Bilevel Derivative-Free Optimization and its Application to Robust Optimization

Andrew R. Conn, IBM Research

(joint work with L. N. Vicente, Univ. Coimbra)

ADVANCED METHODS AND PERSPECTIVES IN NONLINEAR OPTIMIZATION AND CONTROL,

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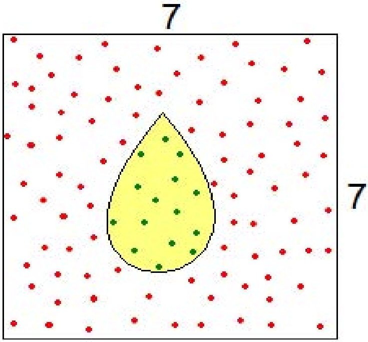
- Legacy codes (written in the past and not maintained by the original authors).
- Lack of sophistication of the user (users need improvement but want to use something simple).

Simple Example with Unavailable Derivatives

Computation of areas of figures by random generation of points (the derivatives of the area function are clearly unavailable):



$$\text{Area} = 7 * 7 * \frac{15}{90+15} = 7$$

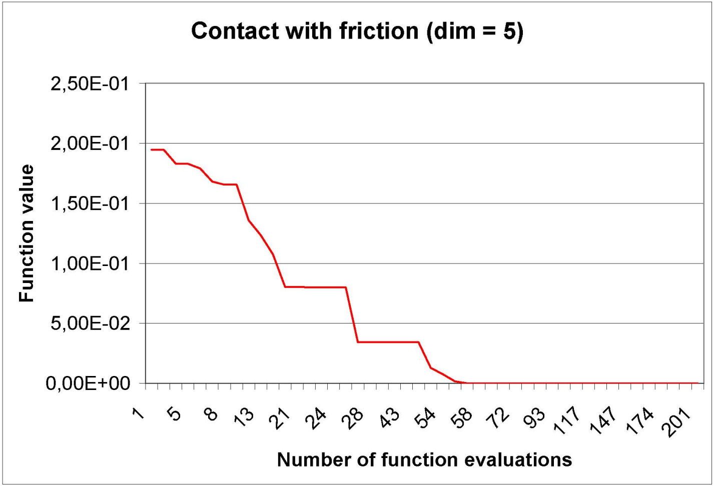
Examples of Problems where Derivatives are Unavailable

Many known applications:

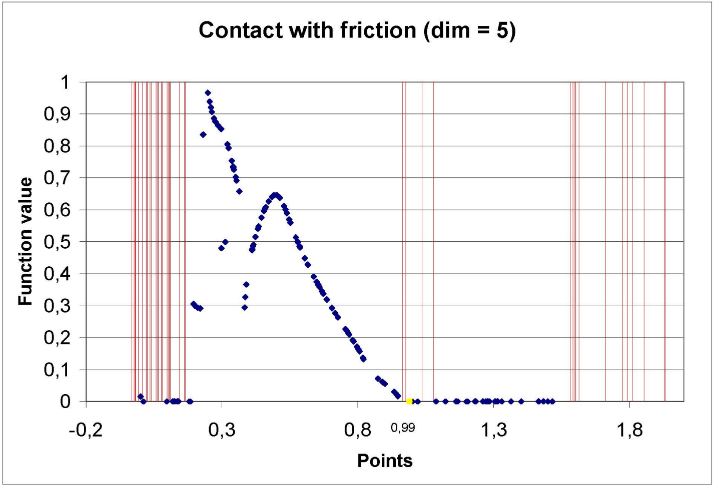
- Engineering design (many examples).
- Circuit design (tuning parameters of relatively small circuits using accurate simulation like PowerSpice).
- Molecular geometry optimization (minimization of the potential energy of clusters).
- Groundwater community problems.
- Medical image registration.
- Dynamic pricing.

- Tuning of algorithmic parameters.
- Automatic error analysis.

