Optimal Design of Groundwater Remediation Systems with Sampling Methods

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Outline

- Collaborators
- General formulation and example problem
  - Formulation
  - Optimization Landscapes
  - Results
- Implicit Filtering
- Community problems
- Conclusions

Collaborators

- IFFCO developers from NCSU Math:
  Tony Choi, Owen Eslinger, Paul Gilmore,
  Alton Patrick, Vincent Bannister
- NCSU Math: Corey Winton, Dan Finkel, Jörg Gablonsky,
  Katie Fowler , Chris Kees, Jill Reese, Todd Coffey
- Other Places:
  - Boeing: Andrew Booker, John Dennis
  - UNC: Casey Miller, Matt Farthing, Glenn Williams
  - ERDC: Stacy Howington
  - Univ. Trier: Astrid Battermann
  - Mich Tech: Alex Mayer

What's the problem.

- Control flow of contaminants in groundwater.
  - Keep plume on site.
  - Keep concentrations at acceptable levels.
  - Minimize cost, mass of contaminant, contaminant concentration . . .
- Control flow and pressure.
  - Municipal water supplies.
  - Agriculture.

Many approaches

- Tightly coupled simulation/optimization (Shoemaker)
- GAs (Mayer, Pinder, Minkser, Yeh . . .)
- Surrogates: response surface, neural nets

Our long-term objectives:

- Examine many formulation, simulator, optimizer combinations in a portable way.
- Build testbed for both groundwater and optimization communities.
- Design new approaches.

Today: one problem/simulator/optimizer triple.

What we do.

- Black-box optimization:
  Use accepted, widely-used, production 3D simulators.
  - Improved portability/documentation relative to research codes.
  - Community might listen to us.
  - No guarantee of differentiability wrt design variables.
- Put problems/solutions on the web.
  http://www4.ncsu.edu/˜ctk/community.html

Flow in the saturated zone

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h) + \mathscr{S},$$

Data:

- BC, IC, spatial domain Ω
- S_s (specific storage coefficient)
- K (hydraulic conductivity)
- $\mathscr{S}$ is the souce/sink term,
  computed from the design variables.

Output: h (hydraulic head)
Typical simulators: ADH, FEMWATER, MODFLOW.

Species Transport

$$\frac{\partial \theta C}{\partial t} = \nabla \cdot (\theta \mathbf{D} \cdot \nabla C) - \nabla \cdot (\theta \mathbf{v} C) + \mathscr{S}^C.$$

Data: porosity θ, interphase
Design: $\mathscr{S}^C$ mass sources/sinks

- C is concentration, solution of PDE;
- v is velocity, computed from h;
- $\mathbf{D}$ is the dispersion tensor, computed from h.

Typical simulator: MT3D

Computing the fluid velocity v

Darcy's law says

$$\theta v = \frac{k}{\mu}(\nabla p + \rho g \nabla z)$$

- $p = \rho g(h - z)$: fluid pressure
- k: intrinsic permeability; μ: dynamic viscosity
- ρ: density; g: gravitational acceleration
- ∇z: vector in vertical direction

What's $\mathbf{D}$

$$\mathbf{D}_{ij} = \delta_{ij}\alpha_t|v| + (\alpha_l - \alpha_t)\frac{v_i v_j}{|v|} + \delta_{ij}\tau D^*$$

- α_l, α_t: longitudinal/transverse dispersivities
- τ: tortuosity of the porous medium
- D^*: free liquid diffusivity.

Design variables

Number and location of wells, pumping rates.
Pumping rates and well locations go in the source term for flow

$$\int_\Omega \mathscr{S}(t)\,d\Omega = \sum_{i=1}^{n} Q_i$$

and for concentration

$$\int_\Omega \mathscr{S}^C(t)\,d\Omega = \sum_{i=1}^{n} C(x_i) Q_i.$$

Examples:

- Sum of δ functions at well locations.
- Well model with well diameter, well type, ...

Example: Hydraulic Capture

Minimize total cost:

$$f^T(Q) = \underbrace{\sum_{i=1}^{n} c_0 d_i^{b0} + \sum_{Q_i < -10^{-6}} c_1 |Q_i{}^m|^{b_1} (z_{gs} - h^{min})^{b_2}}_{f^c} +$$

$$\underbrace{\int_0^{t_f} \left(\sum_{i, Q_i < -10^{-6}} c_2 Q_i (h_i - z_{gs}) + \sum_{i, Q_i > 10^{-6}} c_3 Q_i \right) dt}_{f^o},$$

to keep a contaminant inside a “capture zone”.
$\Omega = [0, 1000] \times [0, 1000]$

Notation

- $\{(x_i, y_i)\}$ are well locations.
- Q_i is pumping rate
  (> 0 for injection, < 0 for extraction.
- d_i is depth of well i
- h_i is head at well i (MODFLOW)
- z_{gs} is elevation of ground surface
- Q^m is design pumping rate.
- h^{min} is minimum allowable pumping rate.

Boundary conditions: Unconfined aquifer

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial y}\right|_{y=0} = \left.\frac{\partial h}{\partial z}\right|_{z=0} = 0, t > 0$$

$$K\frac{\partial h}{\partial z}(x,y,z = h, t > 0) = -1.903 \times 10^{-8} \text{ (m/s)}.$$

$$\begin{aligned} h(1000,y,z,t > 0) &= 20 - 0.001y \text{(m)}, \\ h(x,1000,z,t > 0) &= 20 - 0.001x \text{(m)}, \\ h(x,y,z,0) &= h_s. \end{aligned}$$

Constraints I

Simple bounds:

$$Q^{emax} \le Q_i \le Q^{imax}, \; i = 1, \ldots, n$$

Limits on the pumps.
Simple linear inequality:

$$\sum_i Q_i \ge Q_T^{max},$$

limit on total net extraction rate.

Constraints II

Keep wells away from Dirichlet boundary

$$0 \leq x_i, y_i \leq 800.$$

Bounds on h

$$h^{min} \leq h_i \leq h^{max}, \; i = 1, \ldots, n$$

No dry holes.
Velocity Highly nonlinear function of well locations.
$50 \times 50 \times 10$ grid.

