Nonlinear Programming: Concepts and Algorithms for Process Optimization

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Nonlinear Programming and Process Optimization

Introduction

Unconstrained Optimization
- Algorithms
- Newton Methods
- Quasi-Newton Methods

Constrained Optimization
- Karush Kuhn-Tucker Conditions
- Reduced Gradient Methods (GRG2, CONOPT, MINOS)
- Successive Quadratic Programming (SQP)
- Interior Point Methods (IPOPT)

Process Optimization
- Black Box Optimization
- Modular Flowsheet Optimization – Infeasible Path
- The Role of Exact Derivatives

Large-Scale Nonlinear Programming
- rSQP: Process Optimization
- IPOPT: Blending and Data Reconciliation

Summary and Conclusions

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Introduction

Optimization: given a system or process, find the best solution to this process within constraints.

Objective Function: indicator of "goodness" of solution, e.g., cost, yield, profit, etc.

Decision Variables: variables that influence process behavior and can be adjusted for optimization.

In many cases, this task is done by trial and error (through case study). Here, we are interested in a *systematic* approach to this task - and to make this task as efficient as possible.

Some related areas:

- Math programming
- Operations Research

Currently - Over 30 journals devoted to optimization with roughly 200 papers/month - a fast moving field!

Optimization Viewpoints

Mathematician - characterization of theoretical properties of optimization, convergence, existence, local convergence rates.

Numerical Analyst - implementation of optimization method for efficient and "practical" use. Concerned with ease of computations, numerical stability, performance.

Engineer - applies optimization method to real problems. Concerned with reliability, robustness, efficiency, diagnosis, and recovery from failure.

Optimization Literature

Engineering

1. Edgar, T.F., D.M. Himmelblau, and L. S. Lasdon, Optimization of Chemical Processes, McGraw-Hill, 2001.

2. Papalambros, P. and D. Wilde, Principles of Optimal Design. Cambridge Press, 1988.

3. Reklaitis, G., A. Ravindran, and K. Ragsdell, Engineering Optimization, Wiley, 1983.

4. Biegler, L. T., I. E. Grossmann and A. Westerberg, Systematic Methods of Chemical Process Design, Prentice Hall, 1997.

5. Biegler, L. T., Nonlinear Programming: Concepts, Algorithms and Applications to Chemical Engineering, SIAM, 2010.

Numerical Analysis

1. Dennis, J.E. and R. Schnabel, Numerical Methods of Unconstrained Optimization, Prentice-Hall, (1983), SIAM (1995)

2. Fletcher, R. Practical Methods of Optimization, Wiley, 1987.

3. Gill, P.E, W. Murray and M. Wright, Practical Optimization, Academic Press, 1981.

4. Nocedal, J. and S. Wright, Numerical Optimization, Springer, 2007

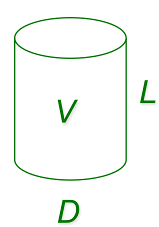
Example: Optimal Vessel Dimensions

What is the optimal L/D ratio for a cylindrical vessel?

Constrained Problem

$$\text{Min} \left\{ C_T \frac{\pi D^2}{2} + C_S \pi DL = \text{cost} \right\} \qquad (1)$$

$$\text{s.t.} \quad V - \frac{\pi D^2 L}{4} = 0$$



Convert to Unconstrained (Eliminate L)

$$\text{Min} \left\{ C_T \frac{\pi D^2}{2} + C_S \frac{4V}{D} = \text{cost} \right\} \qquad (2)$$

$$\frac{d(\text{cost})}{dD} = C_T \pi D - \frac{4VC_s}{D^2} = 0$$

$$D = \left(\frac{4V}{\pi} \frac{C_S}{C_T} \right)^{1/3} \qquad L = \left(\frac{4V}{\pi} \right)^{1/3} \left(\frac{C_T}{C_S} \right)^{2/3}$$

==> $L/D = C_T/C_S$

Note:

