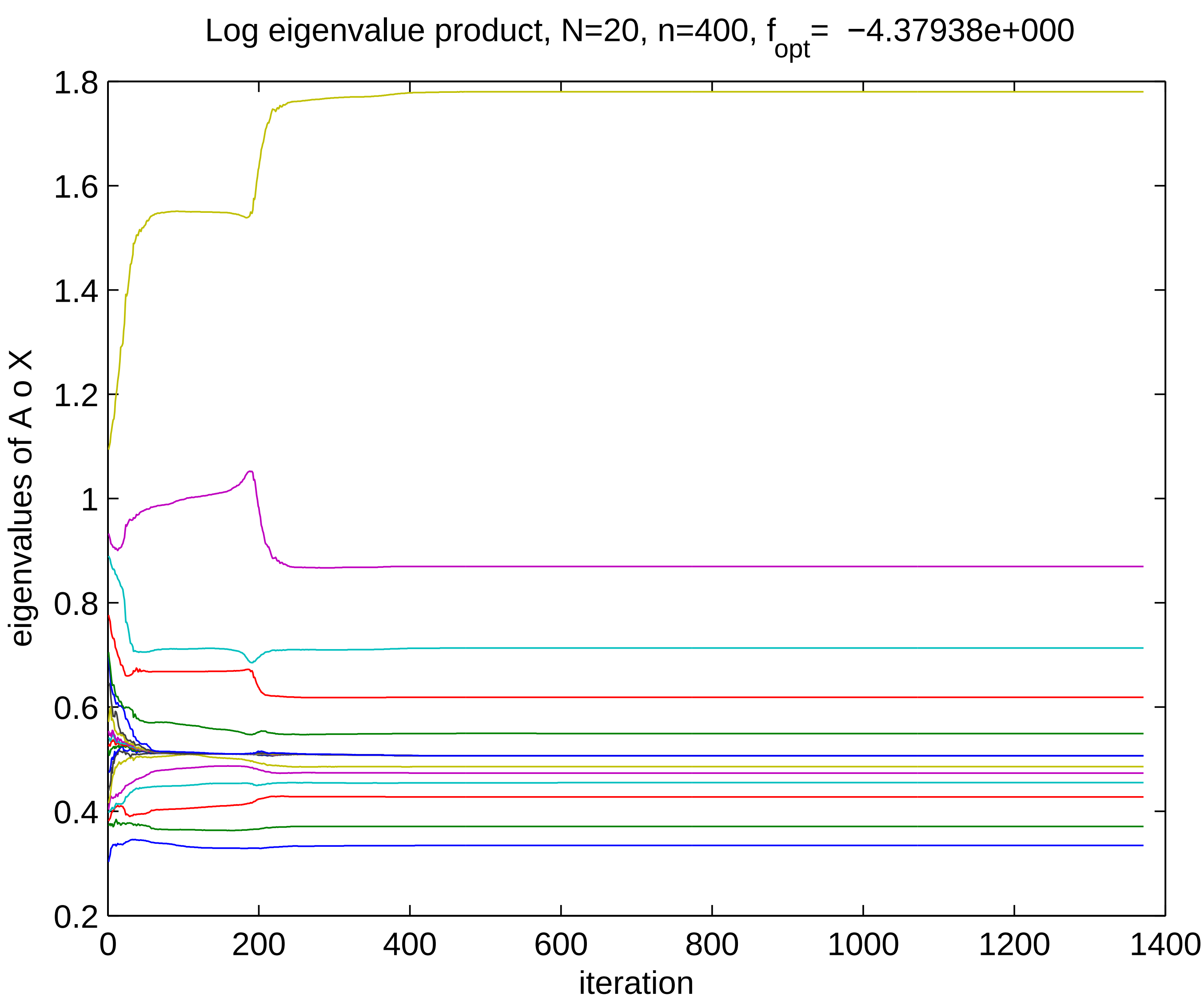
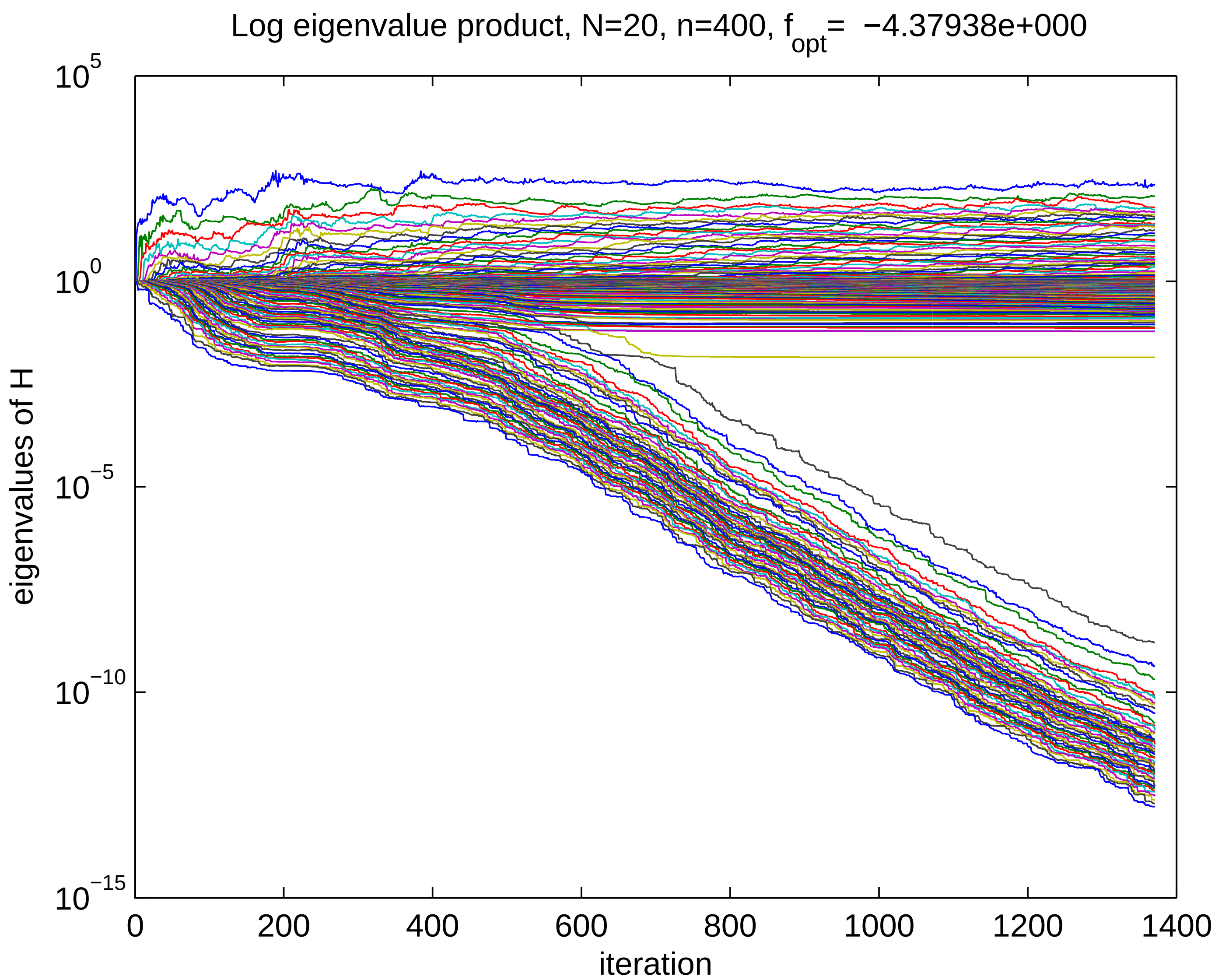


Note that $\lambda_6(X), \ldots, \lambda_{14}(X)$ coalesce

Evolution of Eigenvalues of H



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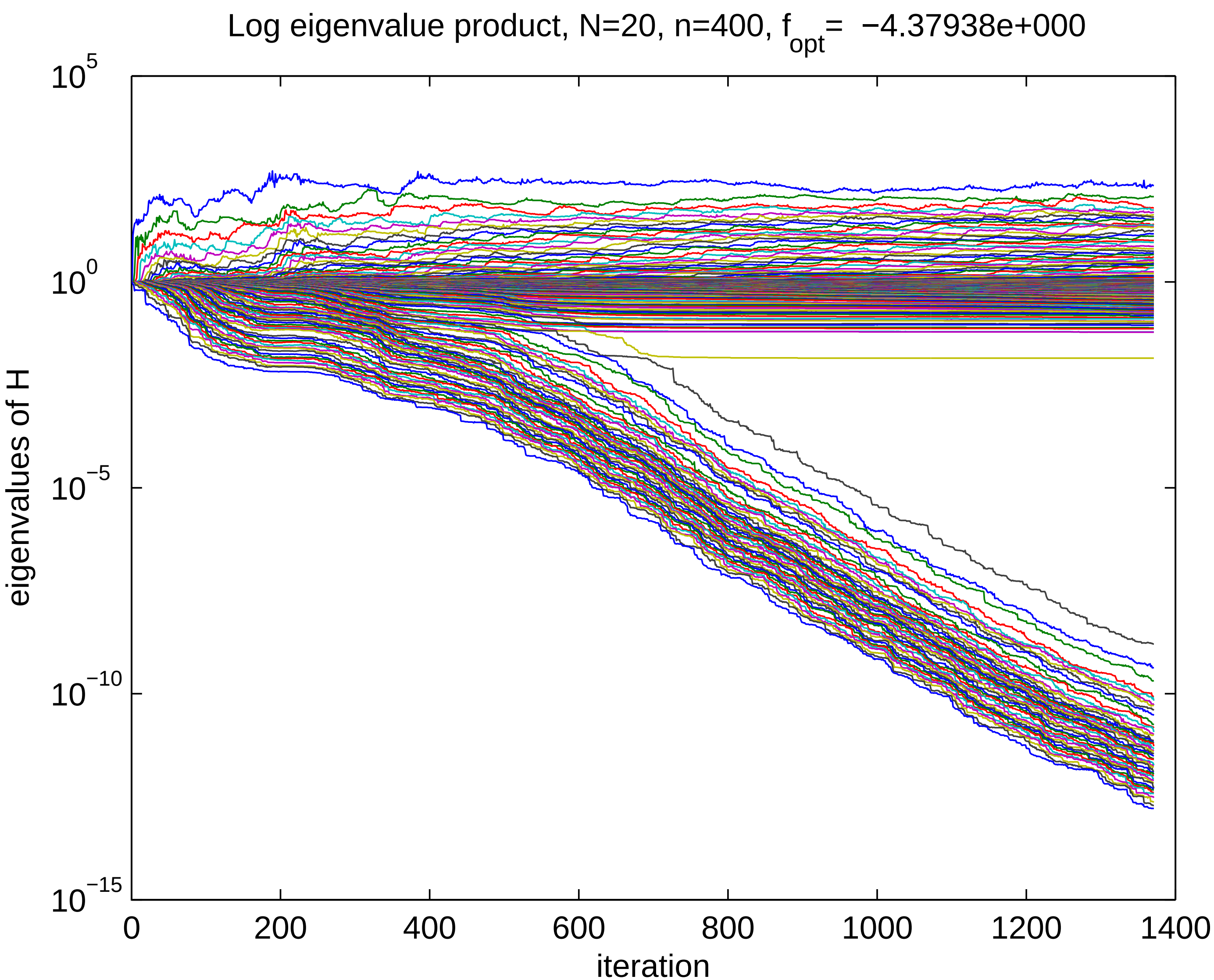

44 eigenvalues of H converge to zero...why???