In DFO convergence/stopping is typically slow (per function evaluation):



The objective function not continuous or not well defined:



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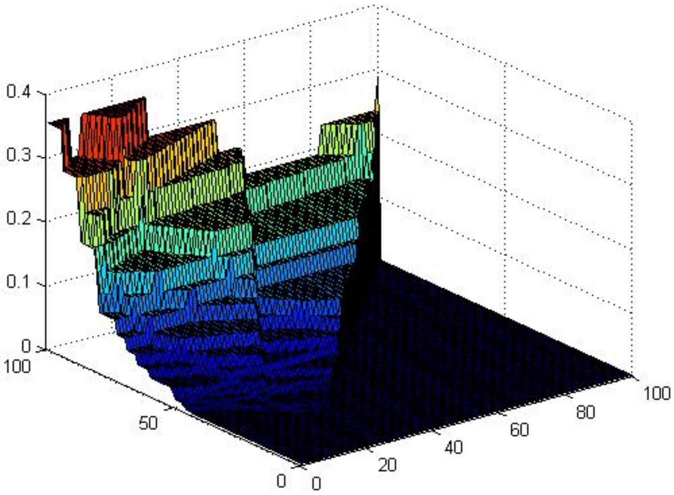

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... making the linear algebra of the algorithms relatively inexpensive.

Illustration of Curse of Dimensionality

Number of points needed to build a complete/determined quadratic polynomial interpolant model:

n	10	20	50	100	200
$(n+1)(n+2)/2$	66	231	1326	5151	20301

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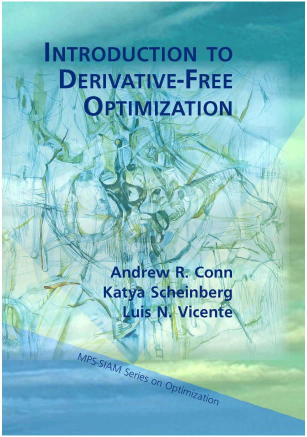
By global convergence, we mean convergence to some form of stationarity from arbitrary starting points.

The Book! (unashamed advertisement)

- A. R. Conn, K. Scheinberg, and L. N. Vicente, Introduction to Derivative-Free Optimization, MPS-SIAM Series on Optimization, SIAM, Philadelphia, 2009.



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- Calculate a step Δx_k by approximately solving the trust-region subproblem (TRS)

$$\min_{\Delta x \in B(x_k;\Delta_k)} \quad m_k(x_k + \Delta x).$$

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and

$$|f(y) - m(y)| \leq \kappa_{ef}\,\Delta^2 \qquad \forall y \in B(x;\Delta).$$

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For a class of fully-linear models, the (unknown) constants $\kappa_{ef}, \kappa_{eg} > 0$ must be independent of x and Δ.

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For a class of fully-quadratic models, the (unknown) constants $\kappa_{ef}, \kappa_{eg} > 0, \kappa_{eh} > 0$, must be independent of x and Δ.

Trust-Region Methods for DFO (basics : continued)

- Set x_{k+1} to $x_k + \Delta x_k$ (successful) or to x_k (unsuccessful) and update Δ_k depending on the value of

$$\rho_k = \frac{f(x_k) - f(x_k + \Delta x_k)}{m_k(x_k) - m_k(x_k + \Delta x_k)}.$$

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- Attempt to accept steps based on simple decrease, i.e., if

$$\rho_k > 0 \iff f(x_k + \Delta x_k) < f(x_k).$$

Trust-Region Methods for DFO (main features)

- Reduce Δ_k only if ρ_k is small and the model is FL/FQ.

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- Allow for model-improving iterations (when ρ_k is not large enough and the model is not certifiably FL/FQ).

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- Incorporate a criticality step (1st or 2nd order) when the 'stationarity' of the model is small.

  $\Longrightarrow$ Internal cycle of reductions of Δ_k.

Analysis of Trust-Region Methods (1st order)

Theorem (Book and SIOPT 2009 paper)

The trust-region radius converges to zero:

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If f is bounded below and has Lipschitz continuous first derivatives then

$$\|\nabla f(x_k)\| \longrightarrow 0.$$

$\Longrightarrow$ True for simple decrease.

$\Longrightarrow$ Use of fully linear models when necessary.