Formulation Decisions I

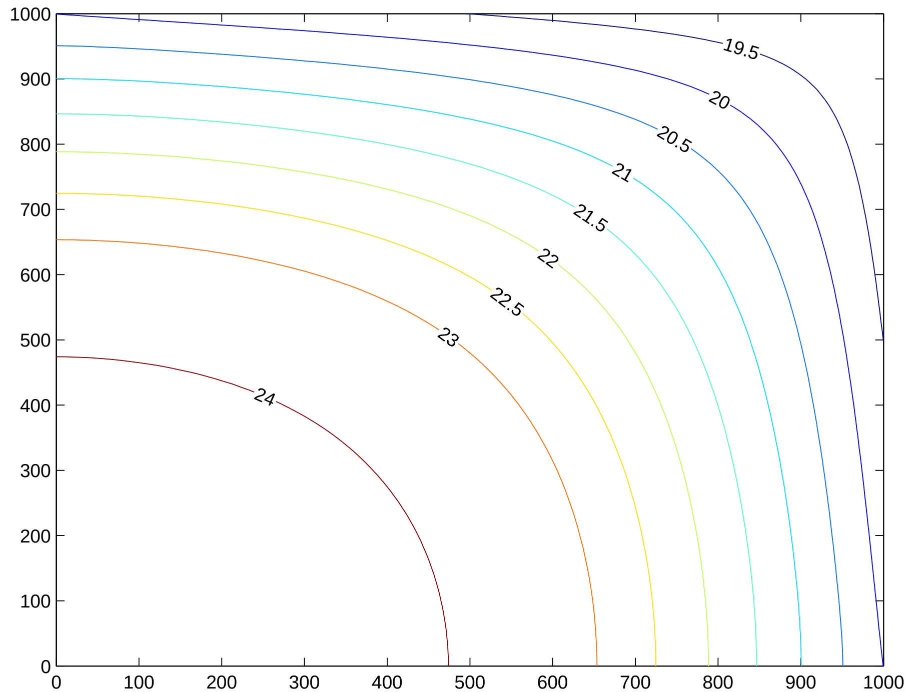
- Contain plume: constrain velocity at zone boundary.
  Test velocity at five downstream locations.
  Approximate velocity with difference of h.
  Five new constraints.
  Need only flow code. Better simulations in progress.
- Implicit filtering deals with bounds naturally.
- Treat constraints as yes/no for sampling method
  - Stratify by cost.
  - Avoid simulator if infeasible wrt cheap (linear) constraints.
- Well is de-installed if pumping rate is suff small.

Formulation Decisions II

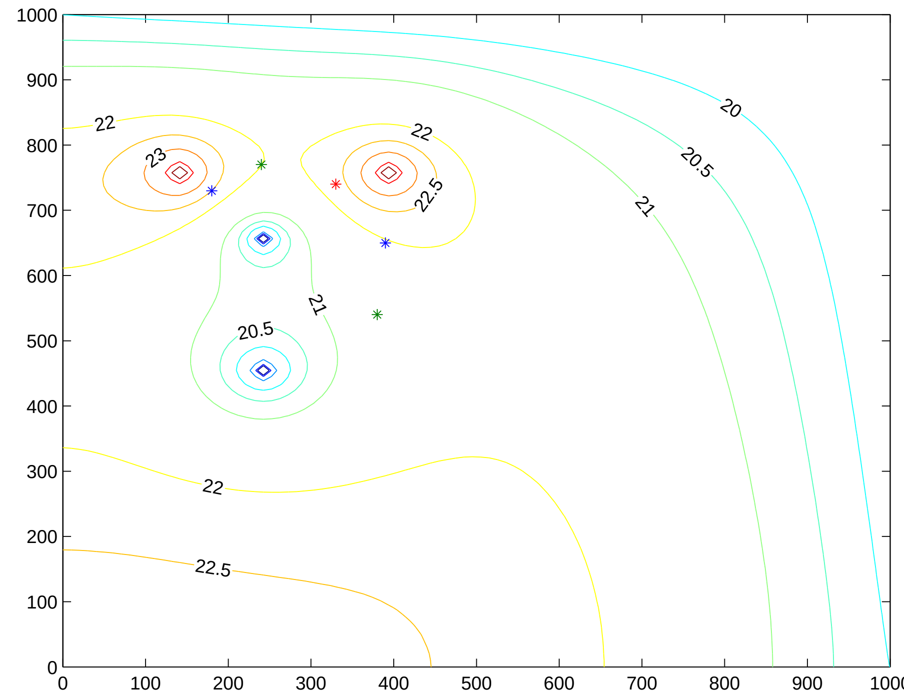
- Discontinuous objective.
  - $50 \times 50 \times 10$ grid. Wells must be on grid nodes. Move to nearest.
  - Remove well from array ($d_i = 0$) if pumping rate is too small.
- Treat head constraint and linear constraints as *hidden* or *yes-no*.
- Initial iterate: two extraction, two injection