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- All convex functions are regular
- All smooth (C^1) functions are regular
- Nonsmooth concave functions are not regular
  Example: $f(x) = -|x|$

Note: this is a somewhat simpler definition of regularity than the one in Lecture 12, but it is less precise: it defines regularity in a neighborhood, not at a point.

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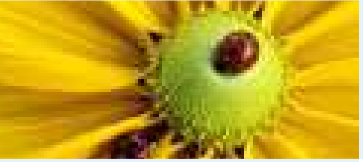

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For nonzero y in the V-space, the mapping $t \mapsto f(x + ty)$ is necessarily nonsmooth at $t = 0$, while for nonzero y in the U-space, $t \mapsto f(x + ty)$ is differentiable at $t = 0$ as long as f is locally Lipschitz.

Partly Smooth Functions: Some Examples, $n = 2$

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Question: What is $\mathcal{M}$ and what are the U and V spaces at $\bar{x} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$?

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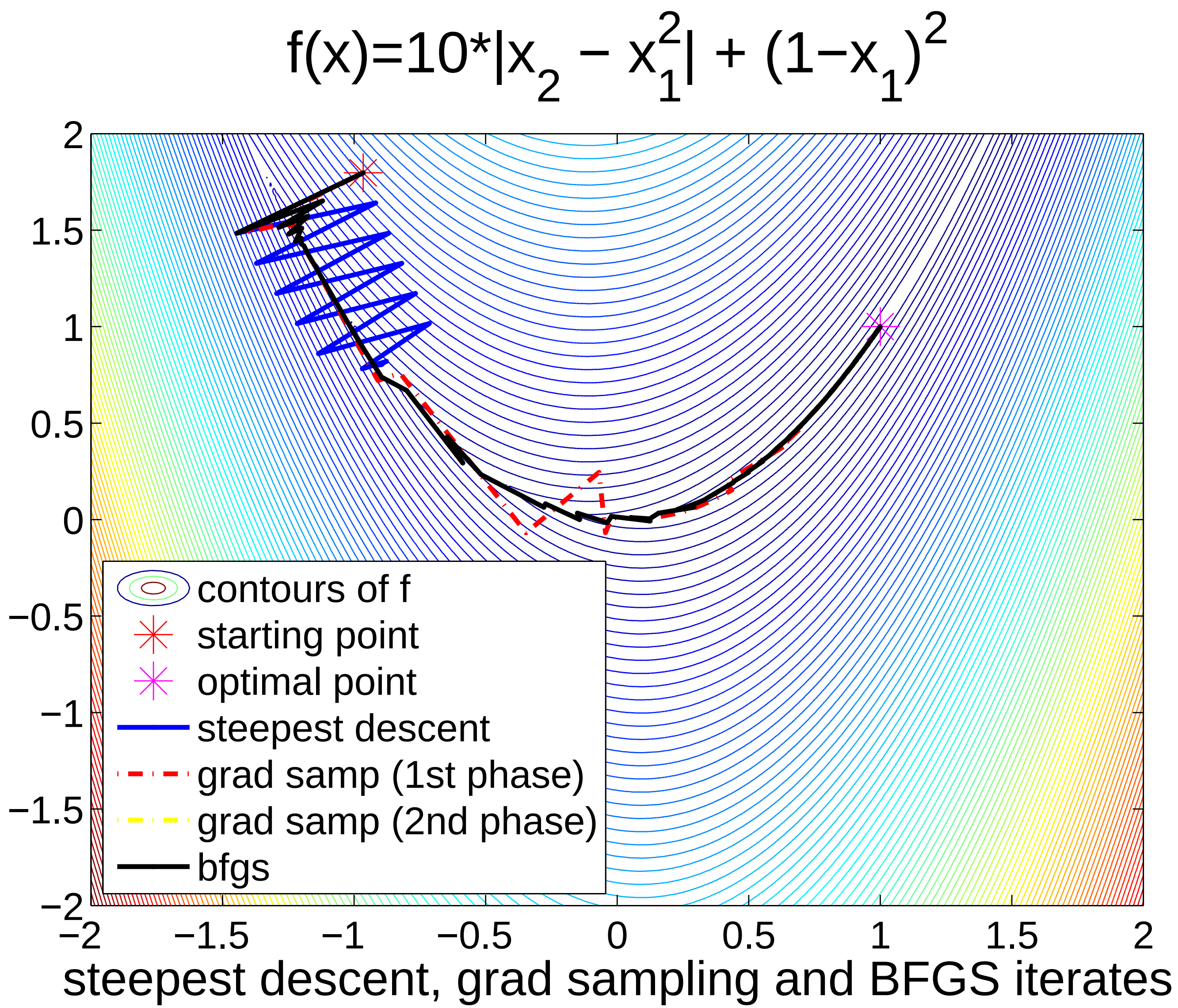
Same Example Again



Why Did 44 Eigenvalues of H Converge to Zero?

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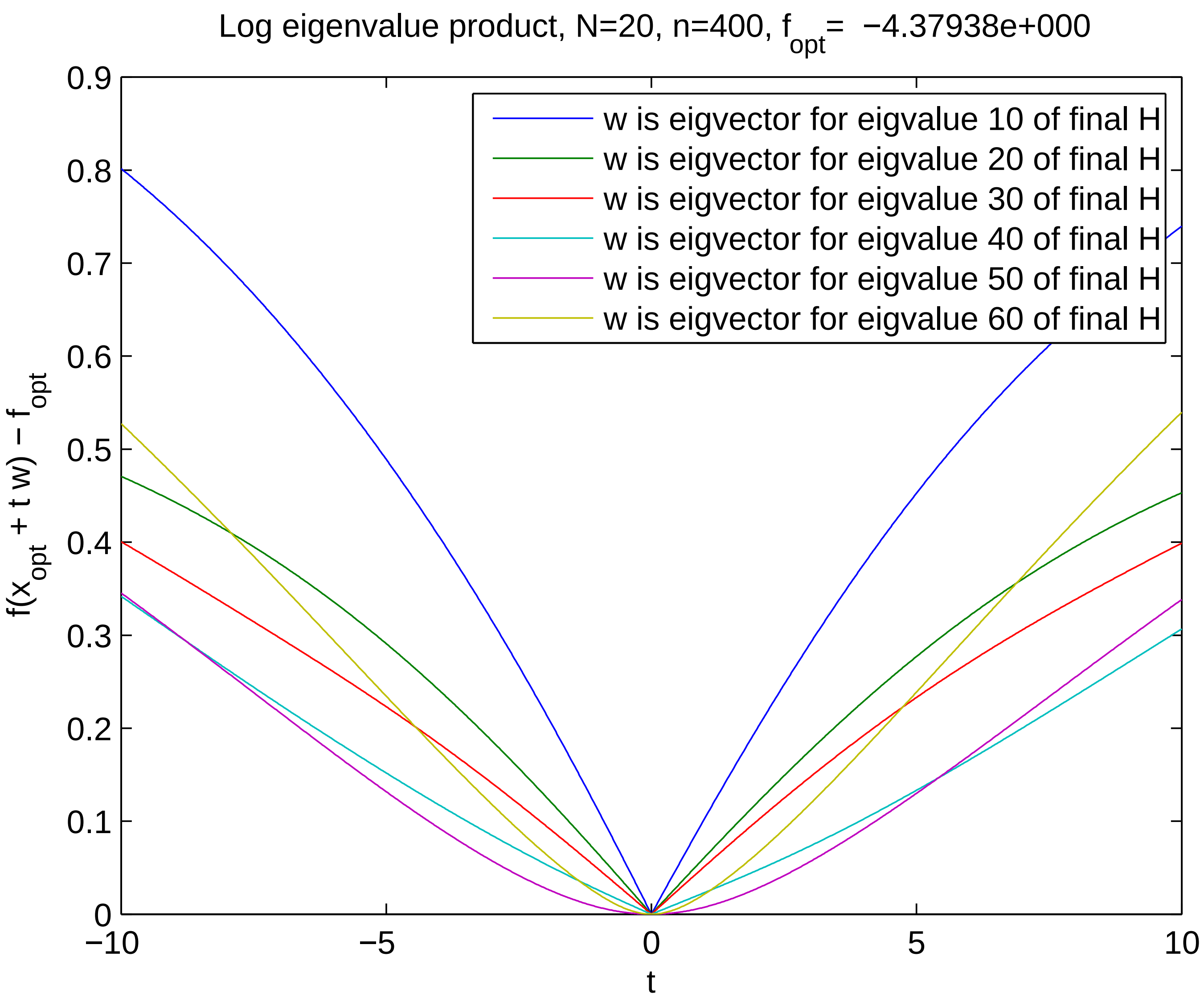
Thus BFGS *automatically* detected the U and V space partitioning without knowing anything about the mathematical structure of f!