Analysis of Trust-Region Methods (2nd order)

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$$\max\left\{\|\nabla f(x_k)\|, -\lambda_{min}[\nabla^2 f(x_k)]\right\} \longrightarrow 0.$$

$\Longrightarrow$ True for simple decrease (under a modification in the trust-region radius update).

$\Longrightarrow$ Use of fully quadratic models when necessary.

Inexact Function Values (dynamic accuracy)

Instead of $f(x)$ suppose we have $\bar{f}(x;\epsilon_x)$ and we can enforce

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then

$$\frac{f(x) - f(x+s)}{m(x) - m(x+s)} \;\geq\; \eta_0' - 2\eta_0 \;>\; 0,$$

with $0 < \eta_0 < \eta_0'/2$ and $\eta_0 < 1$.

Polynomial Models

Given a sample set $Y = \{y^0, y^1, \ldots, y^p\}$, a polynomial basis ϕ, and a polynomial model $m(y) = \alpha^\top \phi(y)$, the interpolating conditions are the following system of linear equations:

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$$M(\phi, Y) = \begin{bmatrix} \phi_0(y^0) & \phi_1(y^0) & \cdots & \phi_p(y^0) \\ \phi_0(y^1) & \phi_1(y^1) & \cdots & \phi_p(y^1) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_0(y^p) & \phi_1(y^p) & \cdots & \phi_p(y^p) \end{bmatrix} \quad f(Y) = \begin{bmatrix} f(y^0) \\ f(y^1) \\ \vdots \\ f(y^p) \end{bmatrix}.$$

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We use the natural basis of monomials, which in 2D is

$$\phi = \{1, x_1, x_2, x_1^2/2, x_2^2/2, x_1 x_2\}.$$

Example of the Interpolation Matrix (underdetermined)

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For instance, when $n = d = 2$, $p = 3$, and

$$\phi \;=\; \{1, x_1, x_2, x_1^2/2, x_2^2/2, x_1 x_2\},$$

the matrix $M(\phi, Y)$ becomes

$$\left[\begin{array}{cccccc} 1 & y_1^0 & y_2^0 & (y_1^0)^2/2 & y_1^0 y_2^0 & (y_2^0)^2/2 \\ 1 & y_1^1 & y_2^1 & (y_1^1)^2/2 & y_1^1 y_2^1 & (y_2^1)^2/2 \\ 1 & y_1^2 & y_2^2 & (y_1^2)^2/2 & y_1^2 y_2^2 & (y_2^2)^2/2 \\ 1 & y_1^3 & y_2^3 & (y_1^3)^2/2 & y_1^3 y_2^3 & (y_2^3)^2/2 \end{array}\right].$$

Underdetermined Polynomial Models

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$$m(y) \;=\; c + g^\top y + \frac{1}{2} y^\top H y$$

built with less than $(n+1)(n+2)/2$ points.

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Theorem (Book)

If Y is Λ_L–poised for linear interpolation/regression then

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$\Longrightarrow$ Linear Λ_L–poisedness is equivalent to $\|M(\phi_L, Y_{scaled})^\dagger\| \leq \Lambda_L$.

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Again,

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Q: What should we do?

A: One should build models by minimizing the norm of H.

Minimum Frobenius Norm Models

Recall the sample set $Y = \{y^0, y^1, \ldots, y^p\}$ and the quadratic model

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MFN models can be built by minimizing the entries of the Hessian (in the Frobenius norm) subject to the interpolation conditions:

$$\begin{array}{ll} \min & \frac{1}{4}\|H\|_F^2 \\ \text{s.t.} & c + g^\top (y^i) + \frac{1}{2}(y^i)^\top H (y^i) \ = \ f(y^i), \quad i = 0, \ldots, p, \end{array}$$

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or, equivalently,

$$\begin{array}{ll} \min & \frac{1}{2}\|\alpha_Q\|^2 \\ \text{s.t.} & M(\phi, Y)\alpha \;=\; f(Y). \end{array}$$

The solution of this QP problem requires a linear solve with:

$$F(\phi, Y) \;=\; \left[\begin{array}{cc} M(\phi_Q, Y) M(\phi_Q, Y)^\top & M(\phi_L, Y) \\ M(\phi_L, Y)^\top & 0 \end{array} \right],$$

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$\Longrightarrow$ Λ_F–poisedness in the minimum Frobenius norm is equivalent to:

$$\|F(\phi, Y_{scaled})^{-1}\| \;\leq\; \Lambda_F.$$

Minimum Frobenius Norm Models (continued)

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where H is, again, the Hessian of the model.