- What if L cannot be eliminated in (1) explicitly? (strange shape)
- What if D cannot be extracted from (2)? (cost correlation implicit)

Unconstrained Multivariable Optimization

Problem: Min $f(x)$ (n variables)

Equivalent to: Max $-f(x),\ x \in R^n$

Nonsmooth Functions
- Direct Search Methods
- Statistical/Random Methods

Smooth Functions
- 1st Order Methods
- *Newton Type Methods*
- Conjugate Gradients

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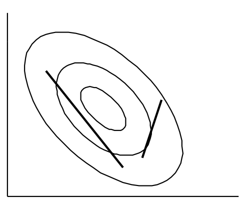
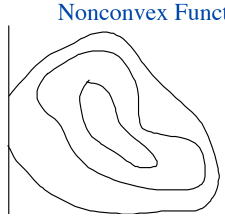
Two Dimensional Contours of F(x)

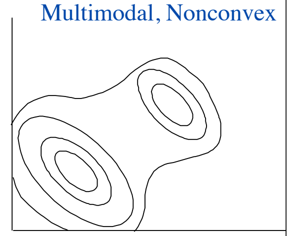
Convex Function

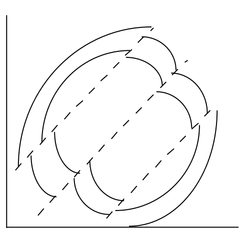


Nonconvex Function

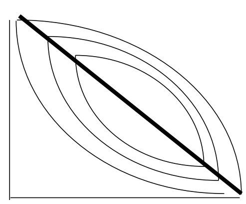


Multimodal, Nonconvex





Discontinuous



Nondifferentiable (convex)

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Local vs. Global Solutions

Convexity Definitions

•a set (region) **X** is convex, if and only if it satisfies:

$$\alpha y + (1-\alpha)z \in X$$

for all α, $0 \leq \alpha \leq 1$, for all points y and z in **X**.

• *f(x)* is convex in domain **X**, if and only if it satisfies:

$$f(\alpha y + (1-\alpha) z) \leq \alpha f(y) + (1-\alpha) f(z)$$

for any α, $0 \leq \alpha \leq 1$, at all points y and z in **X**.

•Find a *local minimum* point x* for f(x) for feasible region defined by constraint functions: $f(x^*) \leq f(x)$ *for all x satisfying the constraints in some neighborhood around* x^* (not for all $x \in \mathbf{X}$)

•Sufficient condition for a local solution to the NLP to be a global is that $f(x)$ is convex for $x \in \mathbf{X}$.

•Finding and verifying *global solutions* will not be considered here.

•Requires a more expensive search (e.g. spatial branch and bound).

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Linear Algebra - Background

Some Definitions

- Scalars - Greek letters, α, β, γ
- Vectors - Roman Letters, lower case
- Matrices - Roman Letters, upper case
- Matrix Multiplication:
  $C = A B$ if $A \in \Re^{n \times m}$, $B \in \Re^{m \times p}$ and $C \in \Re^{n \times p}$, $C_{ij} = \Sigma_k A_{ik} B_{kj}$
- Transpose - if $A \in \Re^{n \times m}$,
  interchange rows and columns --> $A^T \in \Re^{m \times n}$
- Symmetric Matrix - $A \in \Re^{n \times n}$ (square matrix) and $A = A^T$
- Identity Matrix - I, square matrix with ones on diagonal
  and zeroes elsewhere.
- Determinant: "Inverse Volume" measure of a square matrix
  $\det(A) = \Sigma_i (-1)^{i+j} A_{ij} \underline{A}_{ij}$ for any j, or
  $\det(A) = \Sigma_j (-1)^{i+j} A_{ij} \underline{A}_{ij}$ for any i, where $\underline{A}_{ij}$ is the determinant of an order *n-1* matrix with row i and column j removed.
  $\det(I) = 1$
- Singular Matrix: $\det(A) = 0$