Variation of f from Minimizer, along EigVecs of H



Eigenvalues of H numbered *smallest to largest*

BFGS Theory for Special Nonsmooth Functions

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- $f(x) = |x_1| + x_2^2$: remains open!

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4. If $\{x\}$ converges to $\bar{x}$ where f is "partly smooth" w.r.t. a manifold $\mathcal{M}$ then the subspace defined by the eigenvectors corresponding to eigenvalues of H converging to zero converges to the "V-space" of f w.r.t. $\mathcal{M}$ at $\bar{x}$

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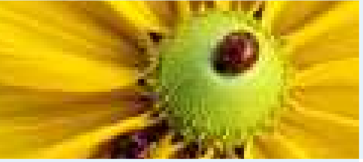

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A Difficult Nonconvex Problem from Nesterov

An Aside: Chebyshev Polynomials

A sequence of orthogonal polynomials defined on $[-1, 1]$ by

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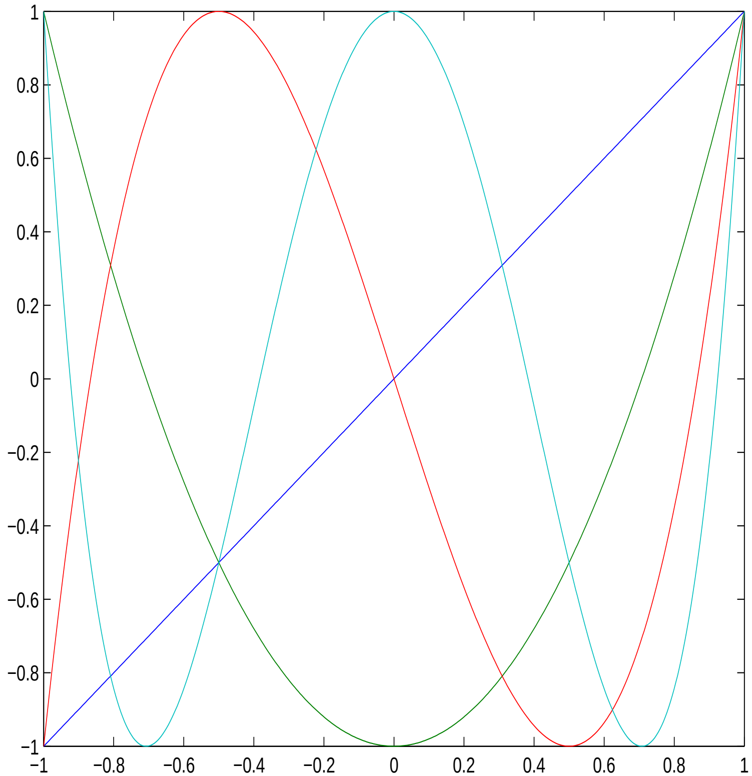
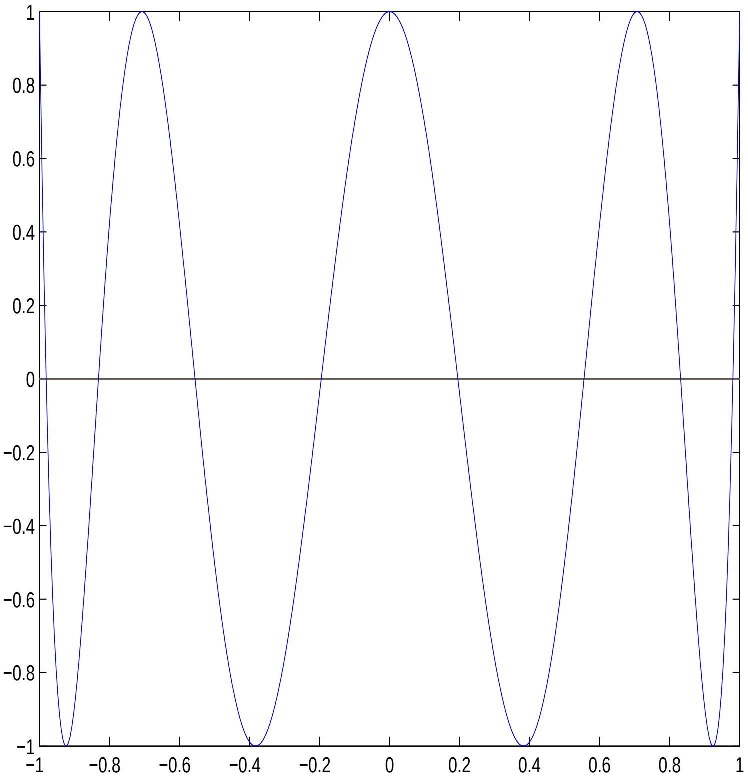
Plots of Chebyshev Polynomials





Left: Plots of $T_0(x), \ldots, T_4(x)$ Right: Plot of $T_8(x)$.

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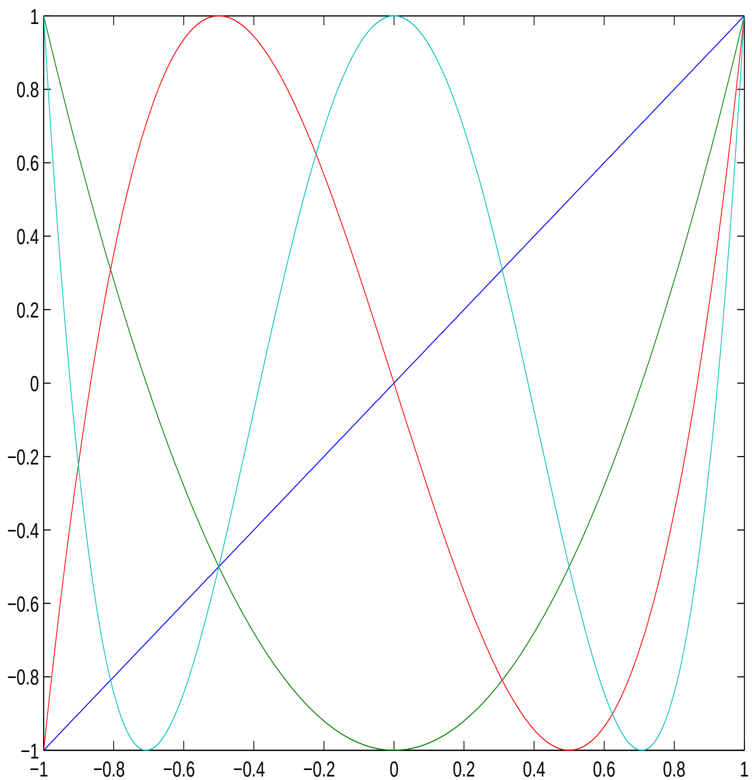

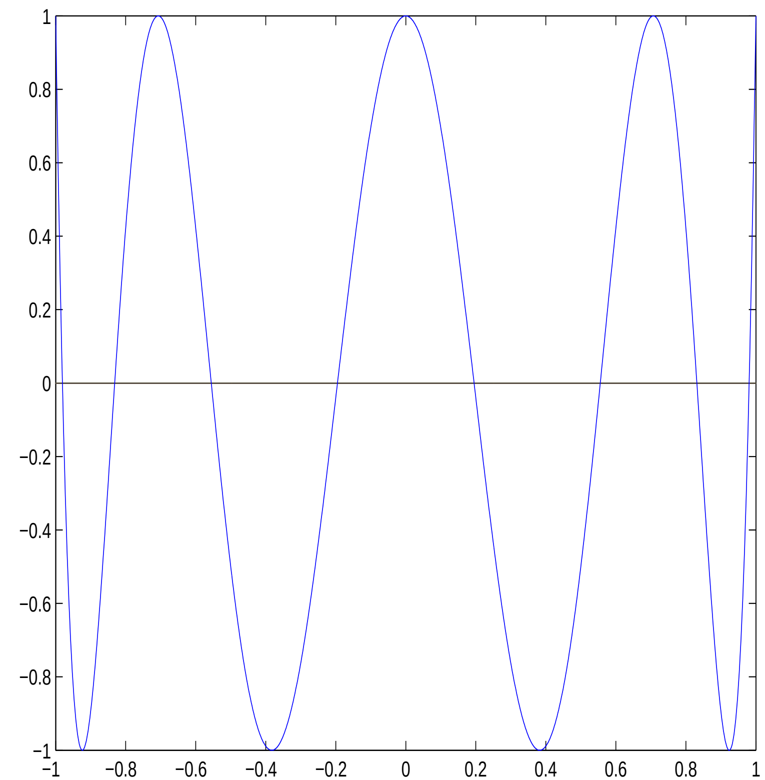

Left: Plots of $T_0(x), \ldots, T_4(x)$ Right: Plot of $T_8(x)$.

Question: How many extrema does $T_n(x)$ have in $[-1, 1]$?

Nesterov's Chebyshev-Rosenbrock Functions

Consider the function

$$N_p(x) = \frac{1}{4}(x_1 - 1)^2 + \sum_{i=1}^{n-1} |x_{i+1} - 2x_i^2 + 1|^p, \quad \text{where } p \geq 1$$

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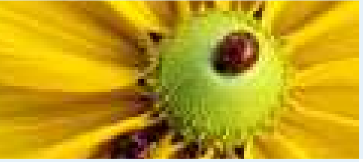

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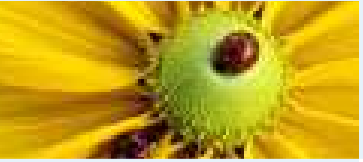

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Newton's method is not much faster, although it converges quadratically at the end.

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The method appears to be converging, very slowly, but may be having numerical difficulties.