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$$\|\nabla f(y) - \nabla m(y)\| \;\leq\; \Lambda_L \left[C_f + C_n C_f \Lambda_F\right] \Delta \quad \forall y \in B(x;\Delta).$$

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$\Longrightarrow$ MFN models are fully linear.

The Bilevel Programming Problem

$$\min_{(x^u, x^\ell) \in \mathbb{R}^{n^u \times n^\ell}} \quad f^u(x^u, x^\ell)$$

$$\begin{aligned} \text{subject to} \quad & c_i^u(x^u, x^\ell) = 0 & i \in \mathcal{E}^u \\ & c_i^u(x^u, x^\ell) \geq 0 & i \in \mathcal{I}^u \end{aligned}$$

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- Applications also appear in engineering (e.g., robust optimization).

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The Reduced Formulation

If we define the set of lower level minimizers (assumed a singleton) as

$$x^\ell(x^u) = \arg\min \left\{ f^\ell(x^u, x^\ell) : \; x^\ell \in \mathbb{R}^{n^\ell} \right\},$$

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We will call $f^u(x^u, x^\ell(x^u))$ the reduced upper level function.

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... which suggests solving the lower level problem using fully quadratic models.

Our DFO Approach for Bilevel Optimization

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Our Trust-Region Interpolation-based Method

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Differently, we start with less than $p_{\max} = (n+1)(n+2)/2$ points and use MFN models.

Thus, until $|$sample set$|$ reaches $p_{\max}$, we never discard points from the sample set and always add new trial points independently of being accepted or not as new iterates.

Our Trust-Region Interpolation-based Method (continued)

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In such situations, we never reduce the trust radius.

Inexact Solution of the Lower Level Problem

Under reasonable assumptions, one can prove

$$|f^u(x^u, x^\ell(x^u)) - f^u(x^u, x^\ell_{dfo}(x^u))| \leq \mathcal{O}(\|\nabla_\ell m^\ell(x^u, x^\ell_{dfo}(x^u))\|) + \mathcal{O}((\Delta^\ell)^2).$$

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Thus, if

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and one can prove that the upper level model stays fully linear.

Dynamic Accuracy Requirements

One way to approximately enforce the dynamic accuracy requirement is to consider only

$$\epsilon_{x^u+s^u} \leq \eta_0'(m^u(x^u) - m^u(x^u + s^u))$$

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Reusing Previous (Upper Level Perturbed) Evaluated Points

Since

$$|f^\ell(x^u, x^\ell) - f^\ell(x^u_{pert}, x^\ell)| \;\leq\; \mathcal{O}(\|x^u - x^u_{pert}\|),$$

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This provide us a criterion to decide whether to accept previously evaluated points in the building of the lower level model.

Matlab Code

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The code handles bilevel problems with any type of linear constraints except upper level constraints on the lower level variables.

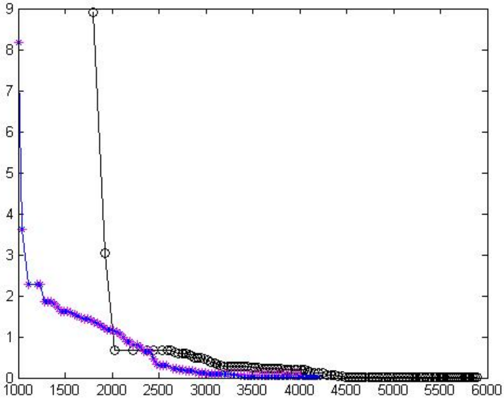
Another feature not described is a warm start procedure for initialization of lower level variables by forming a linear model of $x^\ell(x^u)$.

