Optimization and Water Resources Policy

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Outline

- Water Resource Problems
- Supply Model
- Optimization Problem
  - Hidden Constraints
  - Results from Optimization
  - Algorithm Design
- Implicit Filtering
  - What it's for and what it does
  - Theory
- Code: imfil.m
  - New Features
- Research Issues
- How to Get imfil.m

Why does North Carolina Care?

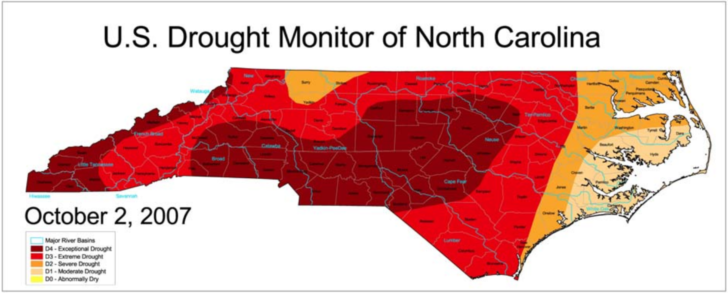
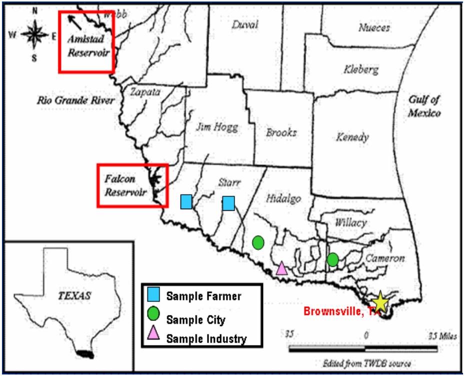


Figure 1. North Carolina Drought Management Council (http://www.ncdrought.org/).

Lower Rio Grande Valley



- City's water supply comes from
  - Permanent rights (hard to sell/buy, fixed on Jan 1)
  - Spot market leases (monthly decisions)
  - Options (purchase Jan 1, exercise May 31)
- Decisions: buy leases, buy/exercise options
  based on expected supply S_E and demand D_E
- Supply/Demand simulated by random sampling of history

Six Design Variables

- Number of rights and options: R, O
- Jan 1 – May 31: $S_E/D_E < \alpha_1$ lease (or exercise options in May) until $S_E/D_E = \beta_1$
- July 1 – Dec 31: $S_E/D_E < \alpha_2$ lease (or exercise options in May) until $S_E/D_E = \beta_2$

Minimize Cost

$$\text{Cost} = R p_R + O p_O + E(X) p_X + E\left(\sum_{months} L_t p_{L_t} \right)$$

R, O are amount of rights and options (design variables) purchased Jan 1.

Prices p_R, p_O known.

X = exercised options, price p_X (depends on data + design)

L_t = leases in month t, price p_L (depends on data + design)

Data randomly generated from historical record using several realizations.

Simple bound constraints and hidden constraints.

Variance Reduction via Control Variates: I

Assume that $f = E(\hat{f})$.
Estimate noise as standard error $\sigma/\sqrt{n}$ in $\hat{f}$
Objective: reduce variance σ; tune number of realizations n
Let Z be a random variable that is well correlated to $\hat{f}$ for which $E(Z)$ is known.
Define

$$\theta = \hat{f}(x) + c(Z - E(Z)),$$

and c is tuned to minimize variance.
We can use $f = E(\theta)$ since $E(Z)$ is known.

Variance Reduction via Control Variates: II

Since

$$Var(\theta) = Var(\hat{f}) - 2cCov(\hat{f}, Z) + c^2 Var(Z)$$

the optimal value of c is

$$c^* = Cov(\hat{f}, Z)/Var(Z).$$

We get an estimate of $Var(\theta)$ too:

$$Var(\theta) = (1 - \rho^2) Var(\hat{f})$$

where ρ is the correlation between $\hat{f}$ and Z.

Variance Reduction via Control Variates: III

One can use more than one control variate:

$$\theta = \hat{f} + \sum c_i (Z_i - E(Z_i)).$$

So, how to you invent the Z's?