Second Nonsmooth Variant of Nesterov's Function

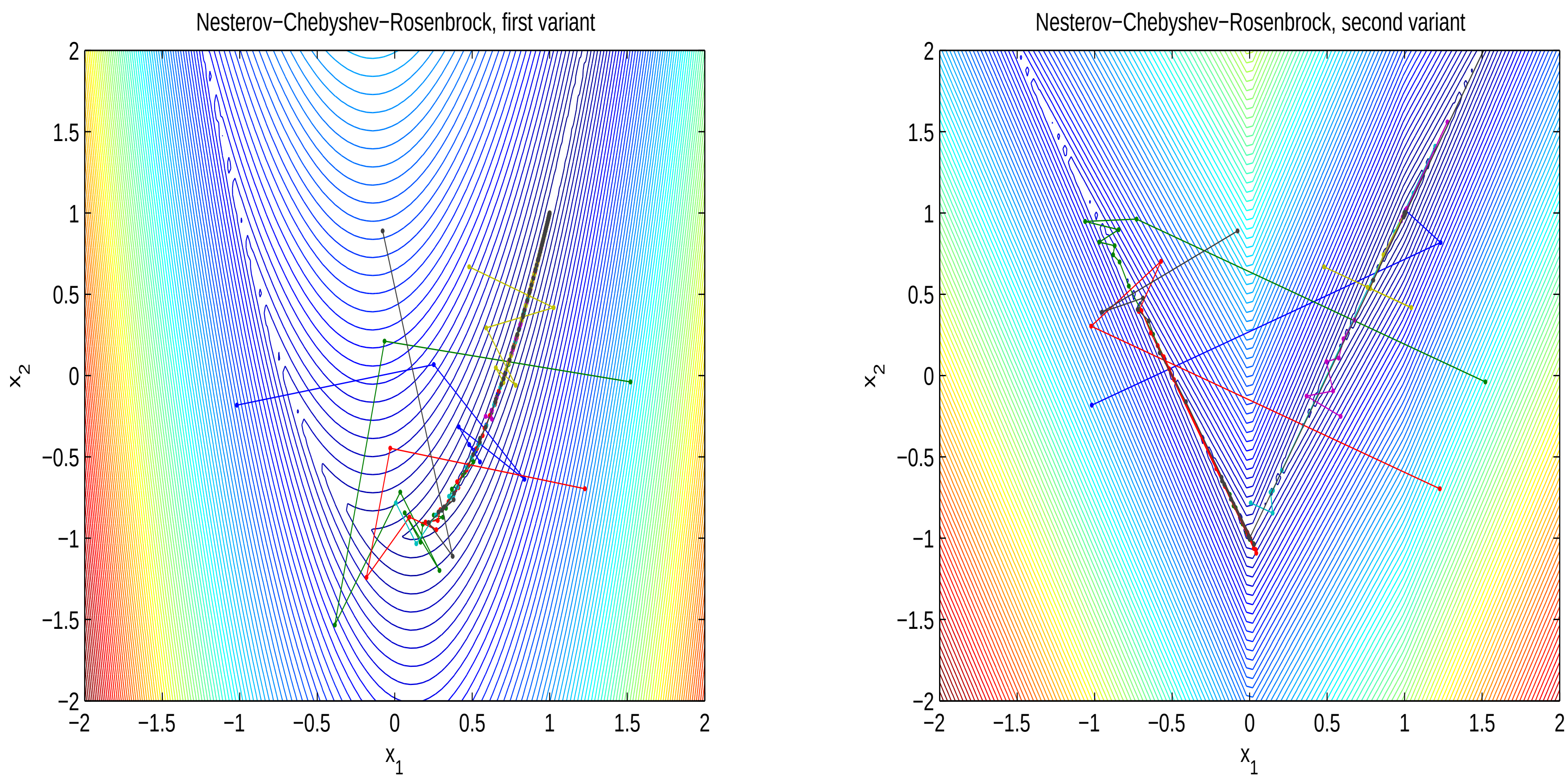
$$\widehat{N}_1(x) = \frac{1}{4}|x_1 - 1| + \sum_{i=1}^{n-1} |x_{i+1} - 2|x_i| + 1|.$$

Again, the unique global minimizer is x^*. The second term is zero on the set

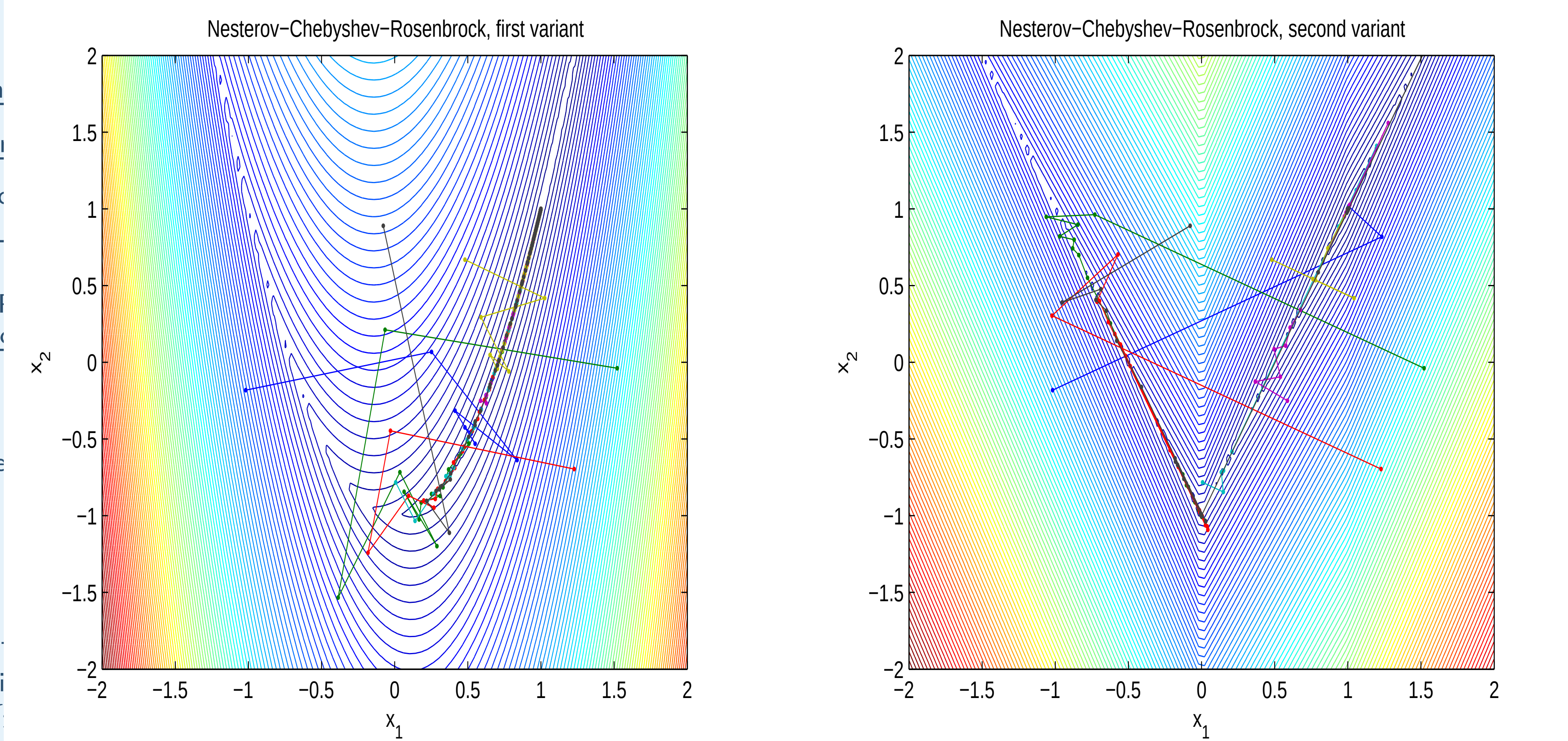
$$S = \{x : x_{i+1} = 2|x_i| - 1, \quad i = 1, \ldots, n-1\}$$

but S is not a manifold: it has "corners".

Contour Plots of the Nonsmooth Variants for $n = 2$



Contour plots of nonsmooth Chebyshev-Rosenbrock functions N_1 (left) and $\widehat{N}_1$ (right), with $n = 2$, with iterates generated by BFGS initialized at 7 different randomly generated points.



Contour plots of nonsmooth Chebyshev-Rosenbrock functions N_1 (left) and $\widehat{N}_1$ (right), with $n = 2$, with iterates generated by BFGS initialized at 7 different randomly generated points.
On the left, always get convergence to $x^* = [1, 1]^T$. On the right, most runs converge to $[1, 1]$ but some go to $x = [0, -1]^T$.

Properties of the Second Nonsmooth Variant $\widehat{N}_1$

When $n = 2$, the point $x = [0, -1]^T$ is Clarke stationary for the second nonsmooth variant $\widehat{N}_1$. We can see this because zero is in the convex hull of the gradient limits for $\widehat{N}_1$ at the point x.