Quadratic/Quartic 5×5 Example

Black: basic version

Red: inexact lower level

Blue: inexact lower level & reuse of points



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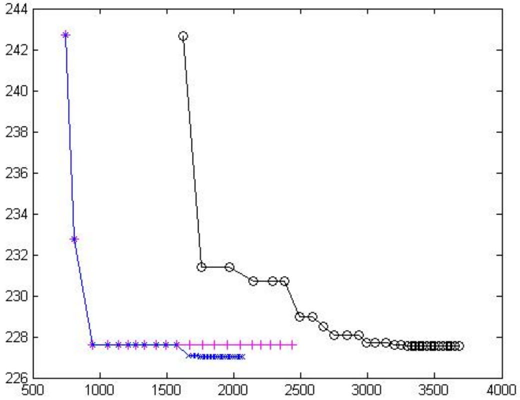

Cubic/Quadratic 20×20 example, with linear constraints

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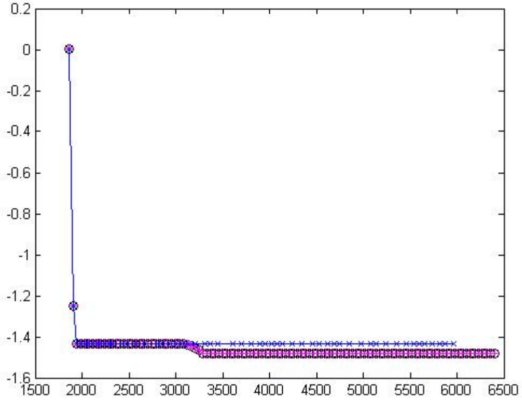

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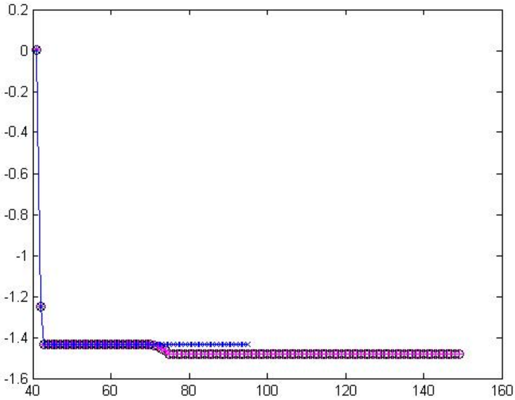

Same $f^u(x^u, x^\ell_{dfo}(x^u))$ values (but now as a function of the # ul evaluations).

Robust Optimization

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Robust optimization also provides a tool for dealing with variables for which the optimal values must be later implemented.

Robust Optimization as Bilevel

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We tested our algorithm in the example reported in Bertsimas, Nohadani, Teo, 2010.

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The robust function is $f(x, p) = g(x + p)$, where $x, p \in \mathbb{R}^2$ and

$$\begin{aligned} g(x) &= 2x_1^6 - 12.2x_1^5 + 21.2x_1^4 - 6.4x_1^3 - 4.7x_1^2 + 6.2x_1 \\ &\quad + x_2^6 - 11x_2^5 + 43.3x_2^4 - 74.8x_2^3 + 56.9x_2^2 - 10x_2 \\ &\quad - 0.1x_1^2x_2^2 + 0.4x_1^2x_2 + 0.4x_2^2x_1 - 4.1x_1x_2. \end{aligned}$$

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The problem has one lower level constraint of the form $\|p\| \leq 0.5$ describing implementation errors:

$$\begin{aligned} \min_{x\in\mathbb{R}^2, p\in\mathbb{R}^2} \quad & g(x+p) \\ \text{s.t.} \quad & p \in \arg\min \left\{ -g(x+p) : \; p \in \mathbb{R}^2, \|p\| \leq 0.5 \right\}. \end{aligned}$$

Bertsimas et al. Example (initial point A)

Black: basic version
Red: inexact lower level
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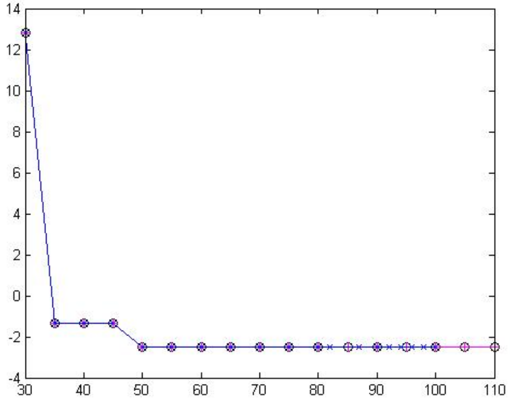