Initial iterate

No wells

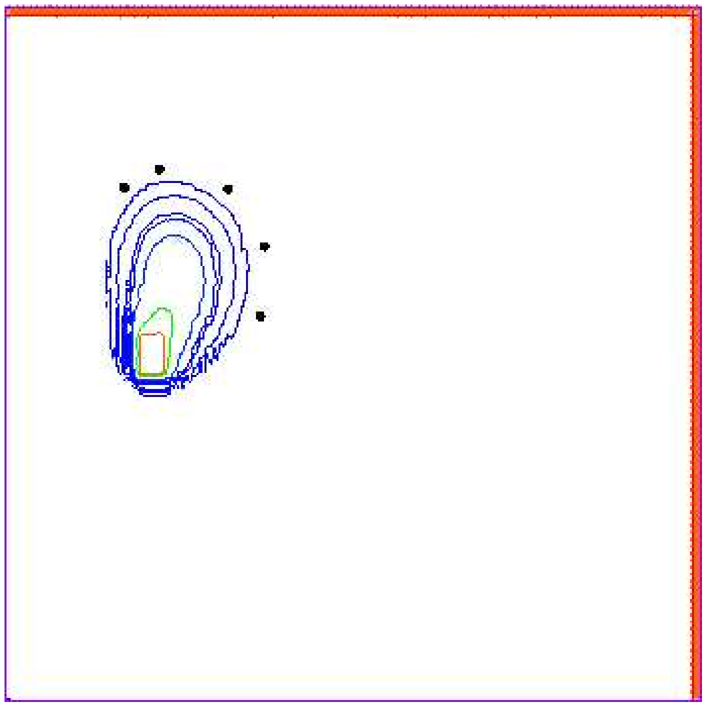


Four well configuration

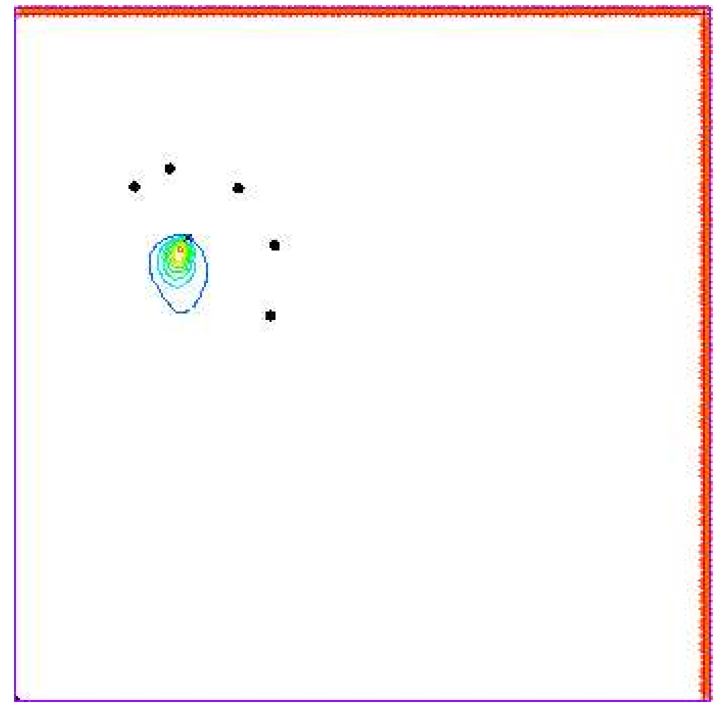


Initial/Final Plumes

Initial Plume

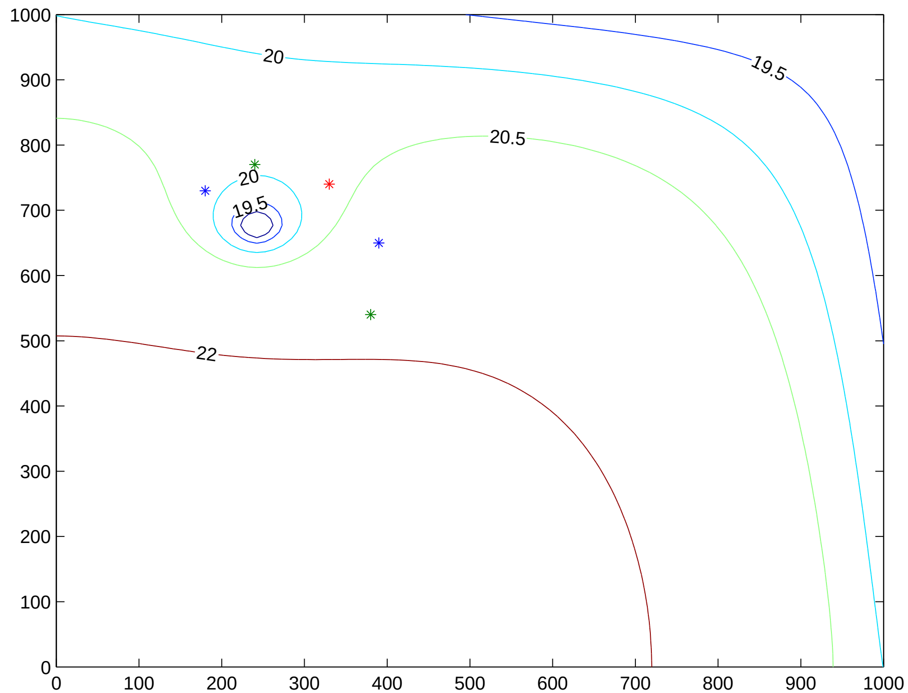


Plume after 5 years

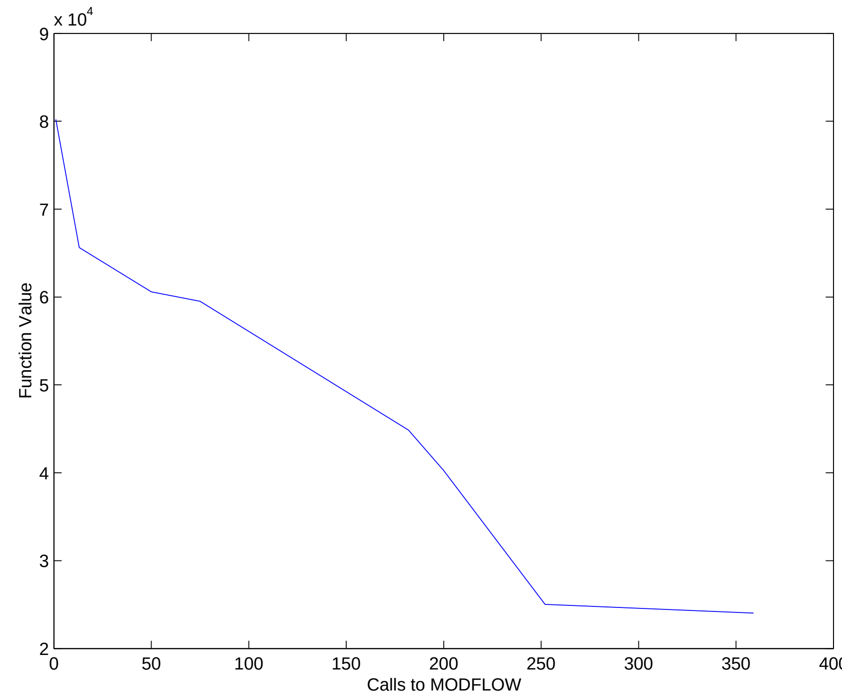


Results

Optimal configuration

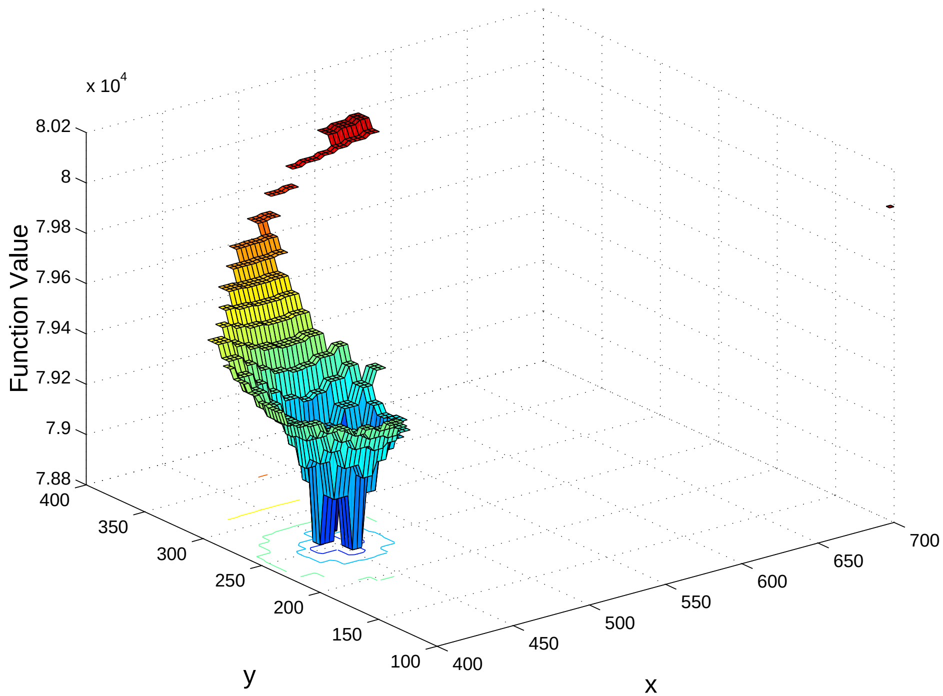


Cost of Optimization

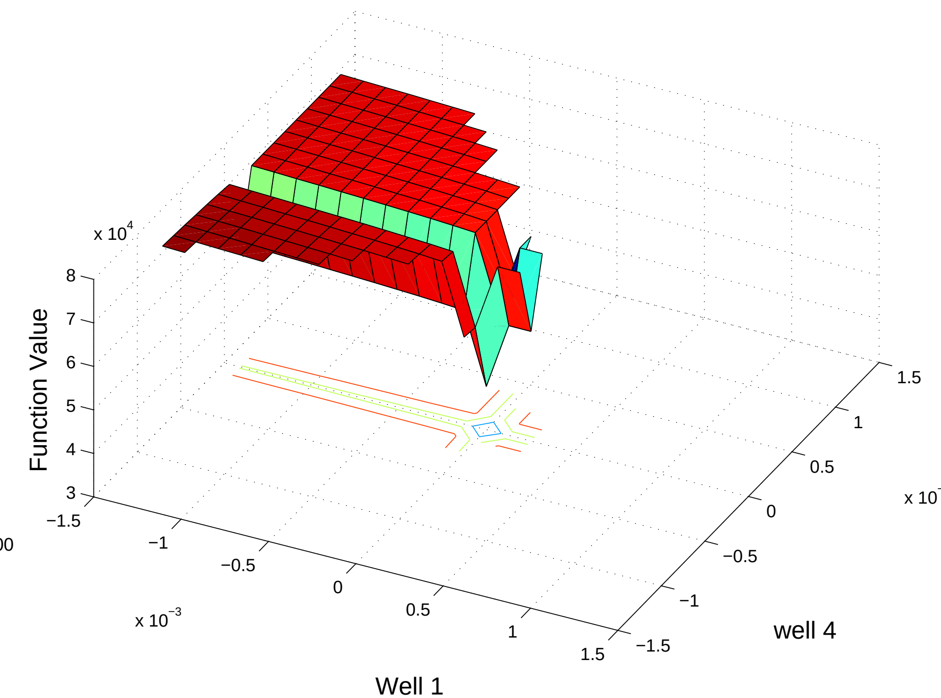


Landscapes

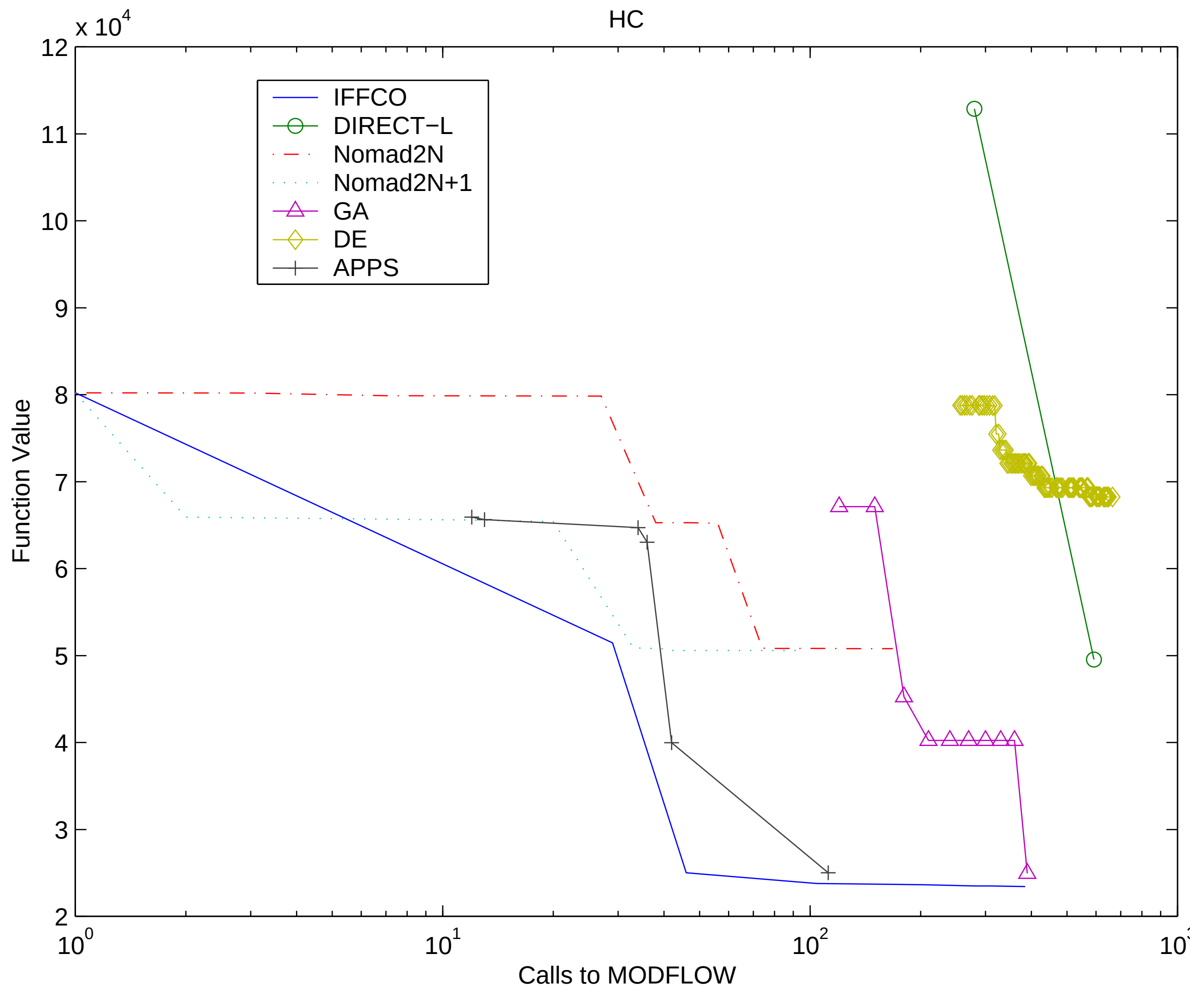
Vary (x_1, y_1) near initial iterate



Vary pumping rate initial iterate



Other Approaches



Wait a minute!

- Optimal point has one well, we start with four.
  Was this fair?
- How does performance depend on initial iterate?
- Do some methods benefit from special choices?
- How can you construct a “rich” set of initial iterates for testing?
- We’re trying:
  - Use DIRECT to find feasible points.
  - Use statistics to identify clusters.
  - Sample wisely within the clusters.

Optimization strategy

$$\min_{x \in \mathscr{D}} f(x)$$

- Conventional gradient-based methods can fail if f is
  - multi-modal,
  - non-convex,
  - discontinuous,
  - non-deterministic, or if
- $\mathscr{D}$ is not determined by smooth inequalities.

