Exploring the Full Flexibility of Pattern Search[1]

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Problem:

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in \mathbf{R}^n, \end{array}$$

where $f : \mathbf{R}^n \to \mathbf{R}$.

This talk will concentrate on the *unconstrained* problem.

But there is a suite of analytical results (with Robert Michael Lewis) to handle classes of constrained problems of the general form:

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in S \subseteq \mathbf{R}^n. \end{array}$$

Generalized Pattern Search:

Given $x_0 \in \mathbf{R}^n$, $f(x_0)$, $P_0 \in \mathbf{R}^{n \times p_0}$, $p_0 \geq n+1$, $\Delta_0 > 0$, and ϵ, for $k = 0, 1, \ldots$ until $\Delta_k < \epsilon$ do $\{$

1. Find a step $s_k = \Delta_k p_k$ using the procedure `Exploratory_Moves`(Δ_k, P_k).

2. If $f(x_k + s_k) < f(x_k)$ then $x_{k+1} = x_k + s_k$; otherwise, $x_{k+1} = x_k$.

3. `Update`(Δ_k, P_k).

$\}$

The Curious Hypotheses:

A key condition for the convergence analysis for pattern search algorithms are the following hypotheses on the result of the `Exploratory_Moves`:

1. $s_k \in \Delta_k P_k \equiv \Delta_k [B\Gamma_k \; BL_k])$.

2. If

$$\min\{f(x_k + y),\ y \in \Delta_k B\Gamma_k\} \quad < \quad f(x_k)$$

   then

$$f(x_k + s_k) < f(x_k).$$

What Do These Hypotheses Say?

1. The s_k returned by the Exploratory Moves must be a column of the matrix $\Delta_k P_k$ (so that $x_k + s_k$ is contained in the rational lattice that underlies all pattern search methods).

2. The step s_k must satisfy either

$$f(x_k + s_k) \quad < \quad f(x_k)$$

   or

$$s_k \quad = \quad 0.$$

   Furthermore, s_k may be 0 *only* if none of the steps in $\Delta_k B \Gamma_k$ yielded simple decrease on $f(x_k)$.

What Makes This Unusual?

1. The simple decrease condition.

   We can accept any step $s_k \in \Delta_k P_k$ that satisfies

   $$f(x_k + s_k) \quad < \quad f(x_k)$$

   and still obtain global convergence.

2. We only need full local information to reduce Δ_k.

   In other words, to set $s_k = 0$, we need to know that for all $y \in \Delta_k B\Gamma_k$,

   $$f(x_k + y) \quad \geq \quad f(x_k).$$

   But for *any* other choice of $s_k \in \Delta_k P_k$, it is sufficient to know that

   $$f(x_k + s_k) \quad < \quad f(x_k)$$

What Are the Consequences?