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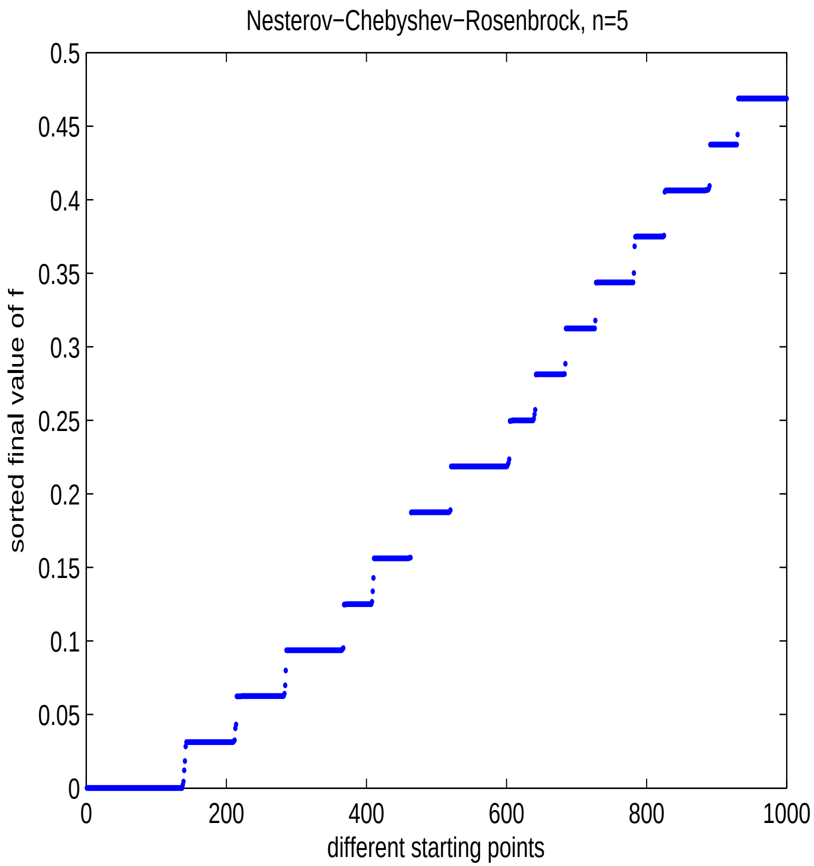
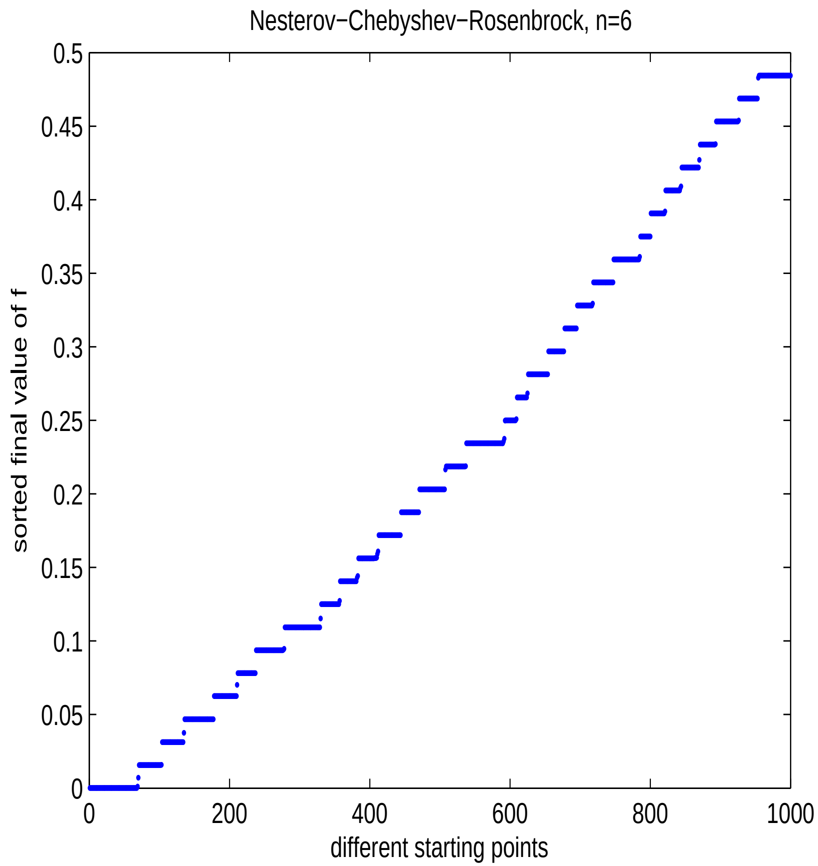
Furthermore, starting from enough randomly generated starting points, BFGS finds all 2^{n-1} Clarke stationary points!

Behavior of BFGS on the Second Nonsmooth Variant





Left: *sorted* final values of $\widehat{N}_1$ for 1000 randomly generated starting points, when $n = 5$: BFGS finds all 16 Clarke stationary points. Right: same with $n = 6$: BFGS finds all 32 Clarke stationary points.

Convergence to Non-Locally-Minimizing Points

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Nonetheless, we don't know whether, in exact arithmetic, the methods would actually generate sequences converging to the nonminimizing Clarke stationary points. Experiments by Kaku (2011) suggest that the higher the precision used, the more likely BFGS is to eventually move away from such a point.

Limited Memory Methods

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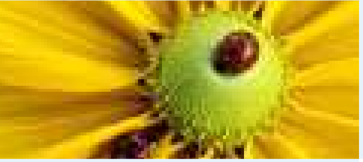
$$(s_j, y_j), \quad j = k-m, \ldots, k-1,$$

where

$$s_j = x_{j+1} - x_j, \quad y_{j+1} = \nabla f(x_{j+1}) - \nabla f(x_j)$$

to an initial inverse Hessian approximation $H_0^{(k)}$.



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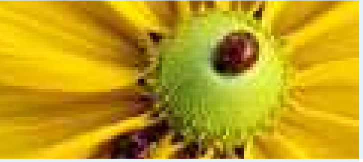

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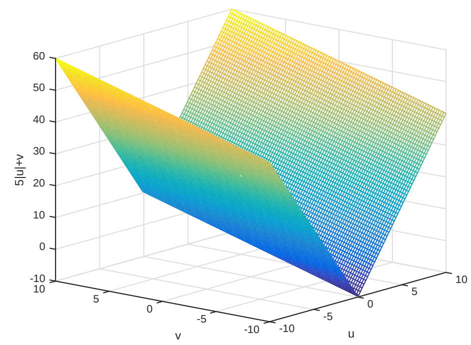
Question: how effective is it on nonsmooth problems?

A Nonsmooth Convex Function, Unbounded Below

Let's reconsider

$$f(x) = a|x_1| + x_2$$

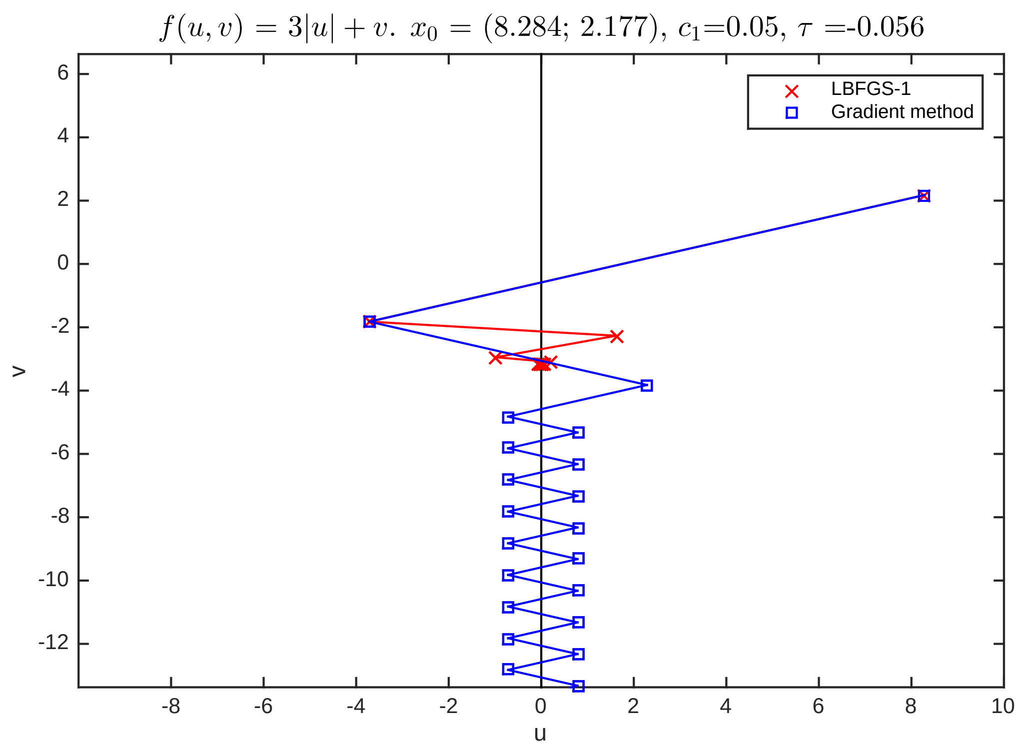
with $a \geq 1$.



Turns out that L-BFGS-1 (saving just one update) with scaling fails for *smaller* values of a than the critical value beyond which Gradient Descent fails!

L-BFGS-1 vs. Gradient Descent

Red: path of L-BFGS-1 with scaling, converges to non-stationary point.
Blue: path of the gradient method with same Armijo-Wolfe line search, generates $f(x) \downarrow -\infty$.



Convergence of the L-BFGS-1 Search Direction

Theorem. Let $d^{(k)}$ be the search direction generated by L-BFGS-1 with scaling applied to $f(x) = a|x_1| + \sum_{i=2}^n x_i$ using an Armijo-Wolfe line search. If $\sqrt{4(n-1)} \leq a$, then $\frac{|d^{(k)}|}{||d^{(k)}||}$ converges to some constant direction d. Furthermore, if