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Linear Algebra - Background

Gradient Vector - ($\nabla f(x)$)

$$\nabla f = \begin{bmatrix} \partial f / \partial x_1 \\ \partial f / \partial x_2 \\ \ldots\ldots \\ \partial f / \partial x_n \end{bmatrix}$$

Hessian Matrix ($\nabla^2 f(x)$ - Symmetric)

$$\nabla^2 f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \cdot\cdot\cdot\cdot & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \ldots. & \ldots. & \ldots. \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} \cdot\cdot\cdot\cdot & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Note: $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$

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Linear Algebra - Background

- Some Identities for Determinant
  $\det(A\,B) = \det(A)\det(B)$; $\det(A) = \det(A^T)$
  $\det(\alpha A) = \alpha^n \det(A)$; $\det(A) = \Pi_i \lambda_i(A)$

- Eigenvalues: $\det(A - \lambda I) = 0$, Eigenvector: $Av = \lambda v$
  Characteristic values and directions of a matrix.
  For nonsymmetric matrices eigenvalues can be complex,
  so we often use singular values, $\sigma = \lambda(A^TA)^{1/2} \geq 0$

- Vector Norms
  $\| x \|_p = \{\Sigma_i |x_i|^p\}^{1/p}$
  (most common are p = 1, p = 2 (Euclidean) and p = ∞ (max norm = $\max_i|x_i|$))
- Matrix Norms
  $\|A\| = \max \|A x\|/\|x\|$ over x (for p-norms)
  $\|A\|_1$ - max column sum of A, $\max_j (\Sigma_i |A_{ij}|)$
  $\|A\|_\infty$ - maximum row sum of A, $\max_i (\Sigma_j |A_{ij}|)$
  $\|A\|_2 = [\sigma_{max}(A)]$ (spectral radius)
  $\|A\|_F = [\Sigma_i \Sigma_j (A_{ij})^2]^{1/2}$ (Frobenius norm)
  $\kappa(A) = \|A\| \|A^{-1}\|$ (condition number) $= \sigma_{max}/\sigma_{min}$ (using 2-norm)

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Linear Algebra - Eigenvalues

Find v and λ where $Av_i = \lambda_i v_i$, i = i,n
Note: $Av - \lambda v = (A - \lambda I)\, v = 0$ or $\det (A - \lambda I) = 0$
For this relation λ is an eigenvalue and v is an eigenvector of A.

If A is symmetric, all λ_i are real
- $\lambda_i > 0$, i = 1, n; A is positive definite
- $\lambda_i < 0$, i = 1, n; A is negative definite
- $\lambda_i = 0$, some i: A is singular

Quadratic Form can be expressed in Canonical Form (Eigenvalue/Eigenvector)

$x^T A x \quad \Rightarrow \quad A\, V = V\, \Lambda$

V - eigenvector matrix (n x n)

Λ - eigenvalue (diagonal) matrix = $\mathrm{diag}(\lambda_i)$

If A is symmetric, all λ_i are real and V can be chosen orthonormal ($V^{-1} = V^T$).
Thus, $A = V\, \Lambda\, V^{-1} = V\, \Lambda\, V^T$

For Quadratic Function: $Q(x) = a^T x + ½\, x^T A x$

Define: $z = V^T x$ and $Q(Vz) = (a^T V)\, z + ½\, z^T (V^T A V) z$
$= (a^T V)\, z + ½\, z^T\, \Lambda\, z$

Minimum occurs at (if $\lambda_i > 0$) $x = -A^{-1} a$ or $x = Vz = -V(\Lambda^{-1} V^T a)$

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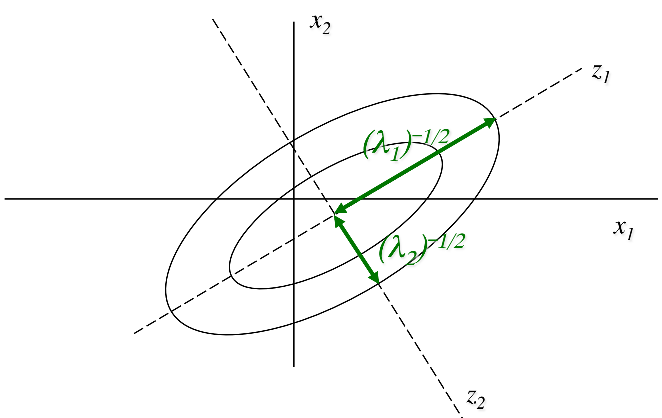
Positive (Negative) Curvature
Positive (Negative) Definite Hessian