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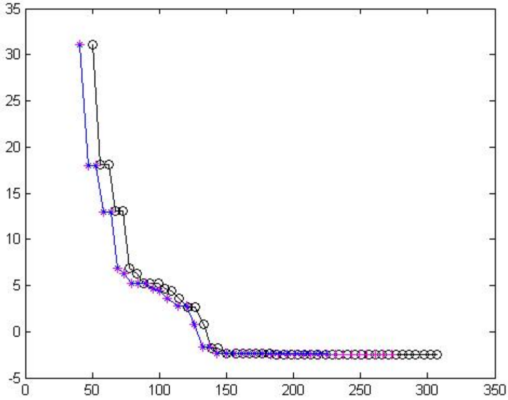
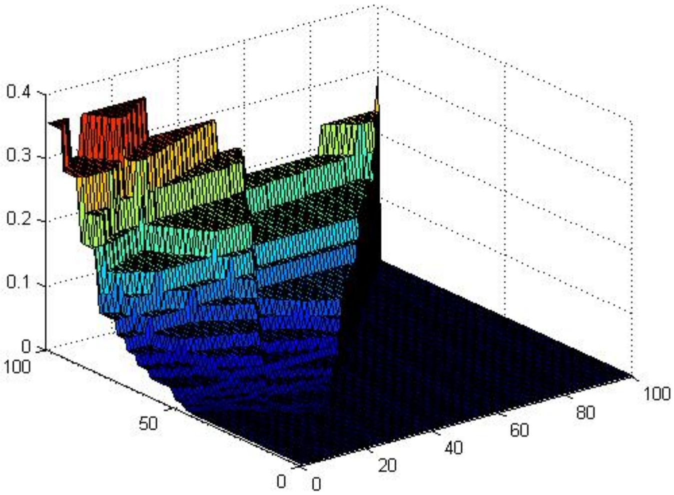


We are currently solving robust portfolio problems involving the Omega function.



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The Omega function is the ratio of the weighted gains (above L) over the weighted losses (below L):

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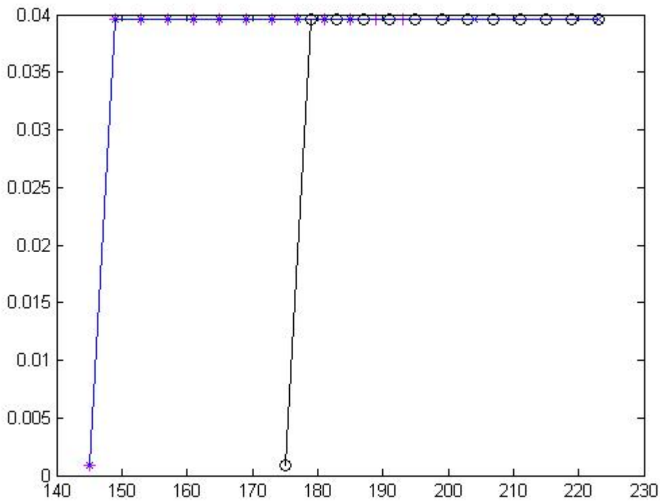
For portfolio optimization, one considers $\Omega(x_1 R_1 + \cdots + x_n R_n)$ and minimize over $x_1 + \cdots + x_n = 1$ and $x_1, \ldots, x_n \geq 0$
and the single threshold parameter L is allowed to vary for robustness in $[0, 0.04]$.

$$\min_{(x^u, x^\ell) \in \mathbb{R}^7 \times [0, 0.04]} \quad -\Omega(x^u; x^\ell)$$
$$\text{s.t.} \quad x^\ell \in \arg\min \left\{ \Omega(x^u; z^\ell) : \; z^\ell \in [0, 0.04] \right\}.$$

Maximizing the Omega Function

8 assets = 7 upper level variables

1 return level = 1 lower level variable / robust variable



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