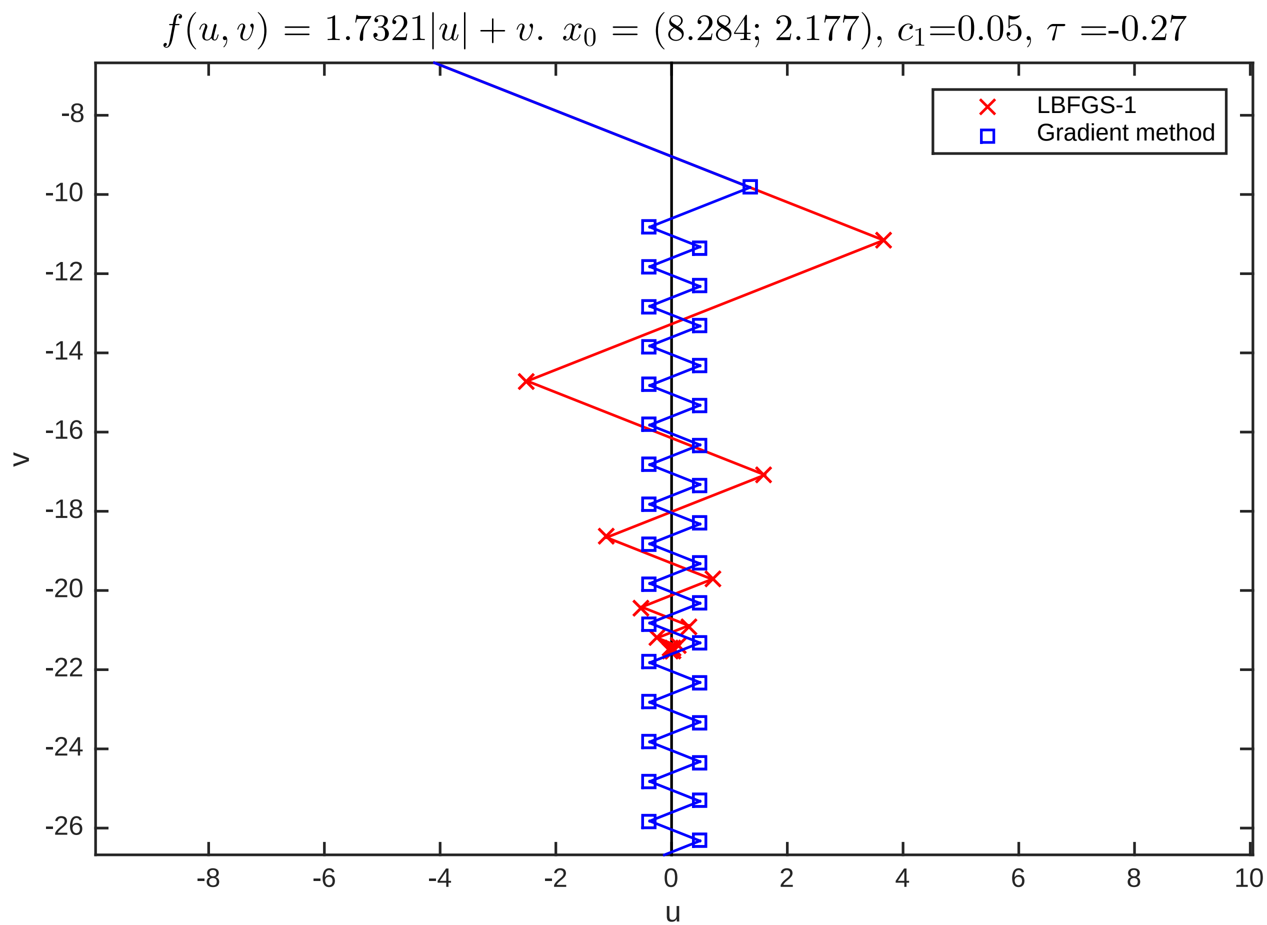
$$a(a + \sqrt{a^2 - 3(n-1)}) > (\frac{1}{c_1} - 1)(n-1),$$

where c_1 is the Armijo parameter, then the iterates $x^{(k)}$ converge to a non-stationary point.

Azam Asl, 2018.

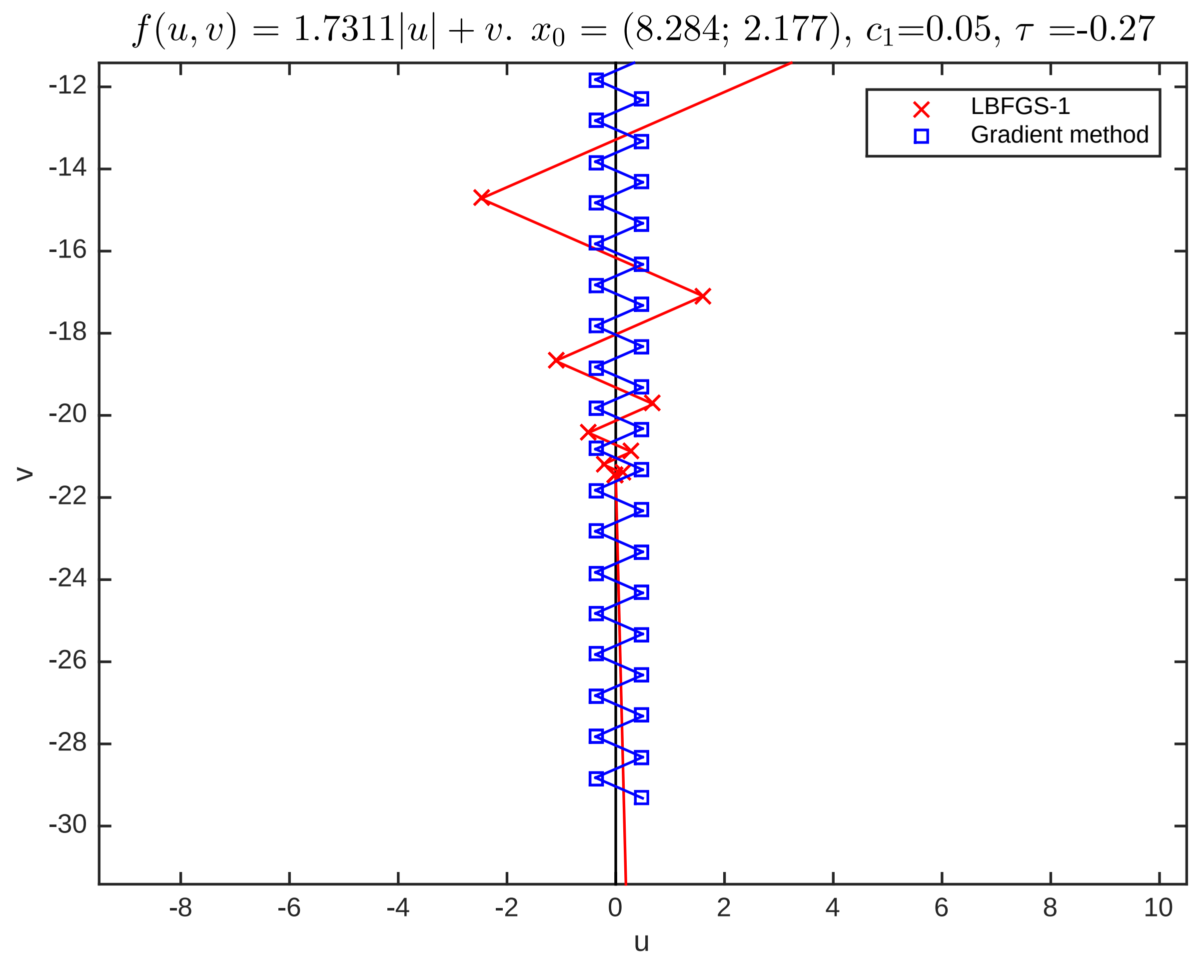
Experiment, with $n = 2$ and $a = \sqrt{3}$

In practice we observe that $\sqrt{3(n-1)} \leq a$ suffices for the method to fail, which is a weaker condition than the previous one. Below with $n = 2$ and $a = \sqrt{3}$ the method fails:



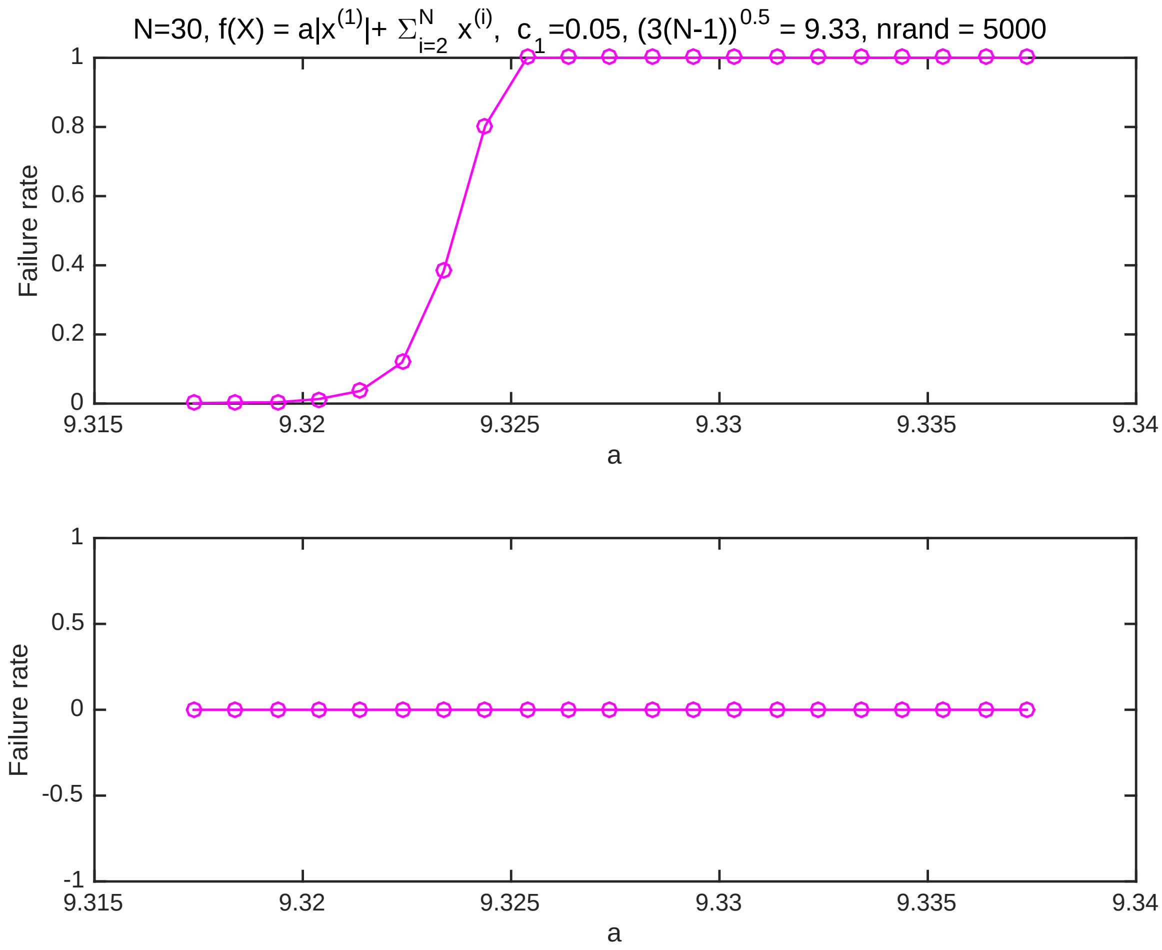
Experiment: slightly smaller a

But if we set $a = \sqrt{3} - 0.001$, it succeeds "at the last minute".