1. We may be able to conclude an iteration with a new iterate using only a single new function evaluation.

2. The necessarily expensive iterations are those that require us to obtain full local information before setting

$$s_k \quad = \quad 0$$

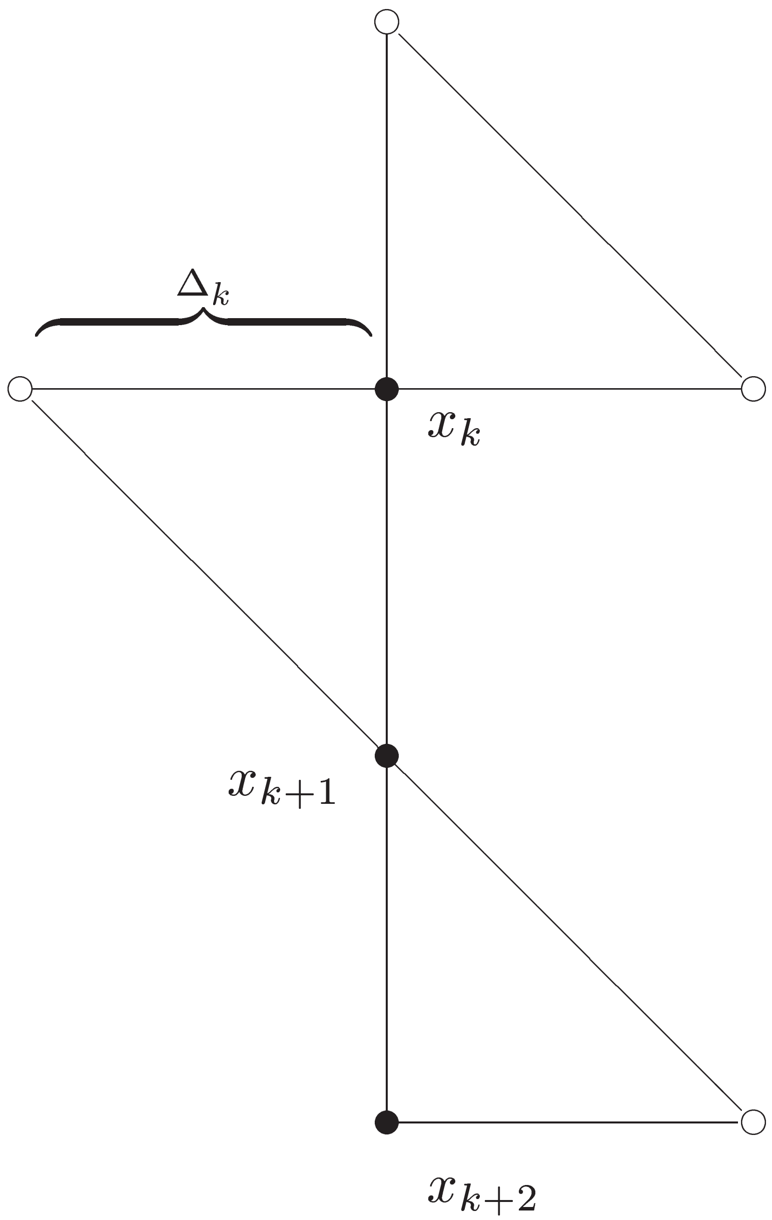
since we must evaluate

$$f(x_k + y) \quad \forall \quad \in \Delta_k B\Gamma_k$$

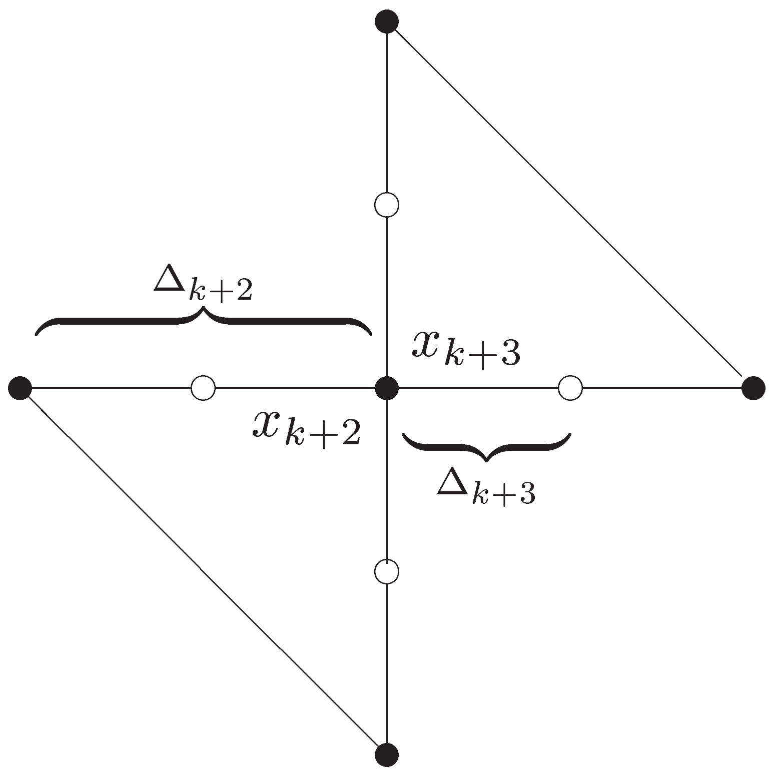
and

$$n + 1 \leq \quad |B\Gamma_k| \quad \leq 2n.$$

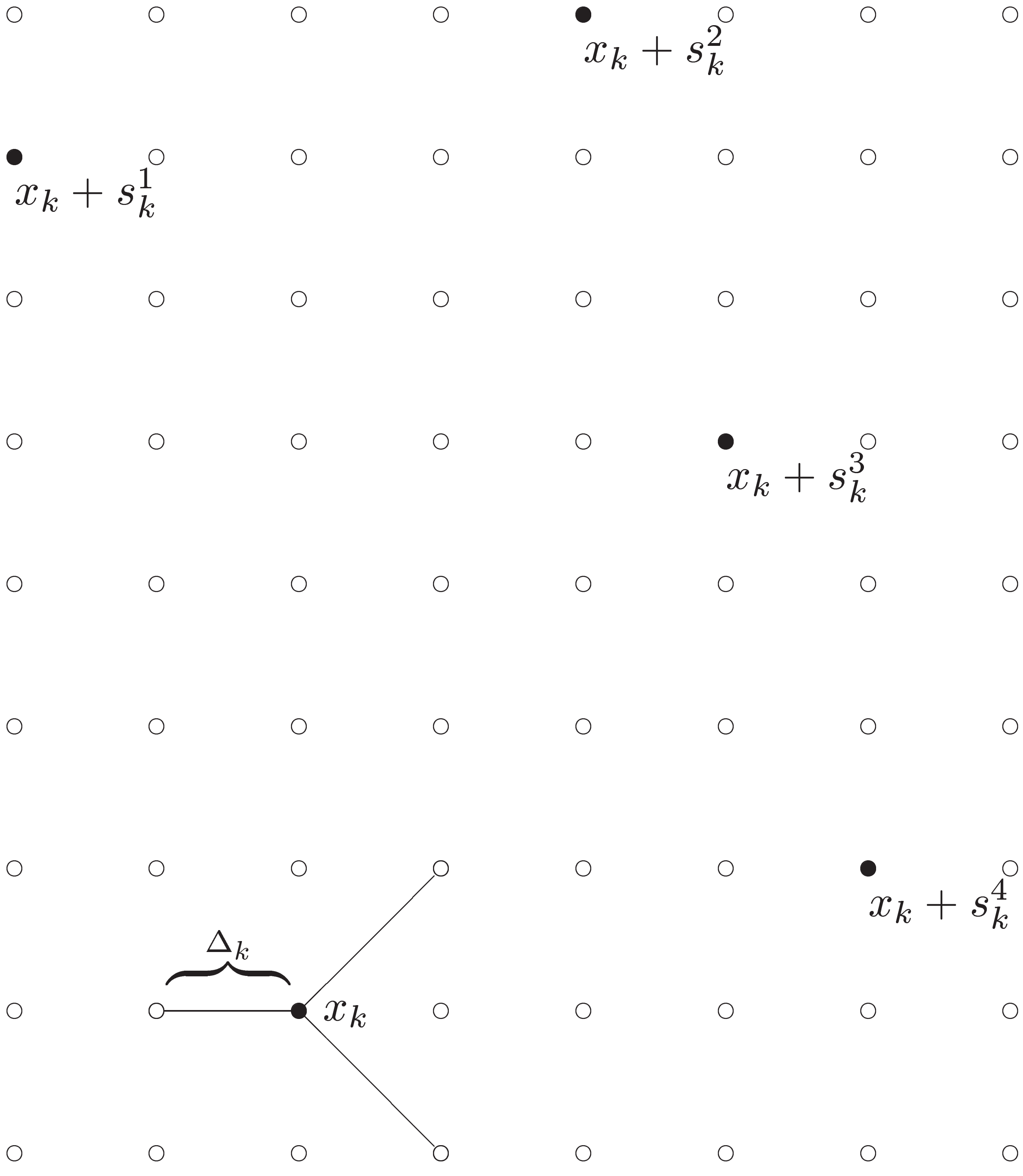
Possible Sequence of “Low-Overhead” Iterations:



What It Takes to Then Reduce Δ:



We Can Have Even More Speculative Strategies:



What Is Their Role?

1. By requiring the iterates to remain on a rational lattice, we ensure that we cannot take steps that are either too long or too short.

2. By requiring full local information before reducing Δ, we ensure that the steps cannot decrease prematurely, but we also ensure that we have at looked along at least one gradient-related direction.

The hypotheses relax the *sufficient decrease* condition to one of *simple decrease*.

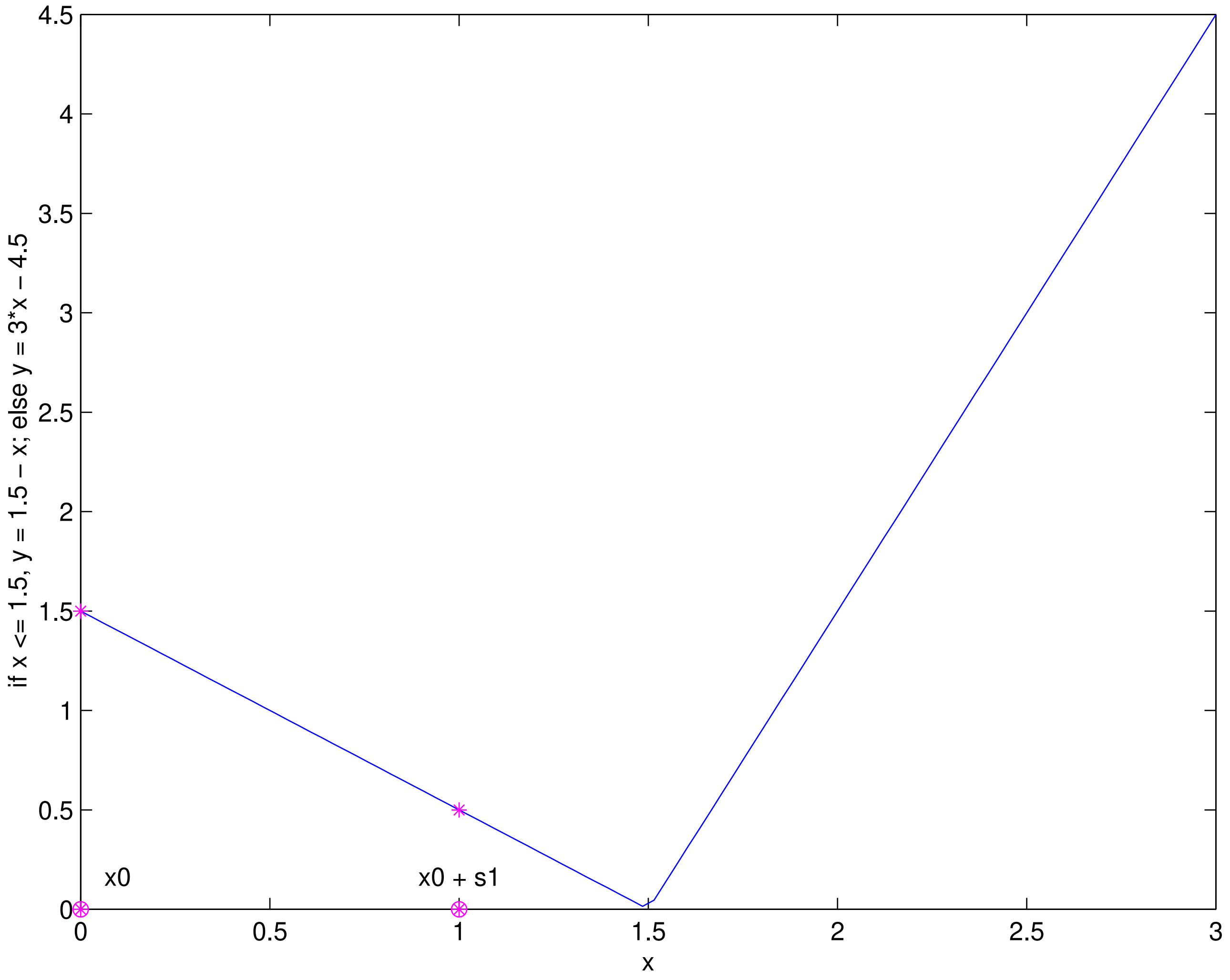
But the trade-off is to place stronger conditions on the form of the step s_k.

Do They Matter in Practice?

The answer is “Yes.”

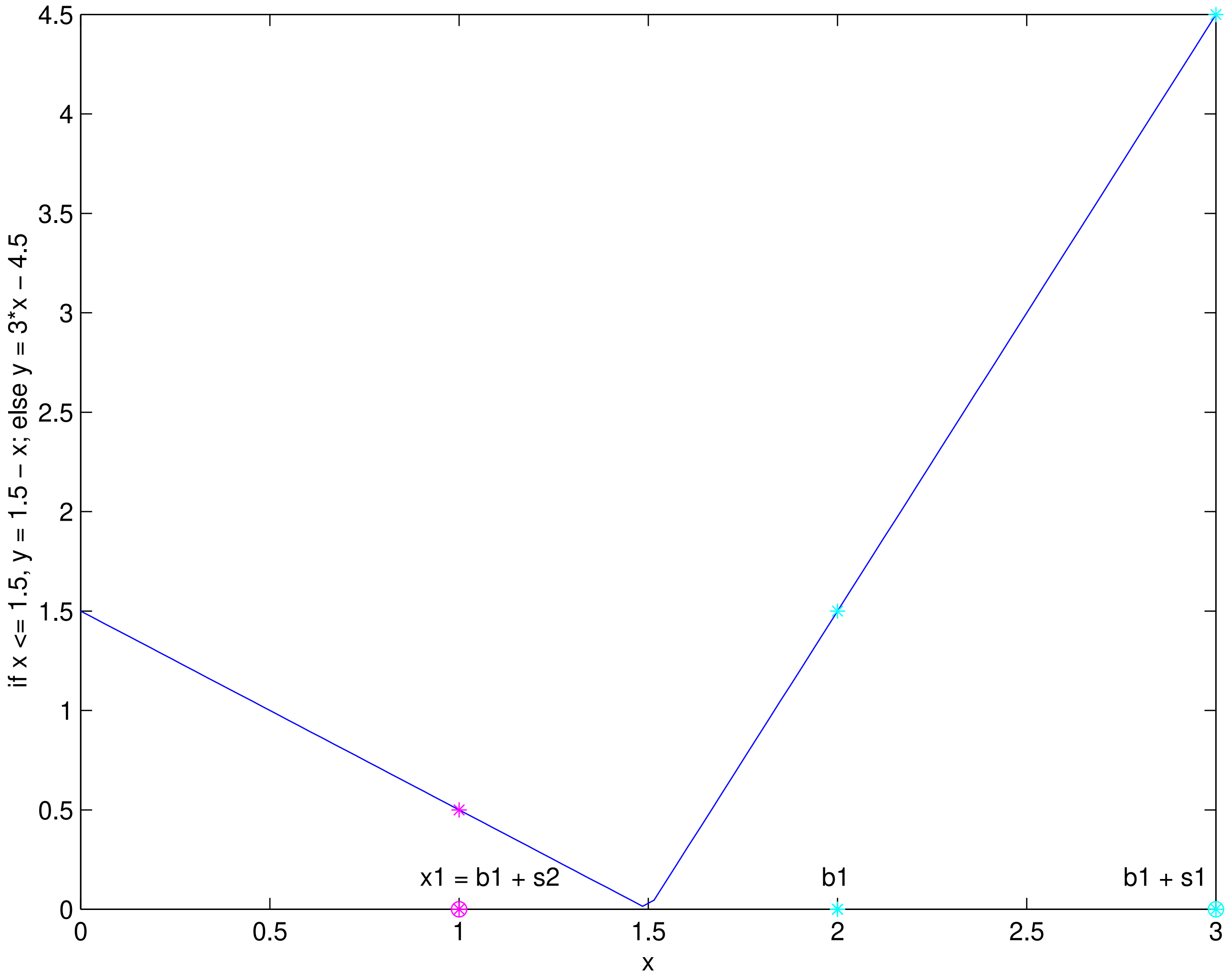
- The tale of Hooke and Jeeves.
- The useful role of Δ.