Sampling methods attempt to address these problems.

Stencil-based sampling methods

- Begin with a base point x.
- Examine points on a stencil;
  reject or adjust points not in $\mathscr{D}$.
- Determine location of next stencil.
- If $f(x)$ is smallest, shrink the stencil.

Examples: Coordinate Search, Nelder-Mead, Hooke-Jeeves, (P)MDS, GPS, Implicit Filtering

This is not global optimization.

Example: coordinate search

Sample f at x on a stencil centered at x, scale=h

$$S(x,h) = \{x \pm he_i\}$$

- Move to the best point.
- If x is the best point, reduce h.

Necessary Conditions: No legal direction points downhill (which is why you reduce h).

What if x is the best point?

Smooth Objective

If $f(x) \leq \min_{z \in S(x,h)} f(z)$ **(stencil failure)**
then
$\|\nabla f(x)\| = O(h)$

So, if (x_n, h_n) are the points/scales generated by coordinate search and f has bounded level sets, then

- $h_n \to 0$ (finitely many grid points/level) and therefore
- any limit point of $\{x_n\}$ is a critical point of f.

Not a method for smooth problems.

Model Problem

motivated by the landscapes.

$$\min_{R^N} f$$

$$f = f_s + \phi$$

- f_s smooth, easy to minimize; ϕ noise
- N is small, f is typically costly to evaluate.
- f has multiple local minima
  which trap most gradient-based algorithms.

Convergence?

Stencil failure implies that

$$\|\nabla f_s(x_n)\| = O\left(h_n + \frac{\|\phi\|_{S(x_n,h_n)}}{h_n}\right)$$

where

$$\|\phi\|_{S(x,h)} = \max_{z \in S} |\phi(z)|.$$

Bottom line

So, if (x_n, h_n) are the points/scales generated by coordinate search, f has bounded level sets, **and**

$$\lim_{n\to\infty}(h_n + h_n^{-1}\|\phi\|_{S(x,h_n)}) = 0$$

then

- $h_n \to 0$ (finitely many grid points/level) and therefore
- any limit point of $\{x_n\}$ is a critical point of f.

Analysis for Hooke-Jeeves, MPS, GPS is similar.
Nelder-Mead is different.

Implicit Filtering

Accelerate coordinate search with a quasi-Newton method.

$\textbf{imfilter}(x, f, pmax, \tau, \{h_n\}, amax)$

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

`fdquasi`$(x, f, pmax, \tau, h_n, amax)$

end for

$pmax$, τ, $amax$ are termination parameters

fdquasi = finite difference quasi-Newton method using a central difference gradient $\nabla_h f$.

fdquasi$(x, f, pmax, \tau, h, amax)$

$p = 1$

while $p \leq pmax$ and $\|\nabla_h f(x)\| \geq \tau h$ **do**

compute f and $\nabla_h f$

terminate with success on stencil failure

update the model Hessian H if appropriate; solve

$Hd = -\nabla_h f(x)$

use a backtracking line search, with at most $amax$ backtracks,

to fi nd a step length λ

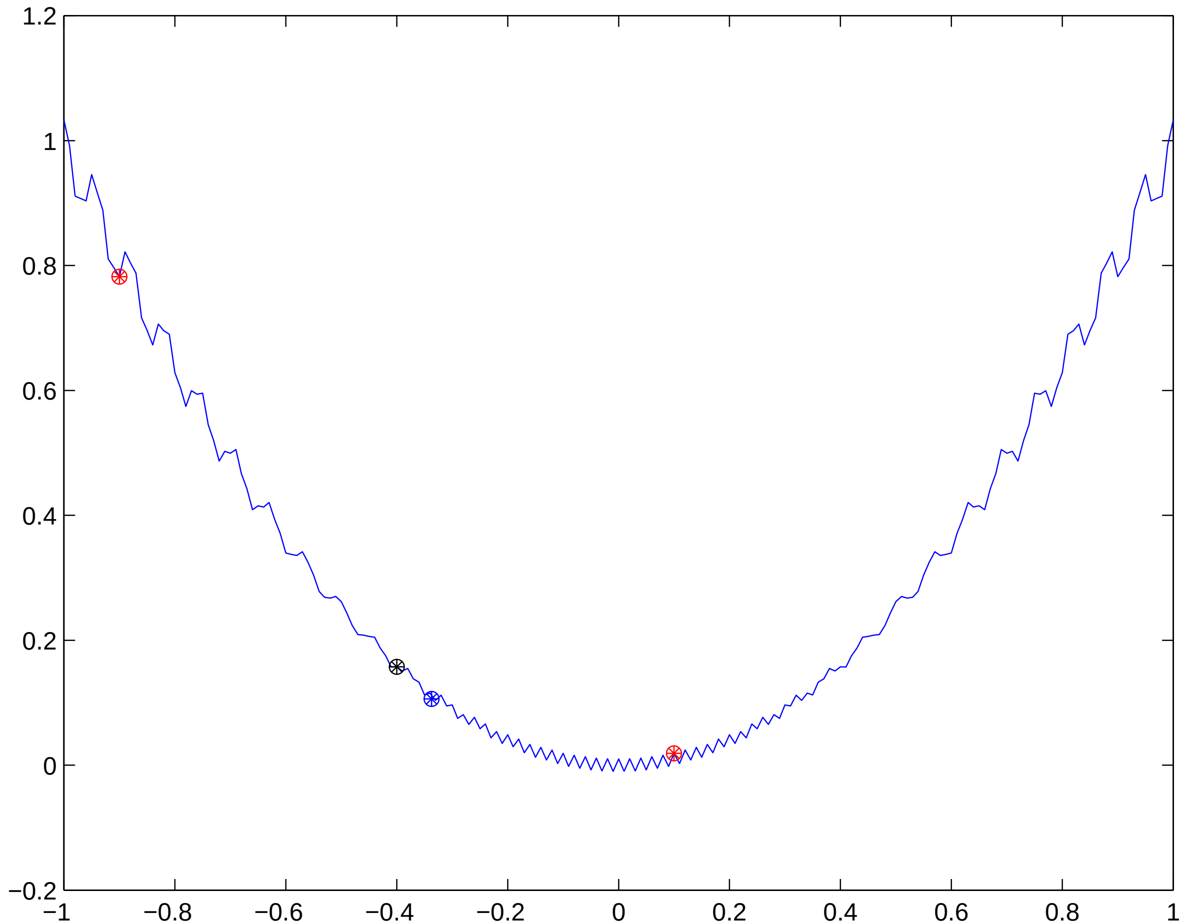
terminate with failure on $> amax$ backtracks