Experiments: Top, scaling on; Bottom, scaling off

$$n = 30, \ \sqrt{3(n-1)} = 9.327$$



Nesterov's Ill-Conditioned Nonsmooth Convex Function

Another Challenging Problem from Nesterov

Consider the nonsmooth, convex function

$$f(x) = \max\left(|x_1|, \quad \{|x_i - 2x_{i-1}|, i = 2, \ldots, n\}\right)$$

and set

$$\tilde{x}_1 = 1, \quad \tilde{x}_i = 2\tilde{x}_{i-1} + 1, i = 2, \ldots, n.$$

Then $f(\tilde{x}) = 1$ although $\|\tilde{x}\| \approx 2^n$.

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$$f_\mu(x) = \mathrm{softmax}\Big(\pm x_1, \pm\{x_i - 2x_{i-1}, i = 2, ..., n\}\Big)$$

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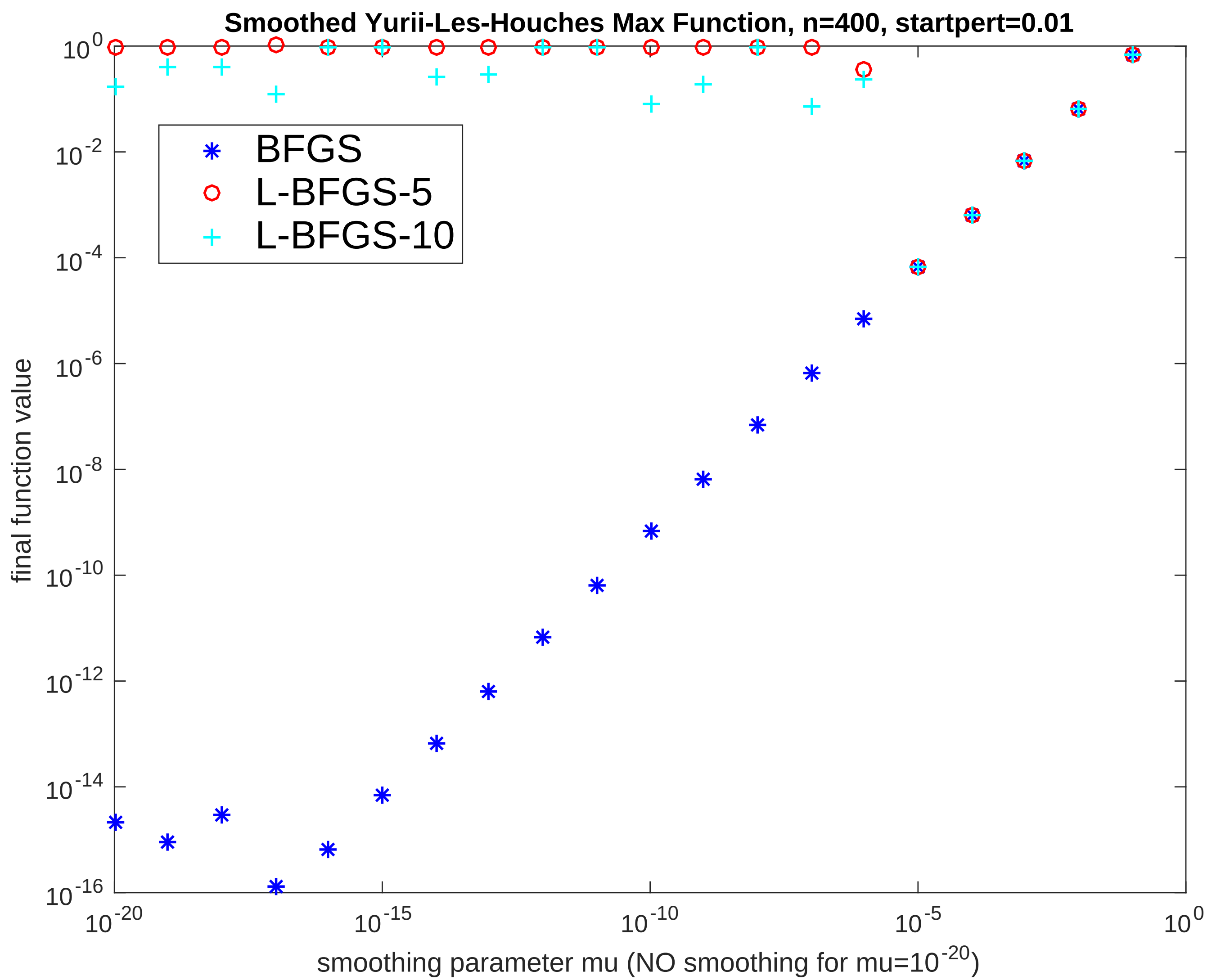
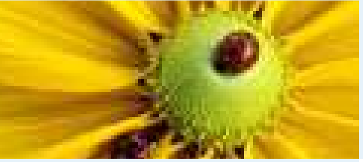
As smoothing parameter $\mu \to 0$, function $f_\mu \to f$.

BFGS and Limited Memory BFGS for $n = 400$



BFGS finds accurate solution independent of conditioning as $\mu \to 0$



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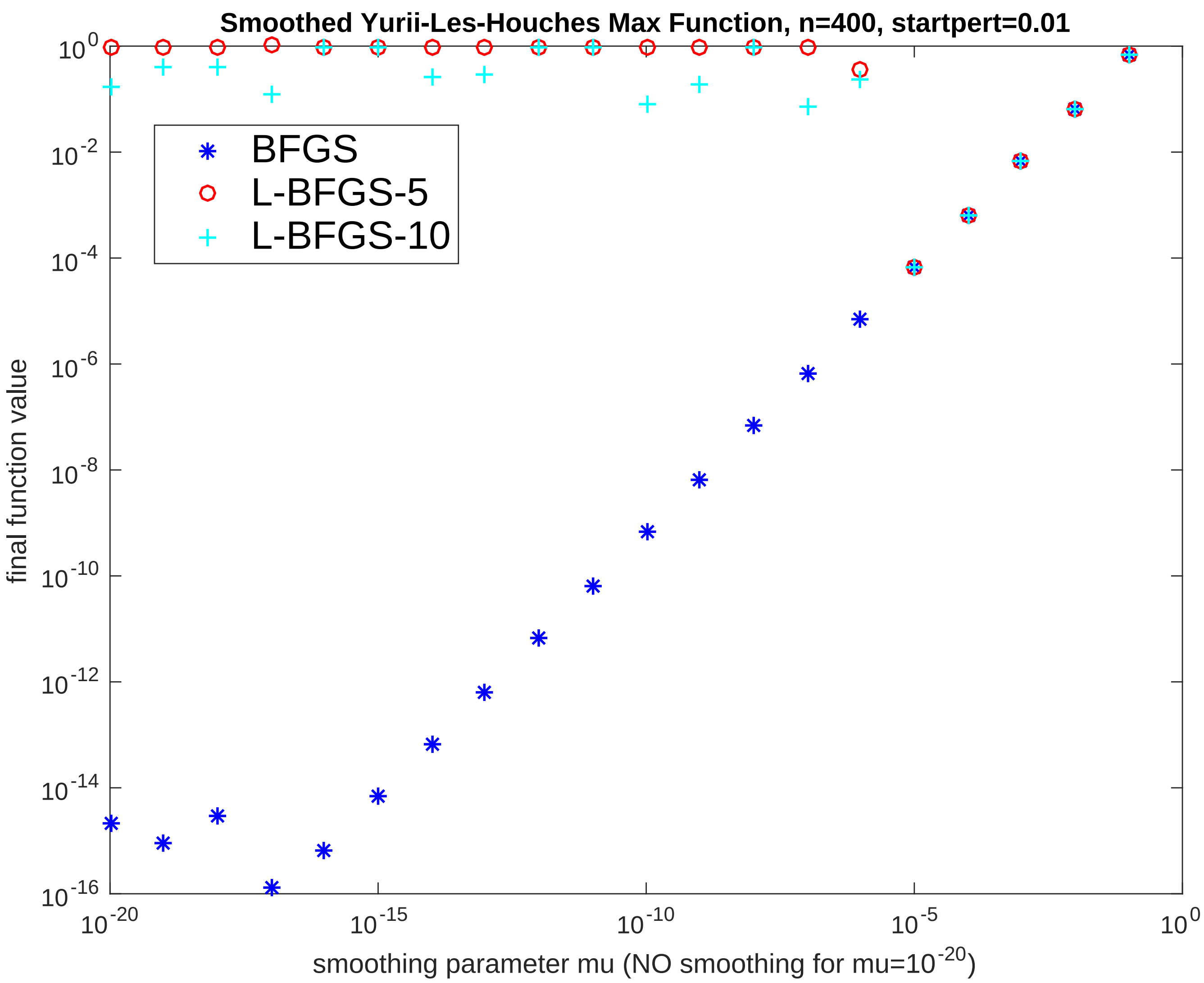