Iteration 1

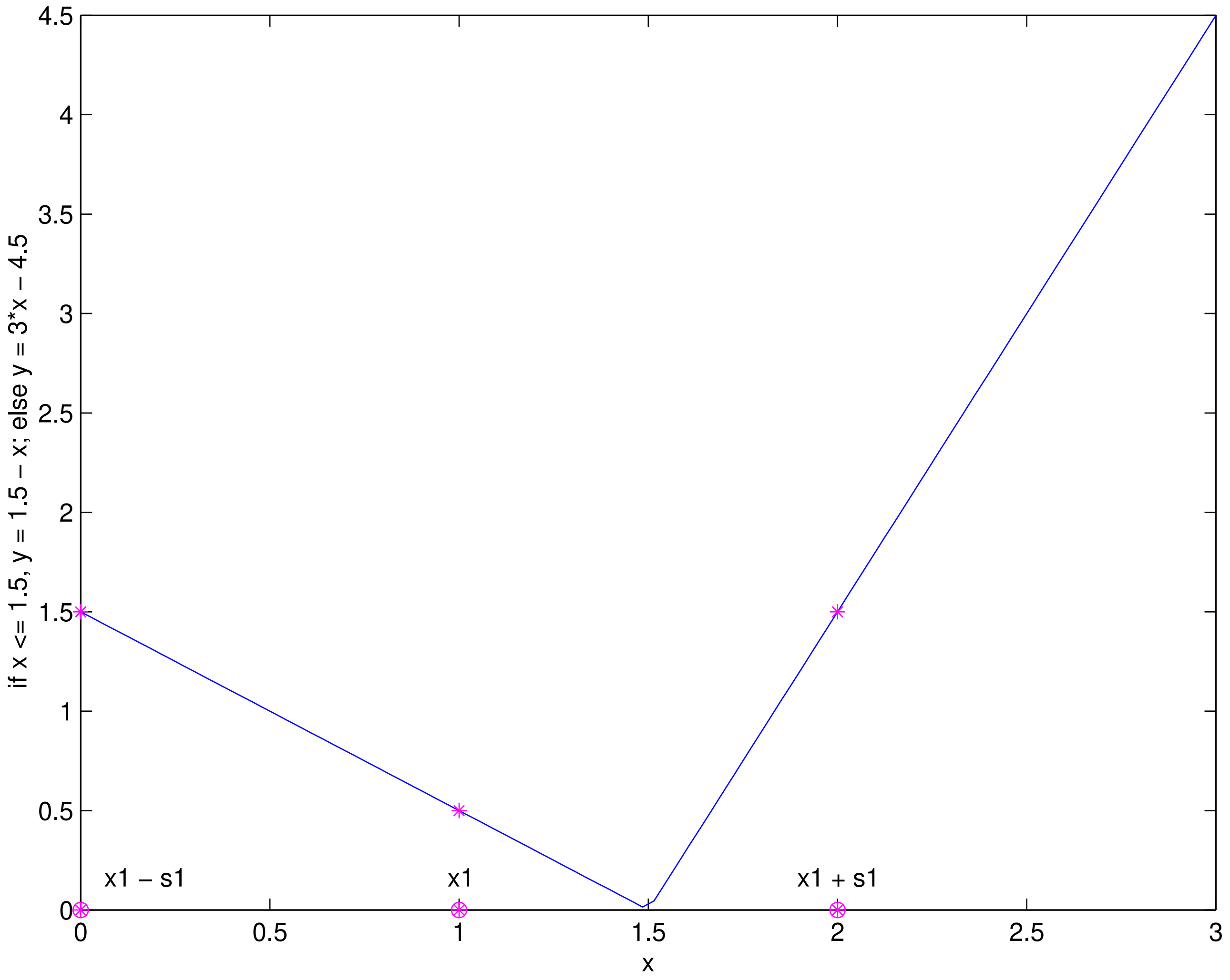


4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
if x <= 1.5, y = 1.5 − x; else y = 3*x − 4.5
x0
x0 + s1
0
0.5
1
1.5
2
2.5
3
x