- Lease price at beginning of the year has known expectation (data).
- Net supply at end of April (prior to option exercise month). Compute from inflows and demand. Expectations known (data).

Then estimate $Var(\hat{f})$ and $Cov(\hat{f}, Z)$ with a small pilot study.

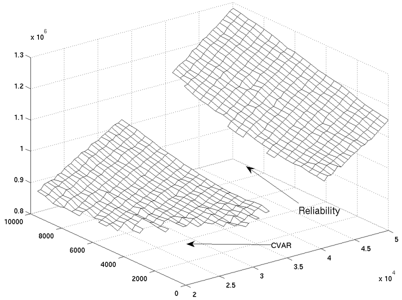
Benefits of Variance Reduction

- Smoother landscape for give number of realizations
- Reduced realizations per function call by 50%
- Promise of coupling to optimization algorithm

Hidden Constraints

- Reliability
  - Probability of serious shortage $< .005$ (every 16.7 years).
  - Tested after simulation runs.
- Conditional value-at-risk (CVAR)
  - Mean of costs above 95th percentile.
  - CVAR $\leq 1.25\times$ total portfolio costs
  - Tested after simulation runs.

Optimization Landscape



Results of Optimization

- Water Resources
  - Leases/Options vs only permanent rights
    lower annual costs with no reliability penalty
  - Leases alone reduce costs even more
    but with higher variability
- Optimization
  - Implicit filtering was robust: could cross gaps
    restarts not necessary
    final costs within 3% for varying initial iterates
  - Feasible initial iterate important

Algorithm Design

- Algorithms based on coordinate search
- Termination
  - budget, estimate of necessary conditions, . . .
- Hidden constraints
- Trivial(?) Parallelism

Noisy Optimization Problems

- Implicit filtering is designed for noisy problems.
  - Perturbations of smooth problems
  - Internal iterations
  - Stochastic models
- Handles Hidden Constraints or failed points

Stencil-Based Sampling Methods

- Given x_c, scale h_c, and directions $V = (v_1, \dots, v_k)$
  - Evaluate f at $x_c + h_c v_j$ for $1 \le j \le k$.
  - Assign NaN, Inf, or artificial value to failed point.
  - Decide what to do next.
  - Example: Coordinate Search
    - Take best point $f(x_c + h_c v_j) = min$ unless ...
    - stencil failure: $f(x_c)$ is best. In that case, reduce h_c.

Coordinate search implicitly filters out noise.

Convergence Theory: smooth f

If

- f has bounded level sets
- $f \in C^1$
- V is a positive basis

Stencil failure implies $\nabla f = O(h)$ and so ...

- $h_n \to 0$ (bounded level sets) therefore
- $\nabla f(x_n) \to 0$

Due to many authors in various forms.
True, but not very exciting.

Convergence Theory: noisy f

If

- f has bounded level sets
- $f = f_{smooth} + \phi$, $f_{smooth} \in C^1$
- V is a positive basis

then $h_n \to 0$, and if

$$\phi(x_n)/h_n \to 0$$

then

$$\nabla f_{smooth}(x_n) \to 0$$

Theory (Audet-Dennis) for Lipschitz f.

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 pictures

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

$$f = f_s + \phi$$

- 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) and therefore
- any limit point of $\{x_n\}$ is a critical point of f.

Simplex Gradient

- Coordinate search is building an approximation of the gradient.
  - Let $\delta f(x : V)_j = f(x + hv_j) - f(x)$
  - Define the simplex gradient

$$Df(x : h, V) = h^{-1}(V^T)^{\dagger}\delta f(x : V)$$

- $Df(x : h, V)$ is the minimum norm least squares solution of

$$\min \|hV^T Df - \delta f\|$$

- If V is a one-sided or centered difference stencil, you get the usual difference gradient.

Exploiting the Simplex Gradient

Since we can compute the simplex gradient with no extra effort, we can

- add $-Df$ to the stencil for the next search,
- do a line search in that direction and mimic steepest descent,
- build a quasi-Newton model Hessian and use that direction, and/or
- reduce h when $\|Df\|$ is small.