Both eigenvalues are strictly positive (negative)
- A is positive (negative) definite
- Stationary points are minima (maxima)



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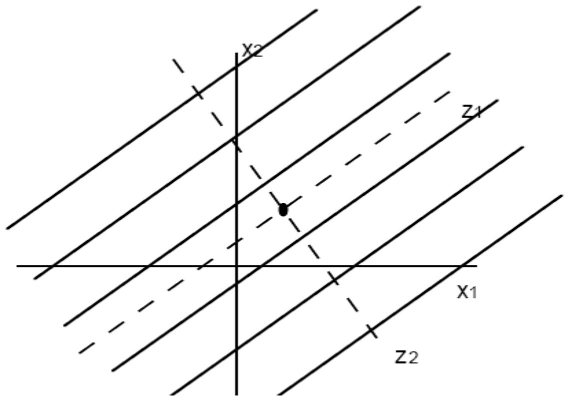
Zero Curvature
Singular Hessian

One eigenvalue is zero, the other is strictly positive or negative

- A is <u>positive semidefinite</u> or <u>negative semidefinite</u>
- There is a ridge of stationary points (minima or maxima)



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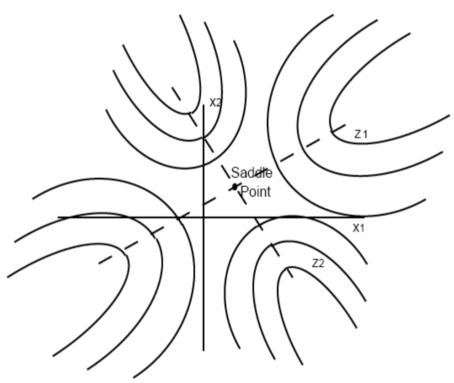
Indefinite Curvature
Indefinite Hessian

One eigenvalue is positive, the other is negative

- Stationary point is a saddle point
- A is indefinite



Note: these can also be viewed as two dimensional projections for higher dimensional problems

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Eigenvalue Example

$$Min\ \ Q(x) = \begin{bmatrix}1\\1\end{bmatrix}^T x + \frac{1}{2}x^T\begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}x$$

$$AV = V\Lambda \quad \text{with}\ \ A = \begin{bmatrix}2 & 1\\1 & 2\end{bmatrix}$$

$$V^T AV = \Lambda = \begin{bmatrix}1 & 0\\0 & 3\end{bmatrix}\ \text{with V} = \begin{bmatrix}1/\sqrt{2} & 1/\sqrt{2}\\-1/\sqrt{2} & 1/\sqrt{2}\end{bmatrix}$$

- **All eigenvalues are positive**
- **Minimum occurs at $z^* = -\Lambda^{-1}V^Ta$**

$$z = V^T x = \begin{bmatrix}(x_1 - x_2)/\sqrt{2}\\(x_1 + x_2)/\sqrt{2}\end{bmatrix} \qquad x = Vz = \begin{bmatrix}(x_1 + x_2)/\sqrt{2}\\(-x_1 + x_2)/\sqrt{2}\end{bmatrix}$$

$$z^* = \begin{bmatrix}0\\-2/(3\sqrt{2})\end{bmatrix} \qquad x^* = \begin{bmatrix}-1/3\\-1/3\end{bmatrix}$$

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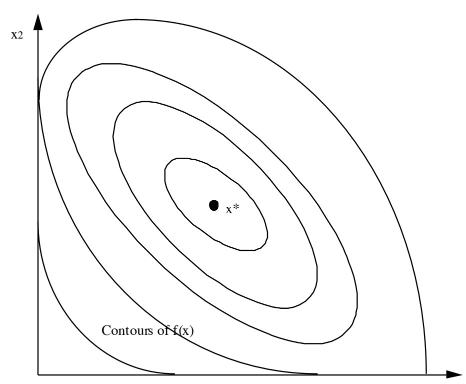
What conditions characterize an optimal solution?