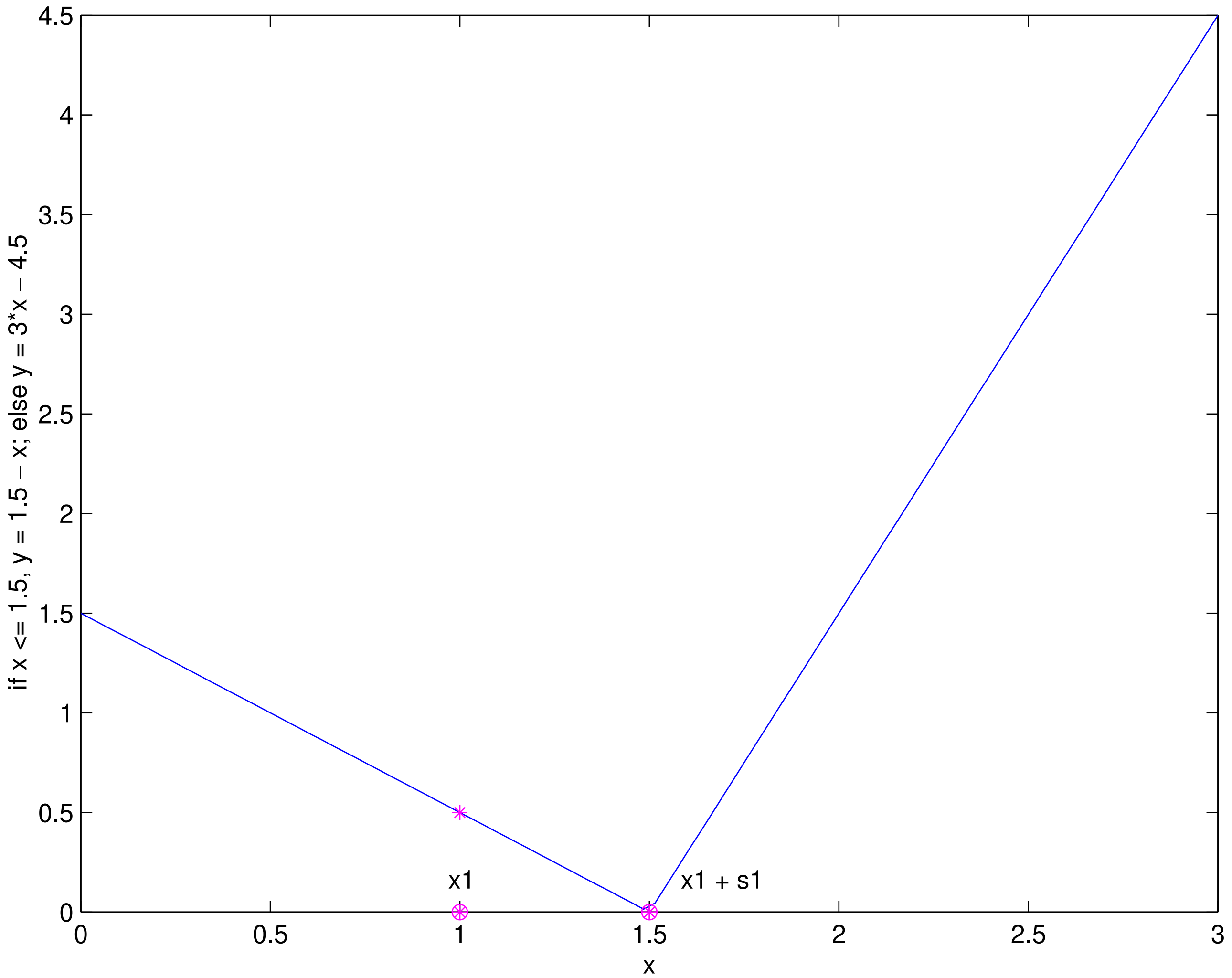
Iteration 2



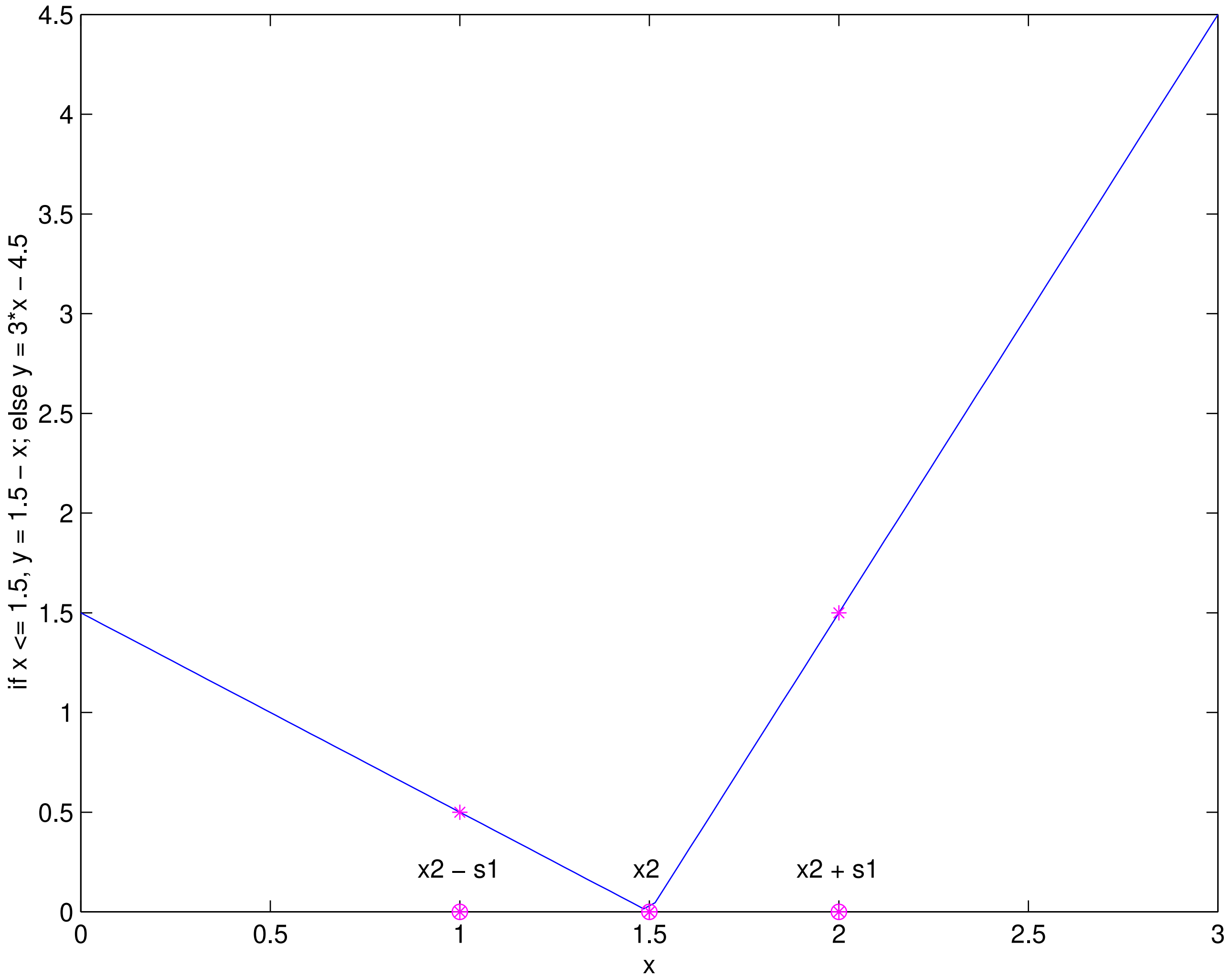
Iteration 2, continued



Iteration 2, resolved

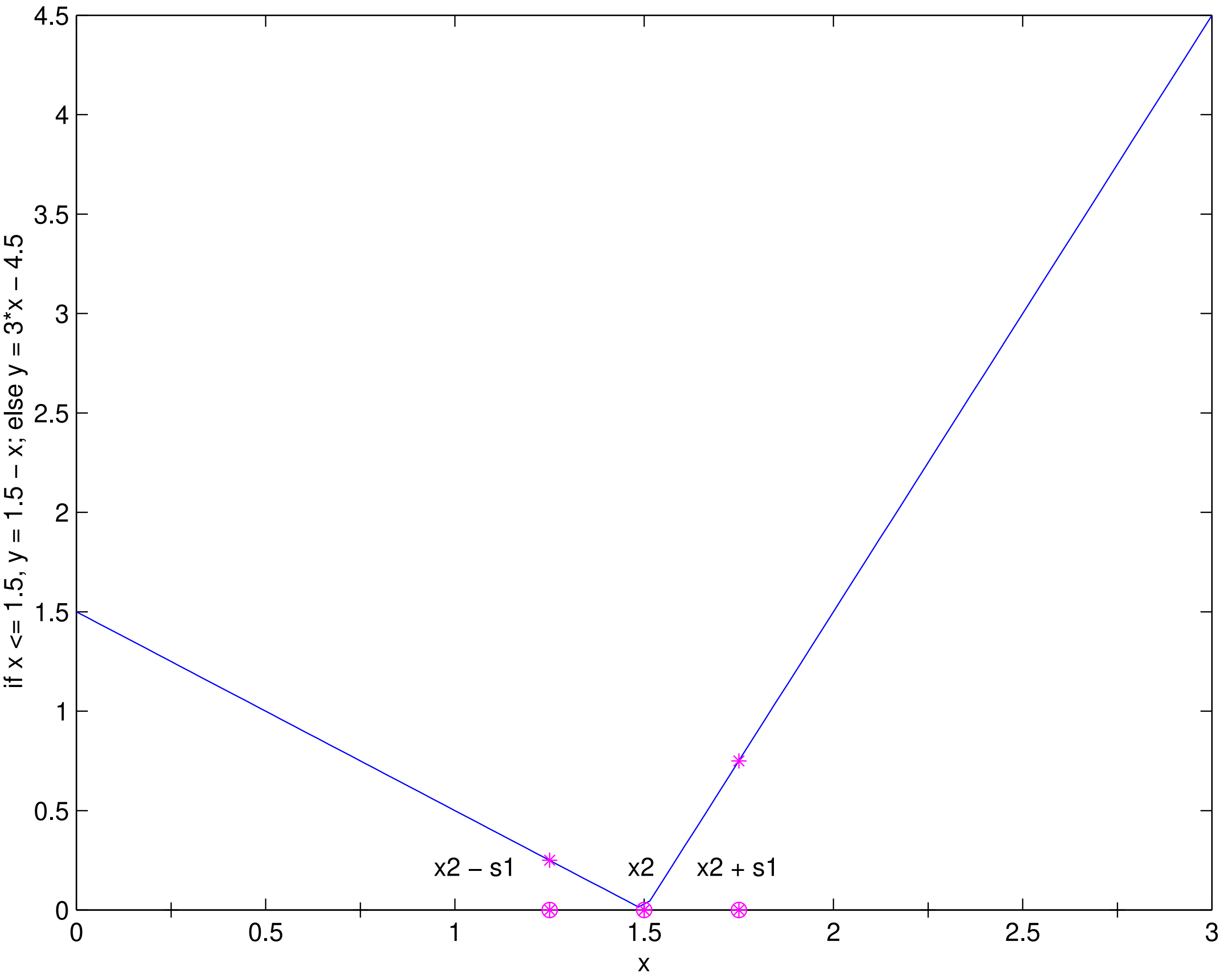


Iteration 3

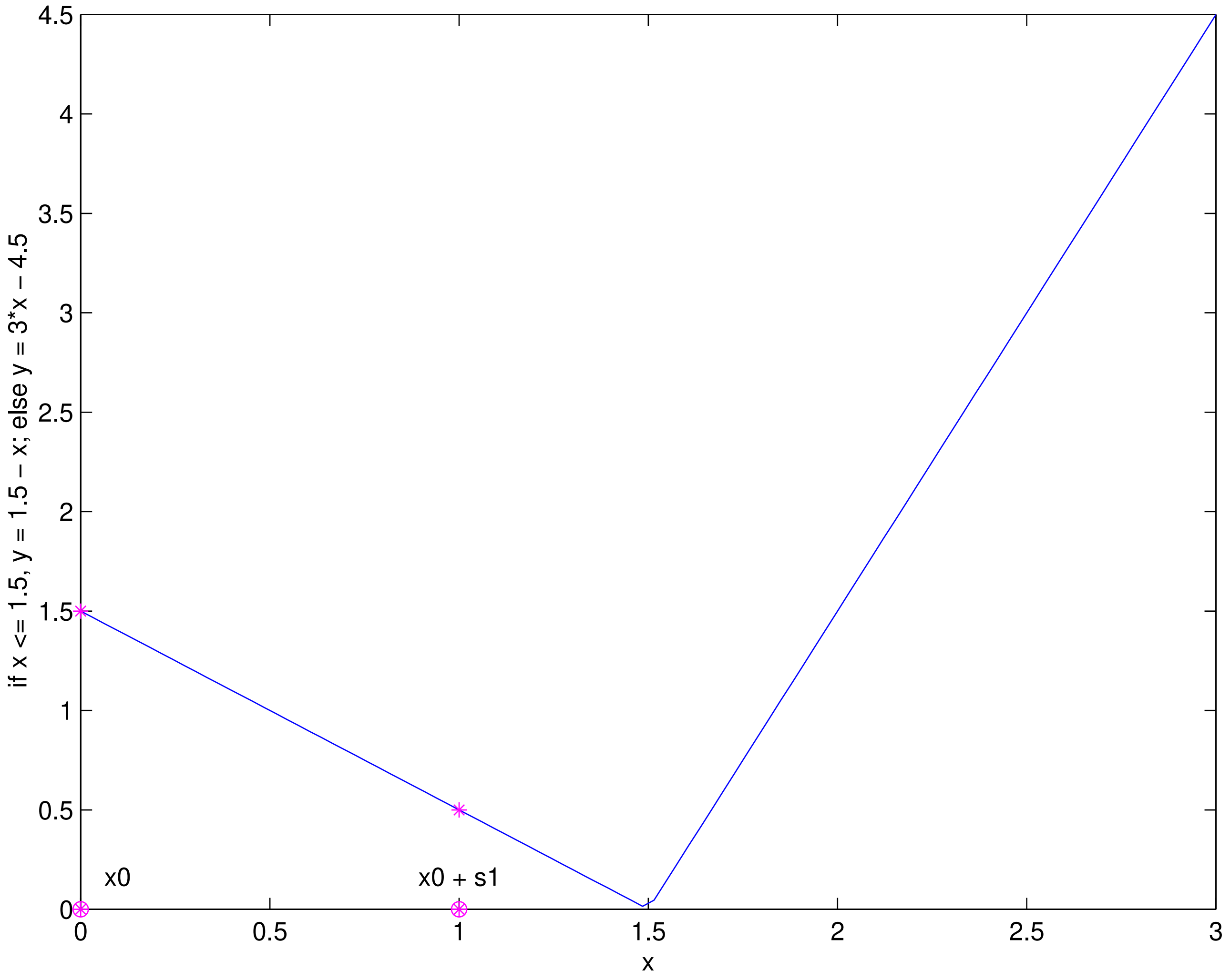