$x \leftarrow x + \lambda d$; $p \leftarrow p + 1$

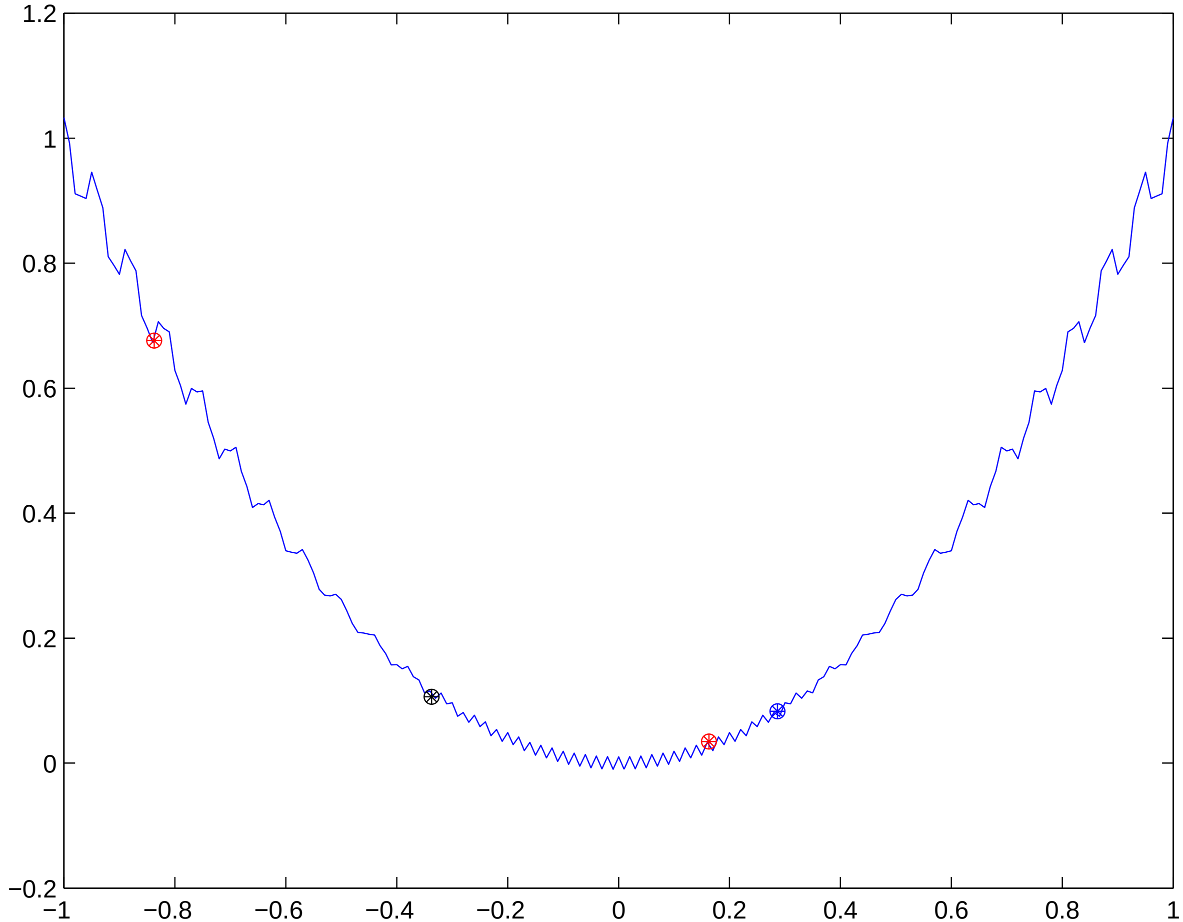
end while

if $p > pmax$ report iteration count failure

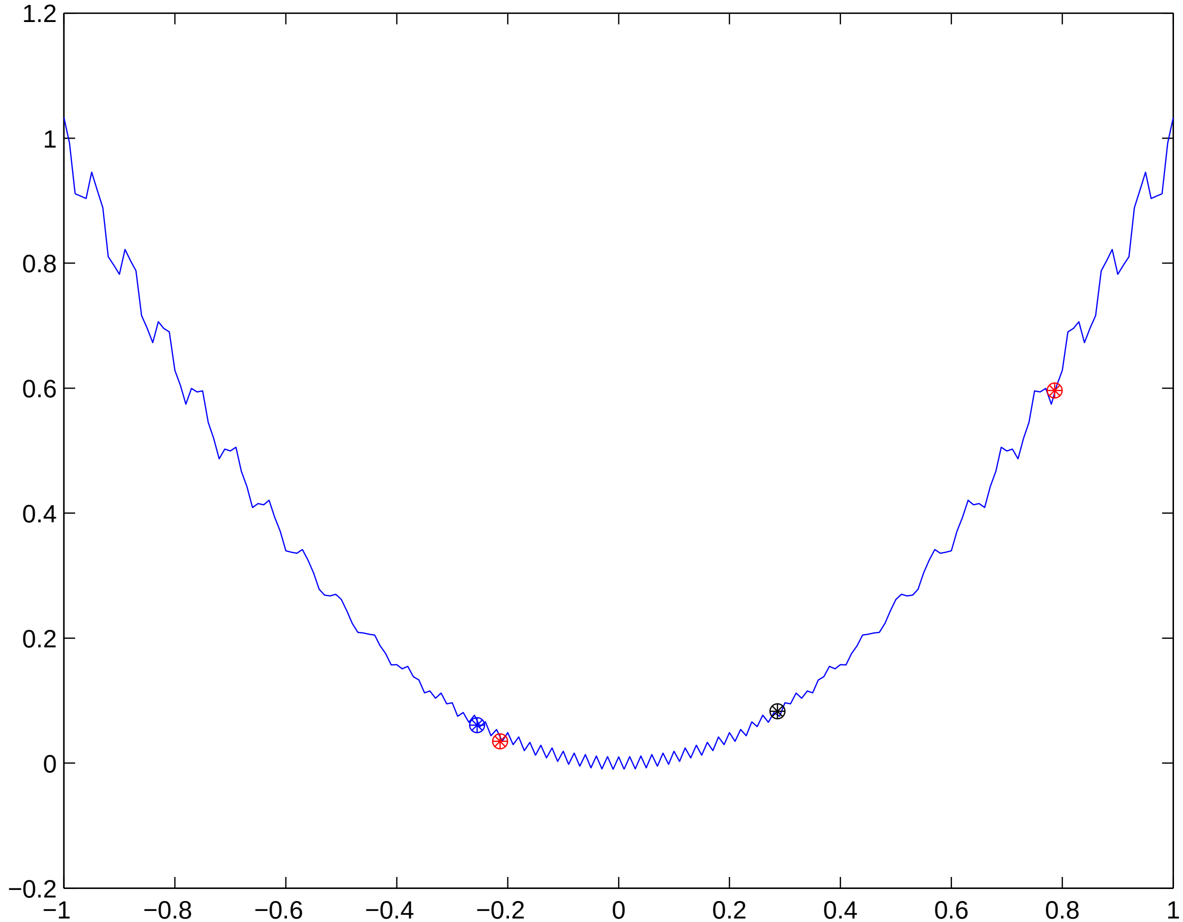
Implicit Filtering: Start



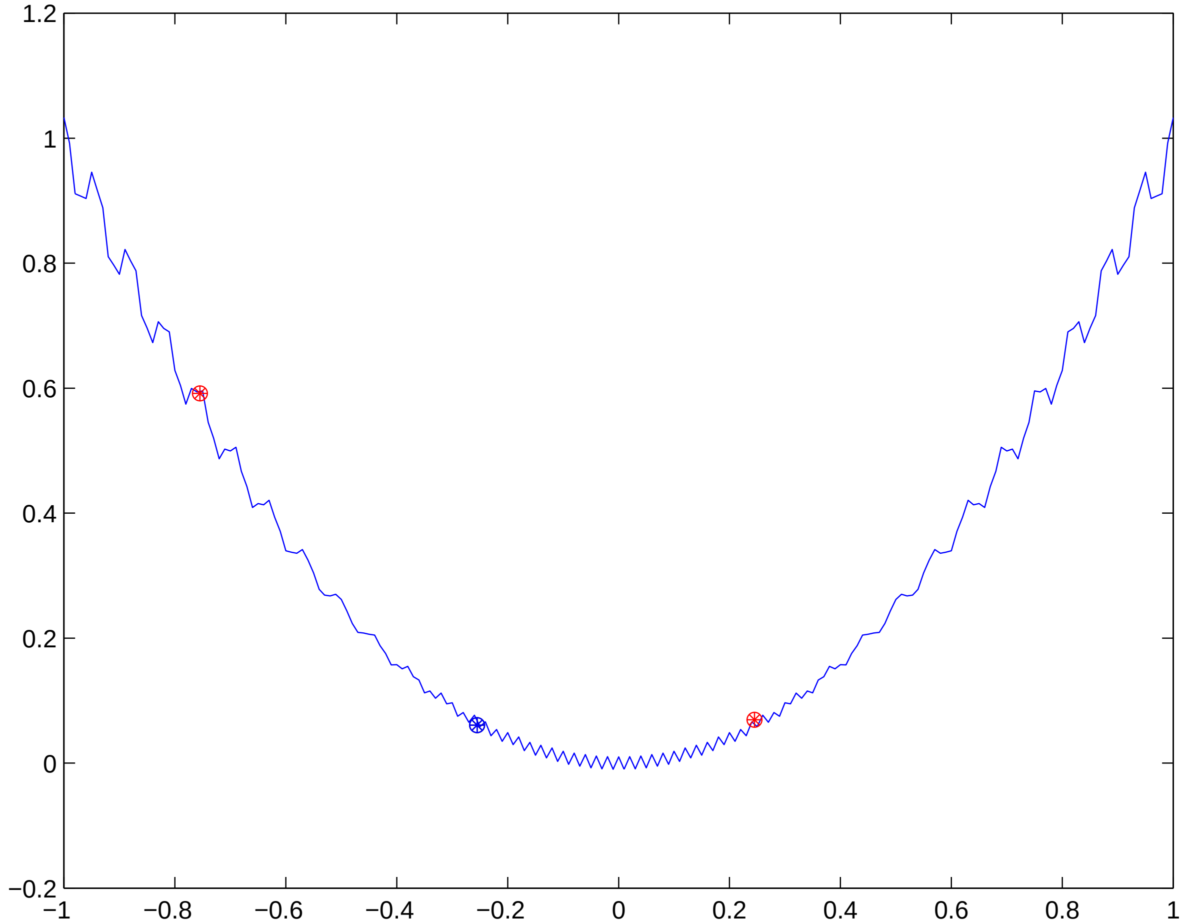
Implicit Filtering: Move



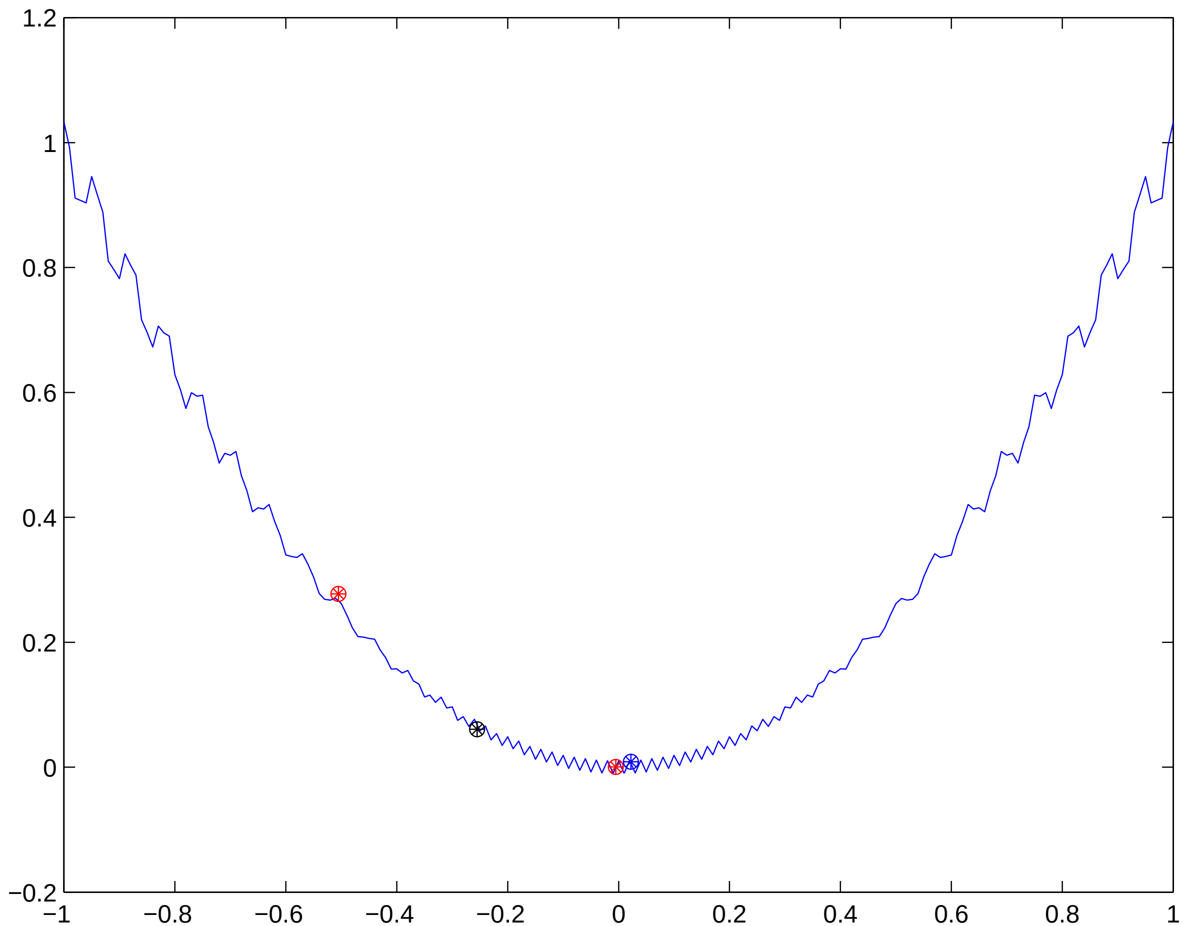
Implicit Filtering: Move



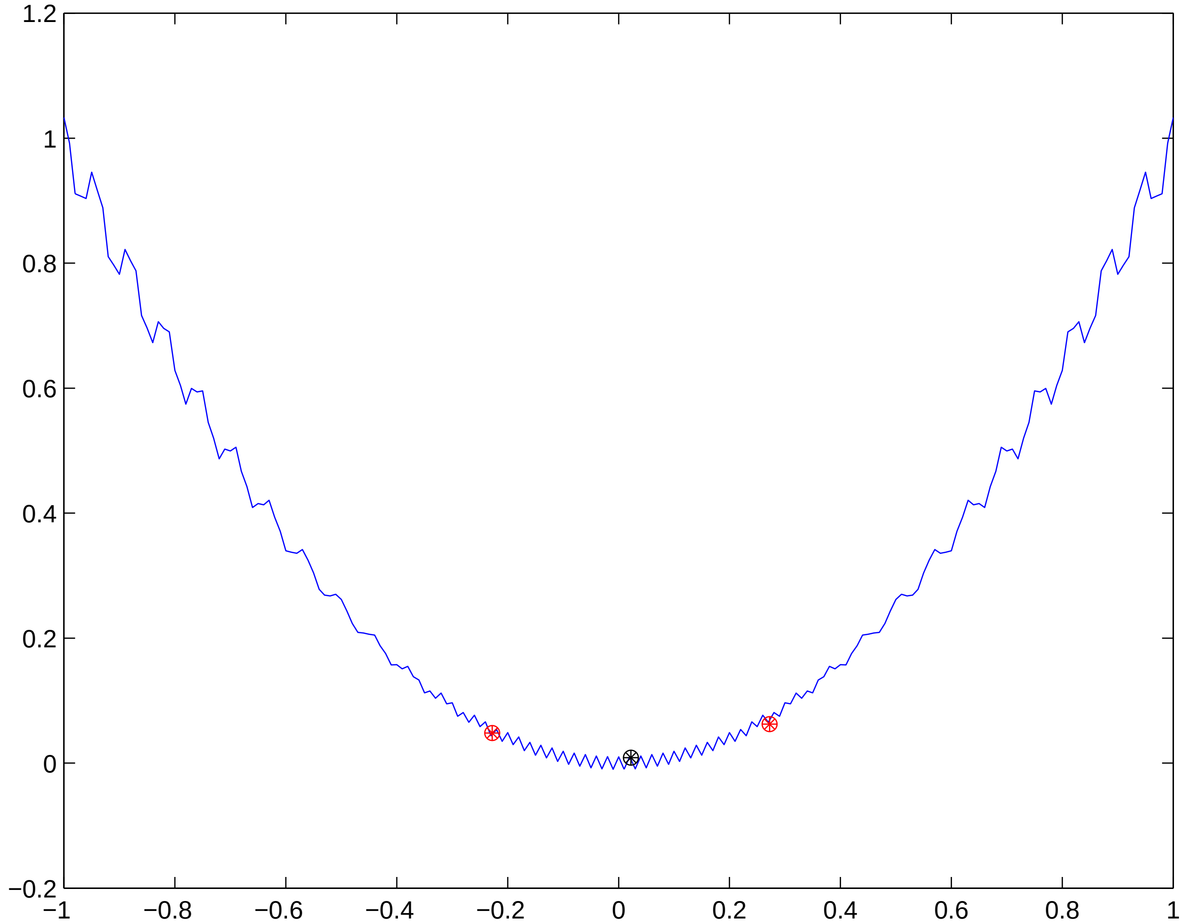
Implicit Filtering: Stencil Failure



Implicit Filtering: Shrink/Move



Implicit Filtering: Termination



Basic Convergence Theorem

Let (x_n, h_n) be the sequence from implicit filtering.
If

- ∇f_s is Lipschitz continuous.
- $\lim_{n \to \infty}(h_n + h_n^{-1} \|\phi\|_{S(x,h_n)}) = 0$
- fdquasi terminates with success for infinitely many n.

then any limit point of $\{x_n\}$ is a critical point of f_s.
Convergence rates need more.

Hidden Constraints

A hidden constraint is violated if the call to f fails.
One can (we do) treat all but bound constraints as hidden.
What to do?

- Assign a large value.