Unconstrained Local Minimum
Necessary Conditions
$\nabla f(x^*) = 0$
$p^T\nabla^2 f(x^*)\, p \geq 0$ for $p \in \Re^n$
(positive semi-definite)

Unconstrained Local Minimum
Sufficient Conditions
$\nabla f(x^*) = 0$
$p^T\nabla^2 f(x^*)\, p > 0$ for $p \in \Re^n$
(positive definite)

For smooth functions, why are contours around optimum elliptical?
Taylor Series in n dimensions about x^*:

$$f(x) = f(x^*) + \nabla f(x^*)^T(x - x^*) + \frac{1}{2}(x - x^*)^T\nabla^2 f(x^*)(x - x^*) + O\left(\|x - x^*\|^3\right)$$

Since $\nabla f(x^*) = 0$, $f(x)$ is purely quadratic for x close to x^*

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Newton's Method

Taylor Series for $f(x)$ about x^k

Take derivative wrt x, set LHS ≈ 0

$$0 \approx \nabla f(x) = \nabla f(x^k) + \nabla^2 f(x^k)\,(x - x^k) + O(||x - x^k||^2)$$
$$\Rightarrow \quad (x - x^k) \equiv d = -\,(\nabla^2 f(x^k))^{-1}\,\nabla f(x^k)$$

- $f(x)$ is convex (concave) if for all $x \in \Re^n$, $\nabla^2 f(x)$ is positive (negative) semidefinite i.e. $\min_j \lambda_j \geq 0$ ($\max_j \lambda_j \leq 0$)
- Method can fail if:
  - x^0 far from optimum
  - $\nabla^2 f$ is singular at any point
  - $f(x)$ is not smooth
- Search direction, d, requires solution of linear equations.
- Near solution:

$$\left\| x^{k+1} - x^* \right\| = O\left\| x^k - x^* \right\|^2$$

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Basic Newton Algorithm - Line Search

0. Guess x^0, Evaluate $f(x^0)$.

1. At x^k, evaluate $\nabla f(x^k)$.

2. Evaluate $B^k = \nabla^2 f(x^k)$ or an approximation.

3. Solve: $\boldsymbol{B^k\, d = -\nabla f(x^k)}$
   If convergence error is less than tolerance:
   e.g., $||\nabla f(x^k)|| \leq \varepsilon$ and $||d|| \leq \varepsilon$ STOP, else go to 4.

4. Find α so that $0 < \alpha \leq 1$ and $f(x^k + \alpha\, d) < f(x^k)$
   sufficiently (Each trial requires evaluation of $f(x)$)

5. $x^{k+1} = x^k + \alpha\, d$. Set $k = k + 1$ Go to 1.

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Comparison of Optimization Methods

1. Convergence Theory

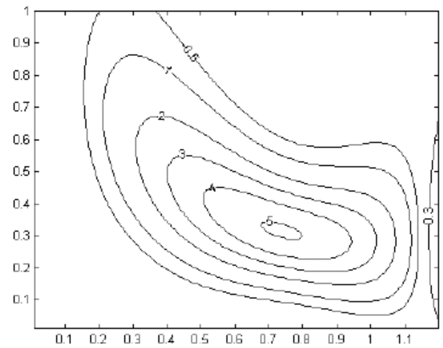
- Global Convergence - will it converge to a local optimum (or stationary point) from a poor starting point?
- Local Convergence Rate - how fast will it converge close to this point?