4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
if x <= 1.5, y = 1.5 − x; else y = 3*x − 4.5
x2 − s1
x2
x2 + s1
0
0.5
1
1.5
2
2.5
3
x

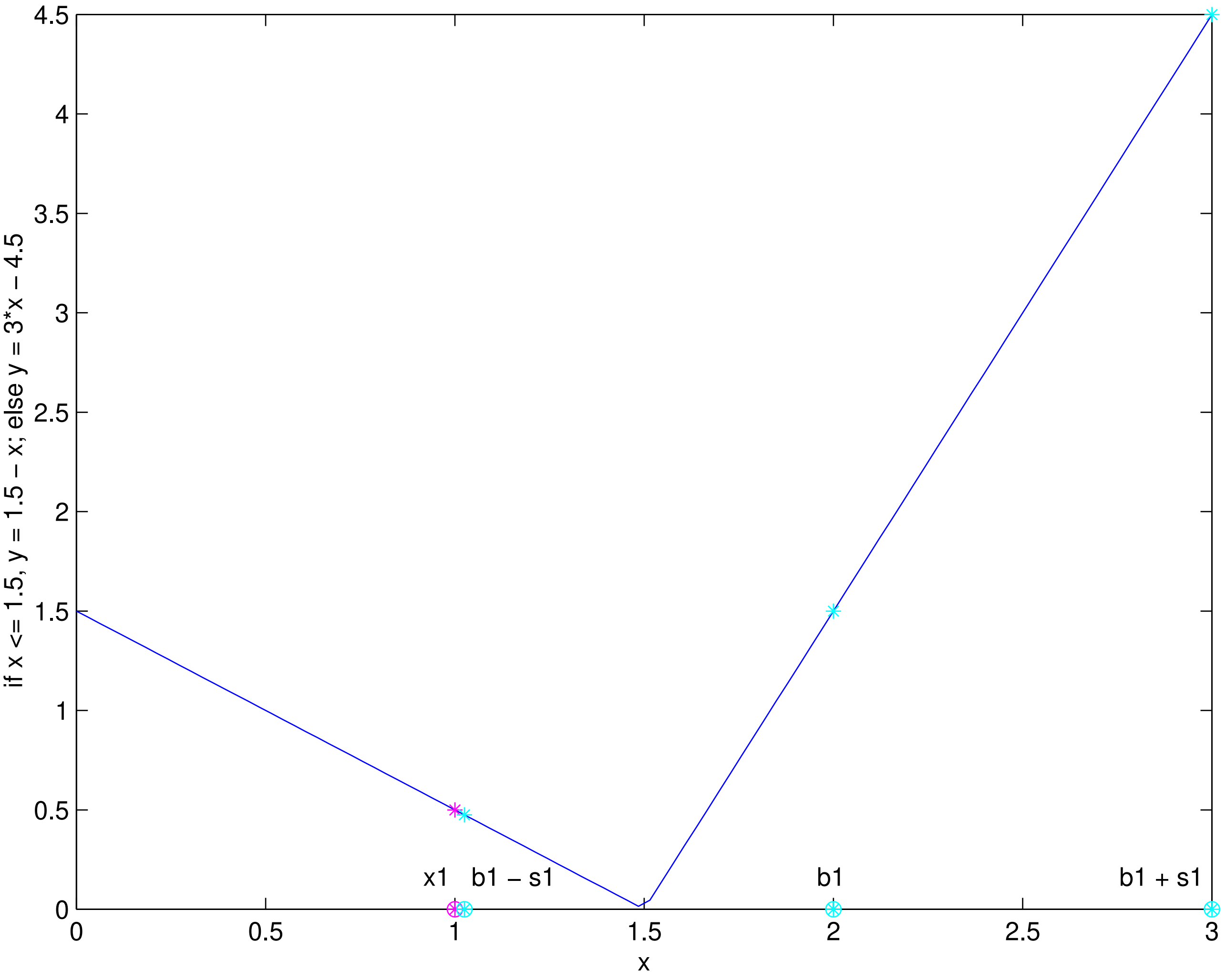
Iteration 3, first reduction...