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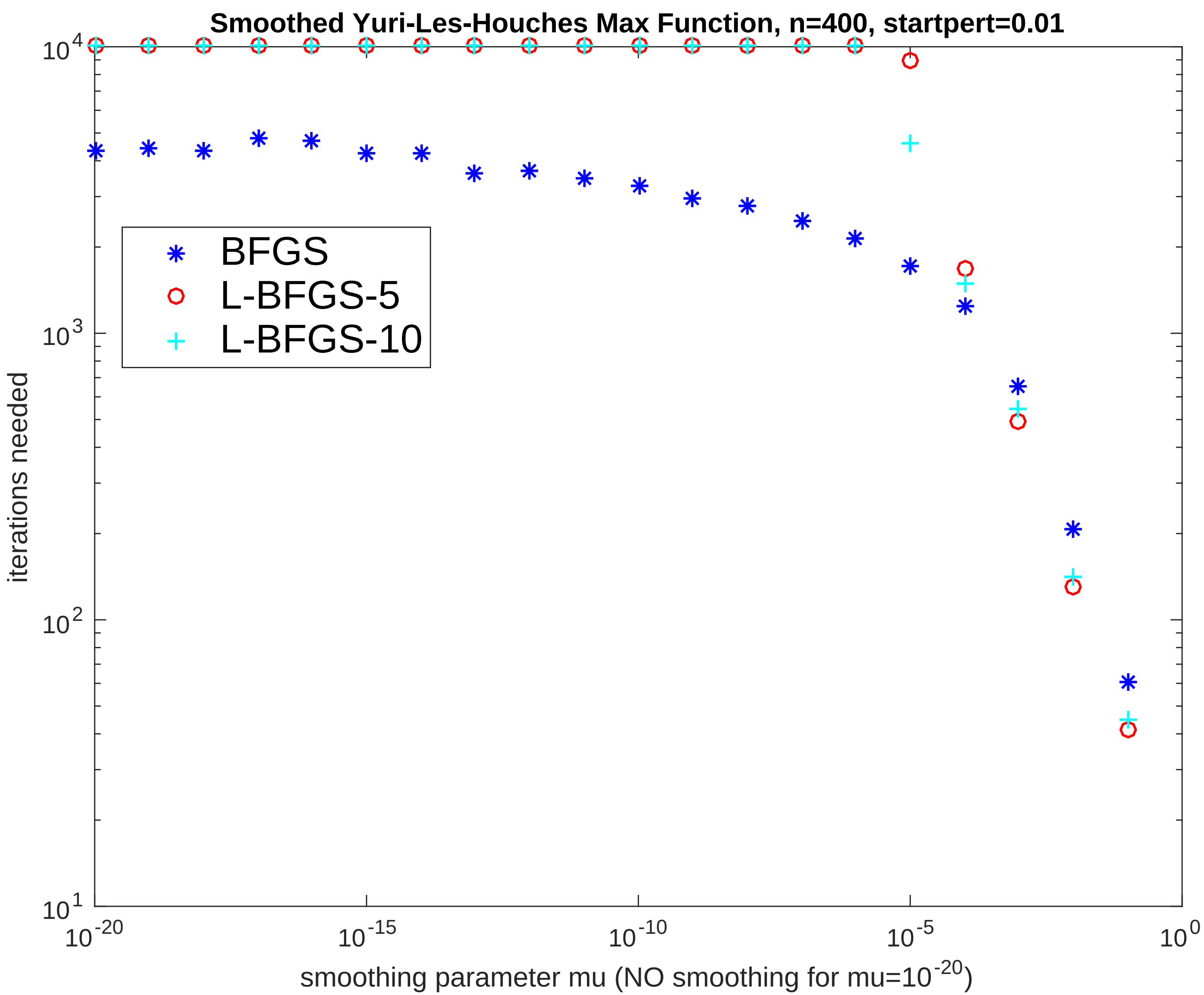
L-BFGS breaks down as $\mu \to 0$

Number of Iterations for $n = 400$



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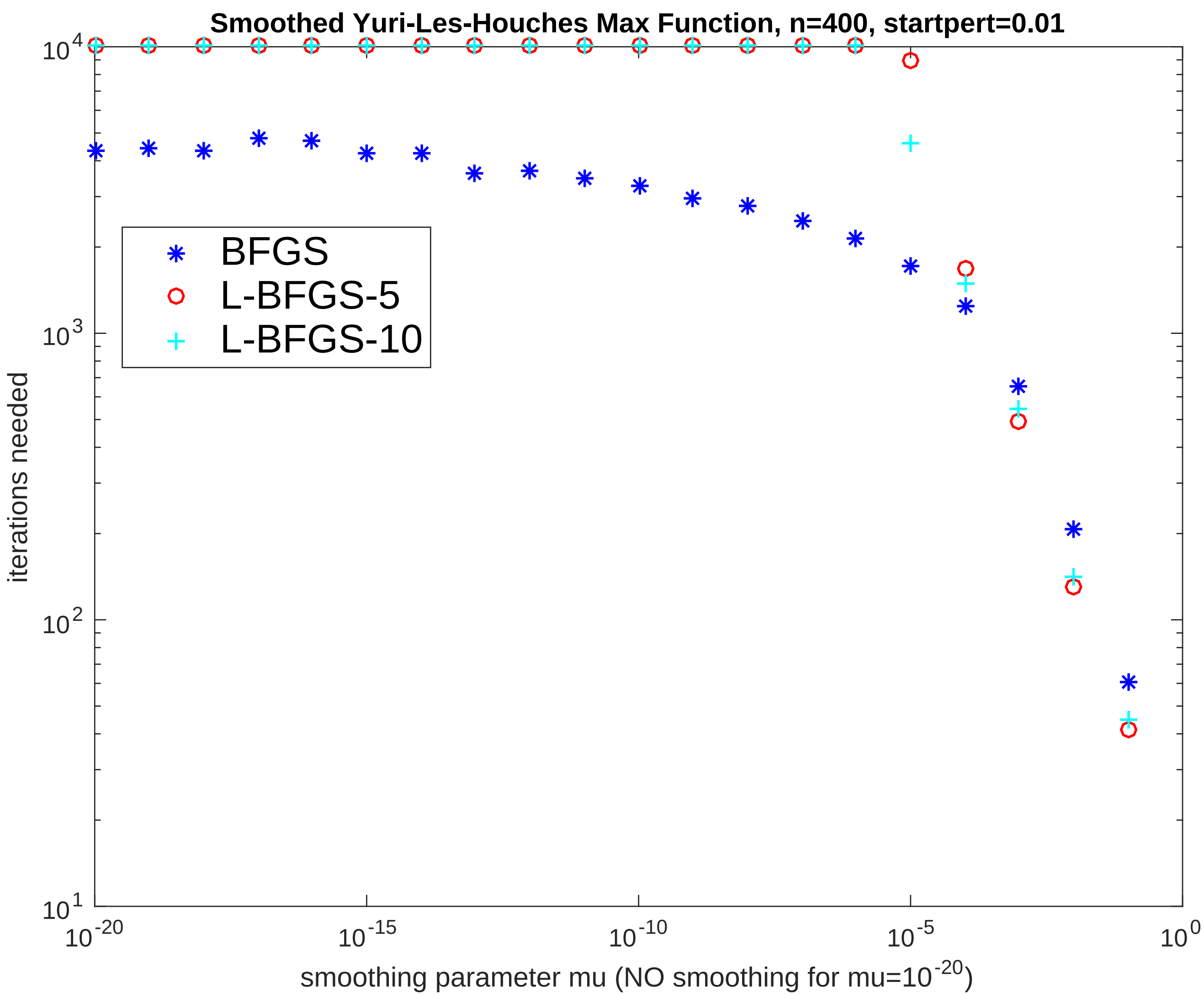

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L-BFGS iterations hits max iteration limit for small μ

Limited Effectiveness of Limited Memory BFGS

We have observed that that addition of nonsmoothness to a problem, convex or nonconvex, creates great difficulties for Limited Memory BFGS, with and without scaling, even when the dimension of the V-space is less than the size of the memory.

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We have observed that that addition of nonsmoothness to a problem, convex or nonconvex, creates great difficulties for Limited Memory BFGS, with and without scaling, even when the dimension of the V-space is less than the size of the memory.

Azam Asl's result establishes failure of L-BFGS-1 for a specific f when scaling is on; no such result is proved yet when scaling is off.

Limited Effectiveness of Limited Memory BFGS

We have observed that that addition of nonsmoothness to a problem, convex or nonconvex, creates great difficulties for Limited Memory BFGS, with and without scaling, even when the dimension of the V-space is less than the size of the memory.

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We have also investigated Limited Memory Gradient Sampling which does not work well either.

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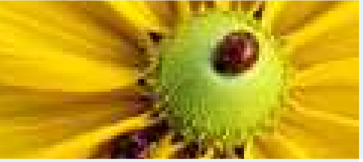

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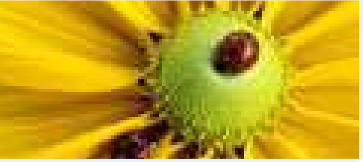

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Concluding Remarks

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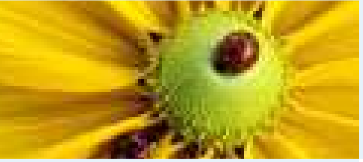

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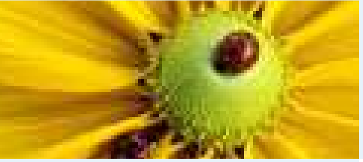

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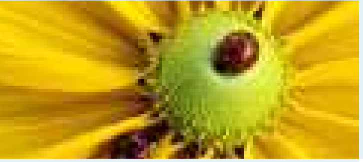

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Our software, HANSO and GRANSO, is available (unconstrained and constrained) along with HIFOO (H-infinity fixed order optimization) for controller design, which has been used successfully in many applications.

Our Papers

J. V. Burke, A. S. Lewis and M. L. Overton, A Robust Gradient Sampling Method for Nonsmooth, Nonconvex Optimization, *SIAM J. Optimization*, 2005

M. Gürbüzbalaban and M. L. Overton, On Nesterov's Nonsmooth Chebyshev-Rosenbrock Functions, *SIAM J. Optimization*, 2012

A. S. Lewis and M. L. Overton, Nonsmooth Optimization via Quasi-Newton Methods, *Math. Programming*, 2013

F. E. Curtis, T. Mitchell and M.L. Overton, A BFGS-SQP Method for Nonsmooth, Nonconvex, Constrained Optimization and its Evaluation using Relative Minimization Profiles, *Optimization Methods and Software*, 2016

A. Asl and M. L. Overton, Analysis of the Gradient Method with an Armijo-Wolfe Line Search on a Class of Nonsmooth Convex Functions, *Optimization Methods and Software*, 2020

A. Asl and M. L. Overton, Analysis of Limited-Memory BFGS on a Class of Nonsmooth Convex Functions IMA J. Numer. Anal., 2020

J. V. Burke, F. E. Curtis, A. S. Lewis, M. L. Overton and L. Simões, Gradient Sampling Methods for Nonsmooth Optimization, in: Numerical Nonsmooth Optimization: State of the Art Algorithms (Springer, 2020).

Papers, software are available at **www.cs.nyu.edu/overton**.