Implicit filtering reduces h when $\|Df(x:h,V)\| \le \tau h$ and uses a quasi-Newton model Hessian.

Quasi-Newton Acceleration

We begin with $H = I$. For the unconstrained case we use two updates.

- SR1

$$H_+ = H_c + \frac{(y - H_c s)(y - H_c s)^T}{(y - H_c s)^T s}$$

- BFGS

$$H_+ = H_c + \frac{yy^T}{y^T s} - \frac{(H_c s)(H_c s)^T}{s^T H_c s}$$

where $s = x_+ - x_c$ and

$$y = Df(x_+ : h_c, V) - Df(x_c : h_c, V)$$

QN Hessians make a huge difference in performance.
Obvious extension for bound constraints.

Implicit Filtering

imfilter$(x, f, pmax, \tau, \{h_n\}, amax)$
  for $k = 0, \dots$ **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 simplex gradient $Df(x : h, v)$

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

$p = 1$
while $p \le pmax$ and $\|Df(x : h, v)\| \ge \tau h$ **do**
  compute f and $Df(x : h, v)$
  terminate with success on stencil failure
  update the model Hessian H if appropriate; solve $Hd = -Df(x : h, v)f(x)$
  use a backtracking line search, with at most *amax* backtracks, to find 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
if $p <= pmax$ report success

Application of Theory

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.

Least squares gradient/Hessian approximation

- Split $H = A + C$. Approximate A with quasi-Newton. Compute C (N_C degrees of freedom).
- Compute part of the Hessian using

$$\delta f(x_c : h, V) = h_c V^T \nabla f(x_c) + \frac{h_c^2}{2} V^T H V + O(h^2)$$

by solving the least squares problem

$$\min \|\delta f(x_c : h_c, V) - h_c V^T Df(x : h, V) - \frac{h_c^2}{2} V^T C V\|$$

for N_C unknowns.

Powell (2006) has a similar idea for DFO.

Diagonal C; V central difference

- $N_C = N$, so if there are no failed points

$$\min \| f(x_+) - V^T \overline{Df} - \frac{1}{2} V^T C V \|$$

is a square system.

Not a finite difference approximation of Hessian diagonal.

Feedback to objective

You can pass h to f. This helps if . . .

- f can control its own accuracy via
  - tolerance in ODE/DAE/PDE models, or
  - number of realizations n in Monte Carlo models.
- f knows its own limiting resolution, so
  - f can tell you when to terminate the iteration.

Using the estimate of the noise

$$Df(x : h, V) = \nabla f_s + O(h + \|\phi\|/h)$$

so the noise renders the gradient estimate useless when

$$\sigma/\sqrt{n} \approx \|\phi\| \geq \|\nabla f\| h \approx \|Df(x : h, V)\| h.$$

So, if f can estimate σ, then one can tune n so that

$$\sigma/\sqrt{n} \leq M_{tune} \|Df(x : h, V)\| h.$$

Termination

Even if the gradient estimate is poor, the search may still produce good results.

However, the search fails if decreases in f do not reflect decreases in f_s:

$$\sigma/\sqrt{n} \approx \|\phi\| \geq |\delta f(x : V)_j|$$

for all j.

So, if f can tell the code what $\sigma/\sqrt{n}$ is, the code can terminate if the estimated noise is larger than the variation in f.

New Mode for Parallelism

- User managed parallelism
- Call multiple instances of objective
- Sample mpi/c/linux cluster code available coming soon

Research Issues

- Algorithms to locate neighborhoods of minimizers
- Analysis
- Asymptotic theoretical results vs tight computational budget
- Parallel computing: I/O, load balancing
- Designing feedback between function and optimization method
  - Noise estimation and control
  - Termination of iteration
- Other Applications
  Electronics, Automotive, Algorithm Tuning

How to get imfil.m

- Email me at tim_kelley@ncsu.edu
- Get it directly from
  http://www4.ncsu.edu/~ctk/imfil.html

Under construction.