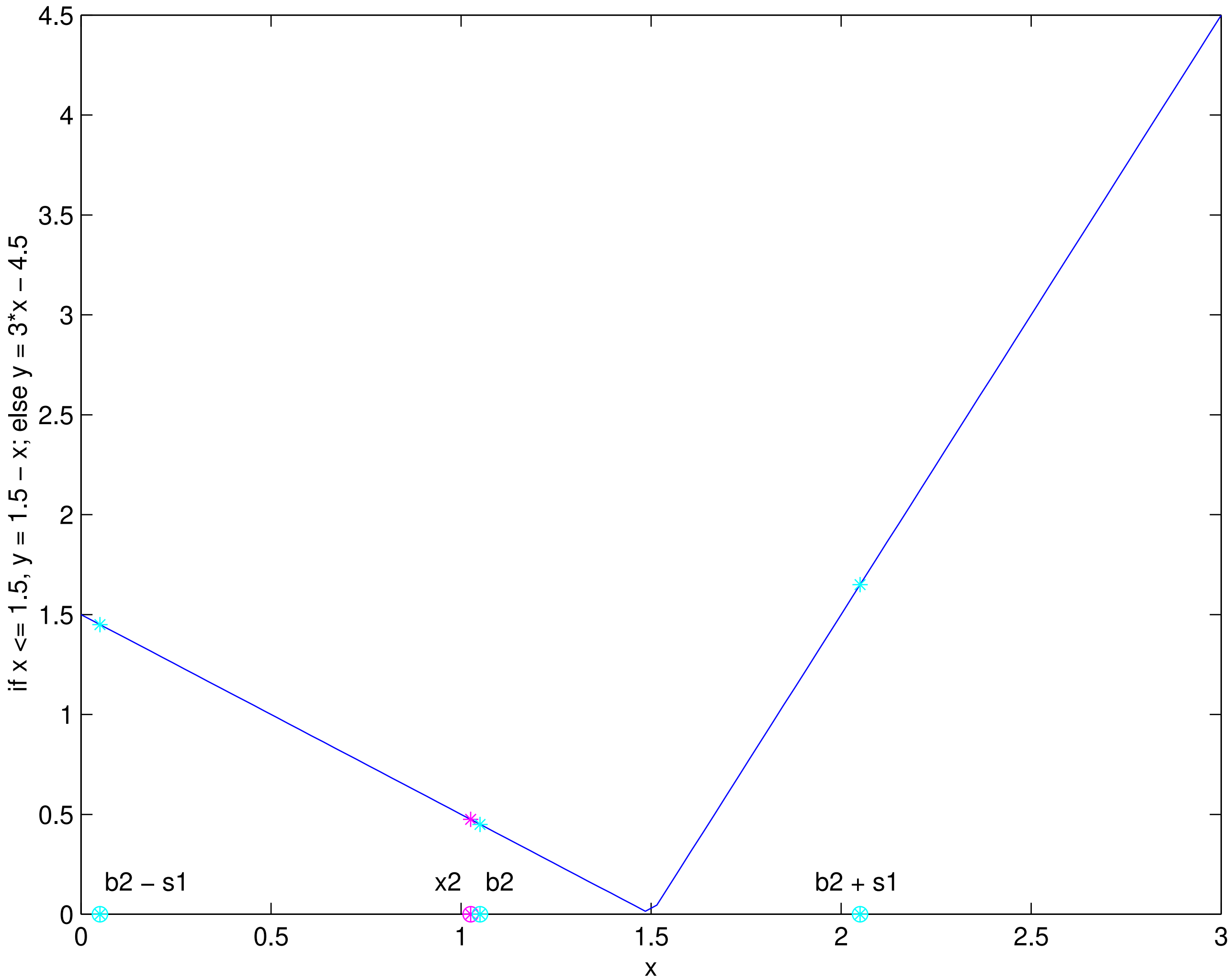
Iteration 1—Revisited



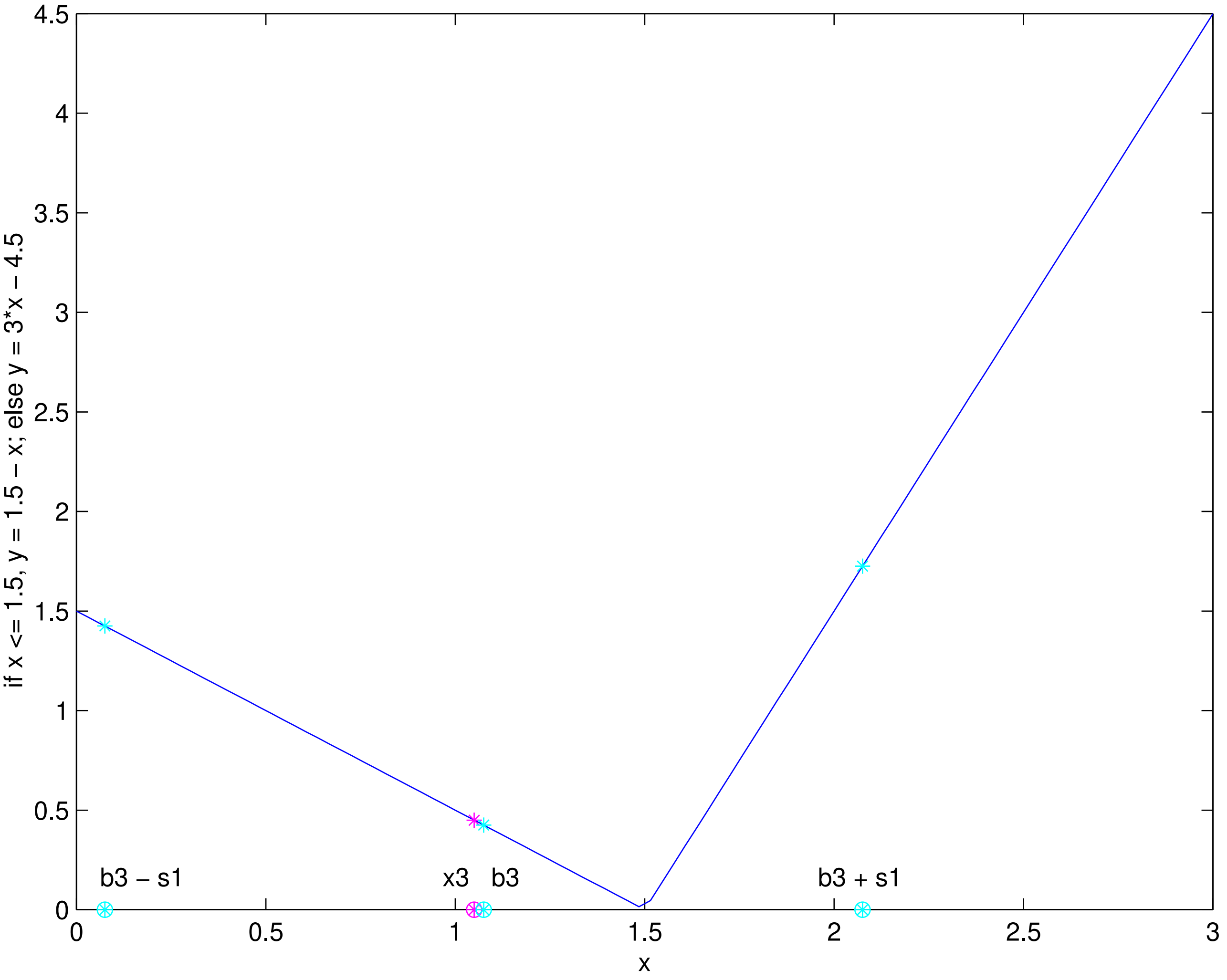
Iteration 2—With One Numerical Error



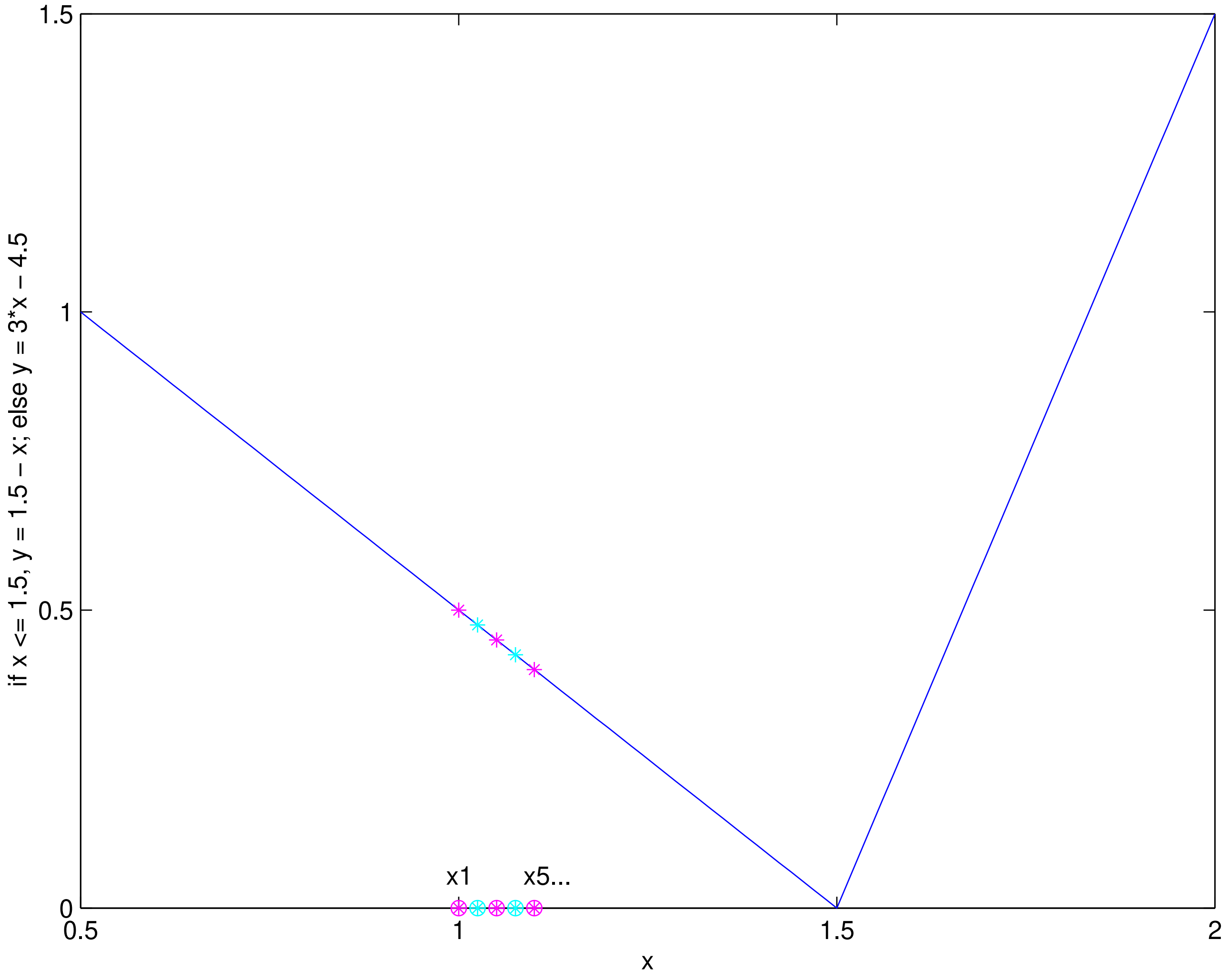
Iteration 3—With One Propagated Error



Iteration 4—With One Propagated Error



Iterates 1–5... (With the Propagated Error)



Note:

- It is not the nondifferentiability of f that is a problem—the iterates are piling up in a neighborhood where the f is continuously differentiable.

- The original Δ is never reduced—and yet the step sizes are $O(\texttt{err})$ (where, typically, $\texttt{err} \approx \texttt{eps}$).

- The problem is not unique to this example. We first (re)discovered the same phenomenon for a quadratic of the form

$$q(x) \quad = \quad H^T H x + c$$

where $H =$

$$\begin{pmatrix} 1.125043498418210 & 2.939352373629113 \\ 0.301824399995522 & 0.772323384033667 \\ -0.704674515756150 & -0.038293989982856 \\ -0.707583376350226 & 0.948456135457931 \end{pmatrix},$$

so that the condition number of

$$H^T H \quad = \quad 7.95551336264464,$$

$\Delta_0 = 6.0,$

$$x_0 \quad = \quad \begin{pmatrix} 0.1123135875305460 \\ 0.9266765162475219 \end{pmatrix},$$

and

$$x_* \quad = \quad \begin{pmatrix} 0.0 \\ 0.0 \end{pmatrix}.$$

What Is Going On?

It is possible in practice for a step to shift off of the rational lattice by $O(\text{eps})$. We see it for other pattern search algorithms, but it never seems to matter in practice.

Why does it matter for Hooke and Jeeves?

In *exact* arithmetic, one can show that the pattern step taken by the Hooke and Jeeves pattern search algorithm will be $\geq \Delta$. Thus—*in exact arithmetic*—the length of any step considered by the algorithm must be $\geq O(\Delta)$.

But *numerical error* can lead to pattern steps that are $O(\text{eps})$. Thus the length of the step taken can be considerably less than Δ.

Inadvertently, we have allowed the step to become too small.

Several Remarks:

1. We were not the first to observe this phenomenon. The observation goes back at least as far as September 1966 in a Remark by Bell and Pike that appeared in *Communications of the ACM*.