- Assign a value of infinity and reject the sample. OK for HJ/MDS, bad for IF.
- Assign a value a bit higher than the nearby points.
- Reject and use least squares to compute $\nabla_h f$.
  - Coming in new version.

NCSU fortran implementation: IFFCO

- Naturally parallel; but watch out for load balancing.
- Use best value in stencil + quasi-Newton search.
- Quasi-Newton model Hessian essential in practice.
- Termination
  - fdquasi: stencil failure, small gradient, amax, pmax
  - overall: list of scales, budget, target
- parameters: IFFCO has reasonable defaults
- hidden constraints: f does not return a value
  IFFCO is prepared
- MATLAB: imfil.m new version coming soon

How to get the software

- IFFCO: Implicit Filtering For Constrained Optimization
- New version released May, 2001
  MPI/PVM/Serial
- ftp to ftp.math.ncsu.edu in
  FTP/kelley/iffco/IFFCO.tar.gz or email to
  Tim_Kelley@ncsu.edu
  http://www4.ncsu.edu/˜ctk
  http://www4.ncsu.edu/˜ctk/iffco.html

Community Problems

- Suite of problems in groundwater remediation
  3D, flow+transport, varying difficulty.
- We provide or point to simulators/optimization codes that will produce a formulation and a solution.
- No pretense that formulation or solution is best possible.
- Portable, good testbed for optimization codes.

How to get the Community Problems

- Constantly updated on
  http://www4.ncsu.edu/˜ctk/community.html
- Packages include problems, makefiles, IFFCO example.
  You need to get the simulators; we tell you how.
- Tested on
  - g77: Solaris, Red Hat 7.3,8.0, MAC OSX, IBM-SP
  - MPI: IBM-SP, several linux clusters
- Three problems in place (only MODFLOW).
- New problems under construction.
- Massive comparison in progress
  GA, NOMAD, Boeing DE, DIRECT, APPS

Conclusions

- Optimal design of groundwater remediation problems
  - Formulation: constraints
    specification of problem
    choice of simulators
  - Community problems
  - Solution: we like sampling methods
- Sampling methods
  - Variants of coordinate search
  - Implicit filtering