2. Benchmarks on Large Class of Test Problems

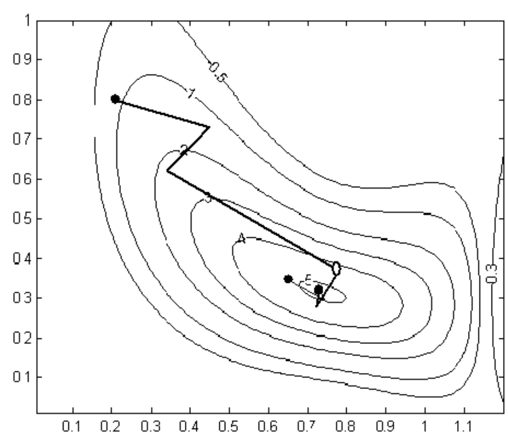
Representative Problem (Hughes, 1981)

$Min\ f(x_1, x_2) = \alpha\ exp(-\beta)$
$u = x_1 - 0.8$
$v = x_2 - (a_1 + a_2 u^2 (1- u)^{1/2} - a_3 u)$
$\alpha = -b_1 + b_2 u^2 (1+u)^{1/2} + b_3 u$
$\beta = c_1 v^2 (1 - c_2 v)/(1+ c_3 u^2)$

$a = [0.3, 0.6, 0.2]$
$b = [5, 26, 3]$
$c = [40, 1, 10]$
$x^* = [0.7395, 0.3144]$ $\quad f(x^*) = -5.0893$



Newton's Method - Convergence Path



Starting Points
[0.8, 0.2] needs steepest descent steps w/ line search up to 'O', takes 7 iterations to $\|\nabla f(x^*)\| \leq 10^{-6}$

[0.35, 0.65] converges in four iterations with full steps to $\|\nabla f(x^*)\| \leq 10^{-6}$

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Newton's Method - Notes

- Choice of B^k determines method.
  - Steepest Descent: $B^k = \gamma I$
  - Newton: $B^k = \nabla^2 f(x)$
- With suitable B^k, performance may be good enough if $f(x^k + \alpha d)$ is sufficiently decreased (instead of minimized along line search direction).
- *Trust region extensions* to Newton's method provide very strong global convergence properties and very reliable algorithms.
- Local rate of convergence depends on choice of B^k.

$$\text{Newton} - \text{Quadratic Rate}: \quad \lim_{k\to\infty} \frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|^2} = K$$

$$\text{Steepest descent} - \text{Linear Rate}: \quad \lim_{k\to\infty} \frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|} < 1$$

$$\text{Desired?} - \text{Superlinear Rate}: \quad \lim_{k\to\infty} \frac{\|x^{k+1} - x^*\|}{\|x^k - x^*\|} = 0$$

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Quasi-Newton Methods

Motivation:

- Need B^k to be positive definite.
- Avoid calculation of $\nabla^2 f$.
- Avoid solution of linear system for $d = -(B^k)^{-1} \nabla f(x^k)$

Strategy: Define matrix updating formulas that give (B^k) symmetric, positive definite and satisfy:

$(B^{k+1})(x^{k+1} - x^k) = (\nabla f^{k+1} - \nabla f^k)$ (Secant relation)

DFP Formula: (Davidon, Fletcher, Powell, 1958, 1964)

$$B^{k+1} = B^k + \frac{(y - B^k s) y^T + y (y - B^k s)^T}{y^T s} - \frac{(y - B^k s)^T s \, y \, y^T}{(y^T s)(y^T s)}$$

$$(B^{k+1})^{-1} = H^{k+1} = H^k + \frac{s s^T}{s^T y} - \frac{H^k y \, y^T H^k}{y H^k y}$$

where: $s = x^{k+1} - x^k$

$y = \nabla f(x^{k+1}) - \nabla f(x^k)$

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Quasi-Newton Methods

BFGS Formula (Broyden, Fletcher, Goldfarb, Shanno, 1970-71)

$$B^{k+1} = B^k + \frac{yy^T}{s^T y} - \frac{B^k s\, s^T B^k}{s\, B^k s}$$

$$\left(B^{k+1}\right)^{-1} = H^{k+1} = H^k + \frac{\left(s - H^k y\right)s^T + s\left(s - H^k y\right)^T}{y^T s} - \frac{\left(y - H^k s\right)^T y\, s\, s^T}{\left(y^T s\right)\left(y^T s\right)}$$