2. The "fix," as both they and we discovered, is easy: before accepting any pattern step, ensure that it is of length $> 0.5\Delta$ (i.e., that it is a "real" step rather than one due to spurious numerical error).

3. This is a problem that only happens with the pattern step—which is unique to the Hooke and Jeeves algorithm.

4. The problem would not have occurred if we were enforcing any reasonable sufficient decrease condition; the difference in function value between the two points was $O(\mathtt{eps})$.

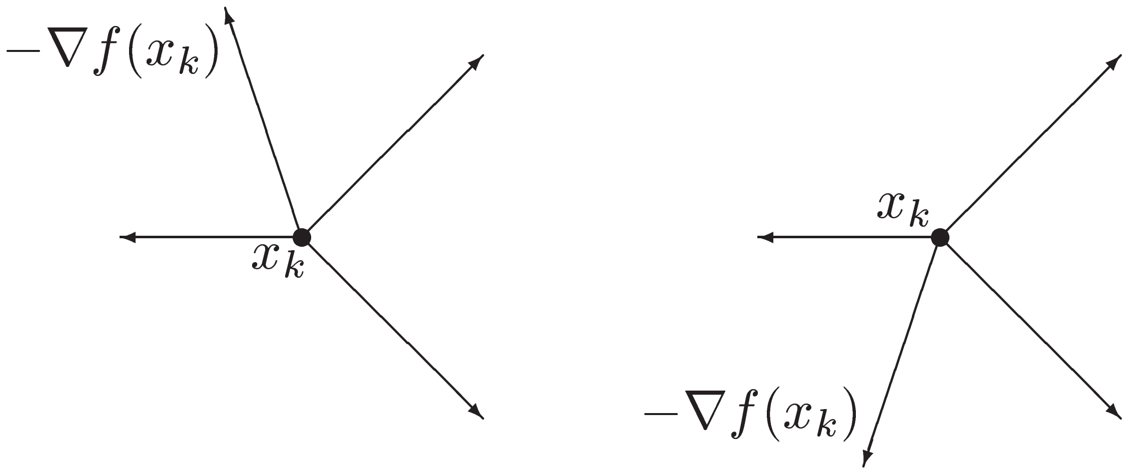
5. In practice, the hypotheses *do* matter to the extent that they help safeguard the length of the step.

   The important thing seems to be that the step accepted is of length $\geq O(\Delta)$.

6. Otherwise, in practice, it *does not* seem to matter whether or not we stay exactly on the rational lattice so long as the length of the step is safeguarded.

Why Full Local Information?

We have always known that the core pattern $B\Gamma_k$ defines a *sufficient* set of search directions to ensure at least one-gradient related direction



—*even though we never explicitly compute an approximation to the gradient*.

What Is New:

- A recent result shows that because we require sufficient local information before reducing Δ_k, when we reduce Δ_k, we have an upper bound on $\|\nabla f(x_k)\|$.
- This result confirms that one only need to check convergence after reducing Δ_k.
- This result also confirms that Δ_k is a reasonable measure of progress toward the solution.
- Further, recent numerical tests show that these observations bear out in practice.

Table 1: **Stopping Criteria vs Function Value** (with correct digits in red)

variance	simplex gradient	Δ	function value
3.0780276899464747	2.8564077075567220	0.7379498442749530	2.4314866861505493
0.0840886692951946	0.4587722065355163	0.3689749221374765	1.5908180895957142
0.0034923677292313	0.0335358610519773	0.1844874610687383	1.4773040257429713
0.0009624353196831	0.3867907025135328	0.0922437305343691	1.4772932399797003
0.0000198901150653	0.0895411558448952	0.0461218652671846	1.4704383882086089
0.0000028553411229	0.0895411558448976	0.0230609326335923	1.4704383882086089
0.0000000607727084	0.0146150464379905	0.0115304663167961	1.4697557553897906
0.0000000069229129	0.0146150464379905	0.0057652331583981	1.4697557553897906
0.0000000003717269	0.0041164809137459	0.0028826165791990	1.4697238142244098
0.0000000000128574	0.0014031259841643	0.0014413082895995	1.4697199463307293
0.0000000000011952	0.0014031259840873	0.0007206541447998	1.4697199463307293
0.0000000000001726	0.0014031259839332	0.0003603270723999	1.4697199463307293
0.0000000000000044	0.0002324055244136	0.0001801635361999	1.4697198389374599
0.0000000000000003	0.0001125699065903	0.0000900817681000	1.4697198337782784
0.0000000000000000	0.0000599178070629	0.0000450408840500	1.4697198322913623
0.0000000000000000	0.0000263260460663	0.0000225204420250	1.4697198320181937
0.0000000000000000	0.0000167958854282	0.0000112602210125	1.4697198319006213
0.0000000000000000	0.0000047650704594	0.0000056301105062	1.4697198318958682
0.0000000000000000	0.0000060153976247	0.0000028150552531	1.4697198318823599
0.0000000000000000	0.0000060154370635	0.0000014075276266	1.4697198318823599
0.0000000000000000	0.0000014421967569	0.0000007037638133	1.4697198318803744
0.0000000000000000	0.0000000946530359	0.0000003518819066	1.4697198318802809
0.0000000000000000	0.0000007685826514	0.0000001759409533	1.4697198318802656
0.0000000000000000	0.0000001400864931	0.0000000879704767	1.4697198318802380
0.0000000000000000	0.0000001388244526	0.0000000439852383	1.4697198318802380
0.0000000000000000	0.0000000858187525	0.0000000219926192	1.4697198318802374
0.0000000000000000	0.0000000302889715	0.0000000109963096	1.4697198318802369
0.0000000000000000	0.0000000201926477	0.0000000054981548	1.4697198318802369
0.0000000000000000	0.0000000403852953	0.0000000027490774	1.4697198318802369
0.0000000000000000	0.0000000807705906	0.0000000013745387	1.4697198318802369
0.0000000000000000	0.0000001615411813	0.0000000006872693	1.4697198318802369
0.0000000000000000	0.0000003230823625	0.0000000003436347	1.4697198318802369
0.0000000000000000	0.0000006461647250	0.0000000001718173	1.4697198318802369
0.0000000000000000	0.0000012923294500	0.0000000000859087	1.4697198318802369
0.0000000000000000	0.0000025846589001	0.0000000000429543	1.4697198318802369
0.0000000000000000	0.0000000000000000	0.0000000000214772	1.4697198318802369
0.0000000000000000	0.0000000000000000	0.0000000000107386	1.4697198318802369

Stopping Criteria vs Function Value (with the accurate digits in red)

variance	**simplex gradient**	**Δ**	**function value**
4.9411598192718458	0.2263891700656974	1.7411233994470423	1.8601023492759197
0.0811996078697978	0.5802488592956152	0.8705616997235212	1.2312578958766123
0.0194966534962939	0.5802488592956146	0.4352808498617606	1.2312578958766123
0.0023720256961172	0.4248714210320179	0.2176404249308803	1.2106577669992014
0.0000284206217874	0.0776887191317999	0.1088202124654401	1.1915680992482827
0.0000069090498631	0.0776887191317958	0.0544101062327201	1.1915680992482827
0.0000003164614125	0.0479513159091597	0.0272050531163600	1.1908299414004579
0.0000000194994980	0.0093396439670933	0.0136025265581800	1.1906986373271959
0.0000000010749623	0.0121041727891894	0.0068012632790900	1.1906625254085708
0.0000000000396487	0.0022185671798555	0.0034006316395450	1.1906541210827679
0.0000000000079770	0.0029096993852857	0.0017003158197725	1.1906536936802317
0.0000000000001623	0.0010165517097722	0.0004250789549431	1.1906526925822196
0.0000000000000241	0.0007737907863992	0.0008501579098863	1.1906526667840798
0.0000000000000005	0.0000349889354527	0.0002125394774716	1.1906526065179295
0.0000000000000001	0.0000781846989614	0.0001062697387358	1.1906526054763062
0.0000000000000000	0.0000565868203412	0.0000531348693679	1.1906526025366604
0.0000000000000000	0.0000553095895545	0.0000265674346839	1.1906526025281774
0.0000000000000000	0.0000006386007673	0.0000132837173420	1.1906526023466188
0.0000000000000000	0.0000033383622352	0.0000066418586710	1.1906526023176558
0.0000000000000000	0.0000033382953730	0.0000033209293355	1.1906526023176558
0.0000000000000000	0.0000026633884371	0.0000016604646677	1.1906526023147586
0.0000000000000000	0.0000008333703238	0.0000008302323339	1.1906526023143786
0.0000000000000000	0.0000008333703238	0.0000004151161669	1.1906526023143786
0.0000000000000000	0.0000001251660178	0.0000002075580835	1.1906526023143038
0.0000000000000000	0.0000001240962228	0.0000001037790417	1.1906526023143038
0.0000000000000000	0.0000001027003223	0.0000000518895209	1.1906526023143023
0.0000000000000000	0.0000000085583602	0.0000000259447604	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000129723802	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000064861901	1.1906526023143014
0.0000000000000000	0.0000000684668815	0.0000000032430951	1.1906526023143014
0.0000000000000000	0.0000001369337631	0.0000000016215475	1.1906526023143014
0.0000000000000000	0.0000002738675262	0.0000000008107738	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000004053869	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000002026934	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000001013467	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000000506734	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000000253367	1.1906526023143014
0.0000000000000000	0.0000000000000000	0.0000000000126683	1.1906526023143014

Table 2: **Stopping Criteria vs Function Value** (with correct digits in red)

std. deviation	simplex gradient	Δ	function value
22.9183504010289383	2.9743637607191737	2.5014767071524533	4.1464661873603124
8.6832469203393288	3.0525104362787010	1.2507383535762266	3.2386547175689682
0.9742534137216189	0.7079812916976593	0.6253691767881133	0.0913657370406688
0.3148834895917984	0.7079812916976596	0.3126845883940567	0.0913657370406688
0.1022307895726505	0.2223733058514898	0.1563422941970283	0.0534052037468748
0.0285932325107842	0.2272574730739602	0.0781711470985142	0.0393810907743447
0.0060453625492211	0.0077732599245623	0.0390855735492571	0.0309003117979746
0.0016903021570746	0.0065522181189447	0.0195427867746285	0.0301593652865318
0.0003390992412607	0.0071627390217534	0.0097713933873143	0.0298266368295058
0.0001309365647018	0.0068574785703491	0.0048856966936571	0.0298172006298319
0.0000181464864324	0.0070101087960513	0.0024428483468286	0.0297779686226221
0.0000036521102920	0.0002582864973020	0.0012214241734143	0.0297738452031370
0.0000011507666769	0.0002582864973006	0.0006107120867071	0.0297738452031370
0.0000004532412662	0.0002582864973063	0.0003053560433536	0.0297738452031370
0.0000000725351831	0.0002678258864045	0.0001526780216768	0.0297737336536433
0.0000000265700146	0.0001864488194325	0.0000763390108384	0.0297737305475209
0.0000000057042037	0.0000383036861745	0.0000381695054192	0.0297737235541039
0.0000000017720984	0.0000394961098672	0.0000190847527096	0.0297737229774112
0.0000000003126184	0.0000178844401704	0.0000095423763548	0.0297737224948635
0.0000000001197997	0.0000105077288229	0.0000047711881774	0.0297737224772656
0.0000000000157681	0.0000035393027747	0.0000023855940887	0.0297737224378923
0.0000000000057364	0.0000035393027747	0.0000011927970443	0.0297737224378923
0.0000000000019638	0.0000000275450570	0.0000005963985222	0.0297737224367684
0.0000000000001968	0.0000000089121494	0.0000002981992611	0.0297737224361492
0.0000000000000504	0.0000000089121494	0.0000001490996305	0.0297737224361492
0.0000000000000137	0.0000000089121494	0.0000000745498153	0.0297737224361492
0.0000000000000044	0.0000000088888801	0.0000000372749076	0.0297737224361492
0.0000000000000018	0.0000000089354187	0.0000000186374538	0.0297737224361492
0.0000000000000002	0.0000000094938824	0.0000000093187269	0.0297737224361487
0.0000000000000001	0.0000000096800369	0.0000000046593635	0.0297737224361487
0.0000000000000000	0.0000000044677094	0.0000000023296817	0.0297737224361487
0.0000000000000000	0.0000000044677094	0.0000000011648409	0.0297737224361487
0.0000000000000000	0.0000000059569458	0.0000000005824204	0.0297737224361487
0.0000000000000000	0.0000000059569458	0.0000000002912102	0.0297737224361487
0.0000000000000000	0.0000000119138916	0.0000000001456051	0.0297737224361487
0.0000000000000000	0.0000000238277832	0.0000000000728026	0.0297737224361487
0.0000000000000000	0.0000000476555665	0.0000000000364013	0.0297737224361487
0.0000000000000000	0.0000000953111330	0.0000000000182006	0.0297737224361487
0.0000000000000000	0.0000000000000000	0.0000000000091003	0.0297737224361487
0.0000000000000000	0.0000000000000000	0.0000000000045502	0.0297737224361487

Stopping Criteria vs Returned Function Value and Distance from the Optimum
(HJSearch in 5 variables with correct digits in red)

std. deviation	Δ	function value	2norm
9.3045897498347561	0.6962268138239019	5.4361106754128041	2.3963015589443808
0.4397293876738081	0.3481134069119510	1.9159086219448116	0.6983895923138458
0.0410391664545333	0.1740567034559755	1.6606319720281675	0.4503869030736324
0.0013106836834532	0.0870283517279877	1.4844950859730970	0.1539439700826097
0.0002155320262490	0.0435141758639939	1.4839329285424792	0.1193151775059503
0.0000103551097665	0.0217570879319969	1.4719532056197253	0.0340026098043645
0.0000004083040040	0.0108785439659985	1.4700097998460036	0.0157919106168492
0.0000000404631436	0.0054392719829992	1.4699006162510915	0.0146783468207784
0.0000000039524363	0.0027196359914996	1.4698655024813616	0.0165829903968097
0.0000000001053694	0.0013598179957498	1.4697300627272001	0.0037575966250456
0.0000000000099616	0.0006799089978749	1.4697241294437269	0.0026128528103905
0.0000000000004175	0.0003399544989375	1.4697203396318461	0.0008546098460838
0.0000000000000347	0.0001699772494687	1.4697203309184161	0.0009857505477117
0.0000000000000027	0.0000849886247344	1.4697198554491324	0.0000742441507744
0.0000000000000001	0.0000424943123672	1.4697198351311140	0.0000435103250214
0.0000000000000000	0.0000212471561836	1.4697198345462448	0.0000326892368369
0.0000000000000000	0.0000106235780918	1.4697198321413172	0.0000138786375838
0.0000000000000000	0.0000053117890459	1.4697198320338560	0.0000174583151828
0.0000000000000000	0.0000026558945229	1.4697198319056393	0.0000058036150574
0.0000000000000000	0.0000013279472615	1.4697198319056393	0.0000058036150574
0.0000000000000000	0.0000006639736307	1.4697198318827320	0.0000018108722900
0.0000000000000000	0.0000003319868154	1.4697198318803228	0.0000002150972866
0.0000000000000000	0.0000001659934077	1.4697198318802984	0.0000001662453937
0.0000000000000000	0.0000000829967038	1.4697198318802445	0.0000000439549373
0.0000000000000000	0.0000000414983519	1.4697198318802440	0.0000000712678851
0.0000000000000000	0.0000000207491760	1.4697198318802382	0.0000000444503609
0.0000000000000000	0.0000000103745880	1.4697198318802382	0.0000000444503609
0.0000000000000000	0.0000000051872940	1.4697198318802376	0.0000000391633863
0.0000000000000000	0.0000000025936470	1.4697198318802376	0.0000000391633863
0.0000000000000000	0.0000000012968235	1.4697198318802376	0.0000000391633863
0.0000000000000000	0.0000000006484117	1.4697198318802376	0.0000000391633863

Stopping Criteria vs Returned Function Value and Distance from the Optimum

(`NLessSearch` in 5 variables with correct digits in red)

std. deviation	Δ	function value	2norm
6.5486433983619570	0.6962268138239019	2.4483717410566310	0.2777276094251399
0.8963664167841120	0.3481134069119510	1.7640603407930924	0.2176549125833814
0.0864294848558236	0.1740567034559755	1.6145138133840160	0.1084697941566830
0.0019435277139807	0.0870283517279877	1.4960316981463304	0.1159039741974479
0.0001572197295223	0.0435141758639939	1.4842980031542836	0.0704179184654578
0.0000095818143977	0.0217570879319969	1.4743470866911506	0.0405719037218861
0.0000002451147079	0.0108785439659985	1.4704546621276158	0.0347609196921366
0.0000000233681897	0.0054392719829992	1.4704546621276158	0.0347609196921366
0.0000000014623741	0.0027196359914996	1.4700532980495444	0.0248115028149709
0.0000000000553148	0.0013598179957498	1.4699489450489640	0.0218490362789150
0.0000000000164568	0.0006799089978749	1.4698667243929047	0.0175966242272939
0.0000000000017077	0.0003399544989375	1.4697677960311799	0.0100138238099774
0.0000000000000594	0.0001699772494687	1.4697270352791718	0.0038904854860887
0.0000000000000036	0.0000849886247344	1.4697216248598952	0.0019382378095814
0.0000000000000001	0.0000424943123672	1.4697201725880154	0.0008493561483688
0.0000000000000000	0.0000212471561836	1.4697199201379811	0.0004321719657023
0.0000000000000000	0.0000106235780918	1.4697198459928282	0.0001688909052103
0.0000000000000000	0.0000053117890459	1.4697198376569938	0.0001089433999276
0.0000000000000000	0.0000026558945229	1.4697198343587019	0.0000721440217908
0.0000000000000000	0.0000013279472615	1.4697198322765974	0.0000289467518772
0.0000000000000000	0.0000006639736307	1.4697198319422011	0.0000113059332085
0.0000000000000000	0.0000003319868154	1.4697198319057987	0.0000073254833814
0.0000000000000000	0.0000001659934077	1.4697198318911258	0.0000047849244202
0.0000000000000000	0.0000000829967038	1.4697198318815330	0.0000016498976358
0.0000000000000000	0.0000000414983519	1.4697198318805513	0.0000008062142814
0.0000000000000000	0.0000000207491760	1.4697198318803257	0.0000004305795219
0.0000000000000000	0.0000000103745880	1.4697198318802669	0.0000002459337107
0.0000000000000000	0.0000000051872940	1.4697198318802593	0.0000002175628883
0.0000000000000000	0.0000000025936470	1.4697198318802593	0.0000002175628883
0.0000000000000000	0.0000000012968235	1.4697198318802593	0.0000002175628883
0.0000000000000000	0.0000000006484117	1.4697198318802593	0.0000002175628883

Conclusions:

- It is worth exploring the flexibility afforded by the theory.

- It is worth exploiting the flexibility afforded by the theory.

- The interaction between the theory and practice can be subtle.

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