Notes:

1) Both formulas are derived under similar assumptions and have symmetry
2) Both have superlinear convergence and terminate in n steps on quadratic functions. They are identical if α is minimized.
3) BFGS is more stable and performs better than DFP, in general.
4) For n ≤ 100, these are the best methods for general purpose problems if second derivatives are not available.

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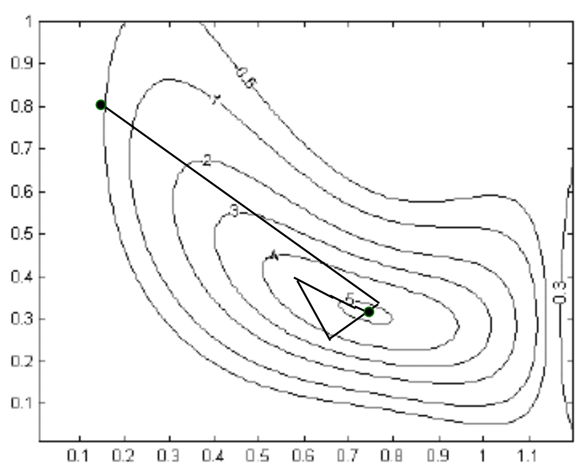
Quasi-Newton Method - BFGS Convergence Path



Starting Point

[0.2, 0.8] starting from $B^0 = I$, converges in 9 iterations to $||\nabla f(x^*)|| \leq 10^{-6}$

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Constrained Optimization (Nonlinear Programming)

Problem: $\quad Min_x \ f(x)$

$\quad$ s.t. $\quad g(x) \le 0$

$\qquad\qquad h(x) = 0$

where:

- $f(x)$ - scalar objective function
- x - n vector of variables
- $g(x)$ - inequality constraints, m vector
- $h(x)$ - meq equality constraints.

Sufficient Condition for Global Optimum

- $f(x)$ must be *convex*, and
- feasible region must be convex,
  i.e. $g(x)$ are all *convex*
  $h(x)$ are all *linear*

Except in special cases, there is no guarantee that a local optimum is global if sufficient conditions are violated.

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Example: Minimize Packing Dimensions

What is the smallest box for three round objects?

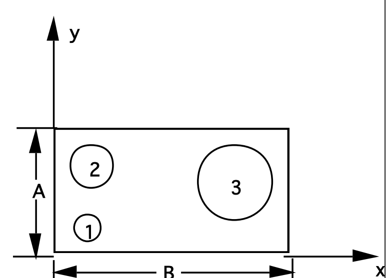
Variables: $A, B, (x_1, y_1), (x_2, y_2), (x_3, y_3)$

Fixed Parameters: R_1, R_2, R_3

Objective: Minimize Perimeter = $2(A+B)$

Constraints: Circles remain in box, can't overlap

Decisions: Sides of box, centers of circles.



$$\begin{cases} x_1, y_1 \ge R_1 & x_1 \le B - R_1, \ y_1 \le A - R_1 \\ x_2, y_2 \ge R_2 & x_2 \le B - R_2, \ y_2 \le A - R_2 \\ x_3, y_3 \ge R_3 & x_3 \le B - R_3, \ y_3 \le A - R_3 \end{cases}$$

in box

$x_1, x_2, x_3, y_1, y_2, y_3, A, B \ge 0$

$$\begin{cases} (x_1 - x_2)^2 + (y_1 - y_2)^2 \ge (R_1 + R_2)^2 \\ (x_1 - x_3)^2 + (y_1 - y_3)^2 \ge (R_1 + R_3)^2 \\ (x_2 - x_3)^2 + (y_2 - y_3)^2 \ge (R_2 + R_3)^2 \end{cases}$$

no overlaps

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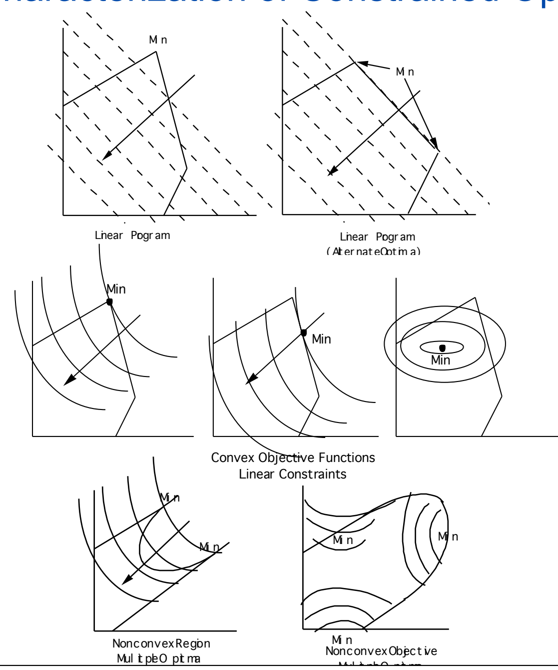
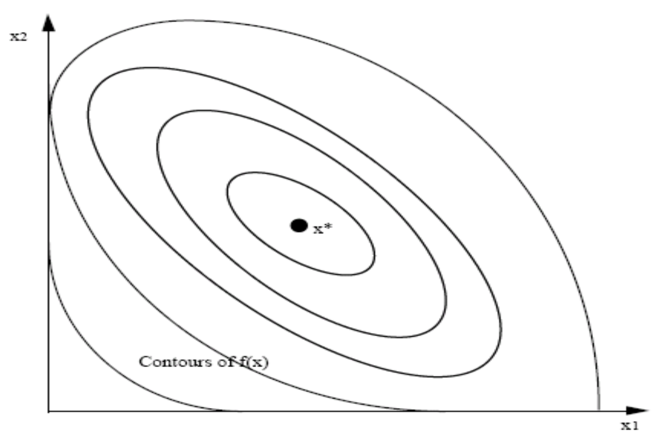
Characterization of Constrained Optima



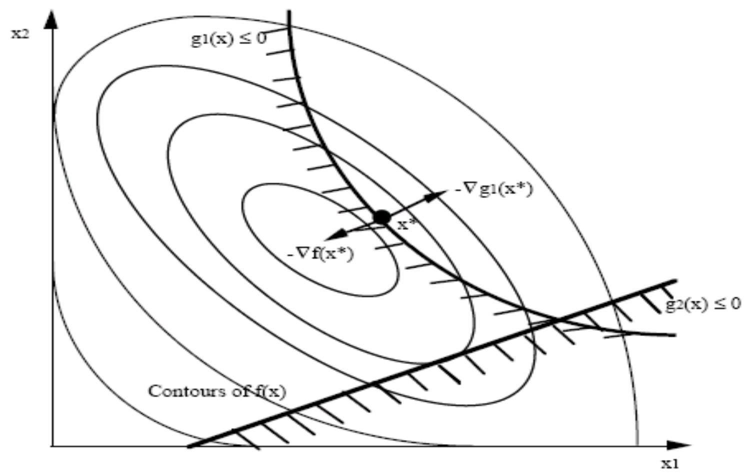
What conditions characterize an optimal solution?



<u>Unconstrained Local Minimum</u>
<u>Necessary Conditions</u>
$\nabla f(x^*) = 0$
$p^T \nabla^2 f(x^*)\, p \geq 0$ for $p \in \Re^n$
(positive semi-definite)

<u>Unconstrained Local Minimum</u>
<u>Sufficient Conditions</u>
$\nabla f(x^*) = 0$
$p^T \nabla^2 f(x^*)\, p > 0$ for $p \in \Re^n$
(positive definite)

Optimal solution for inequality constrained problem



Min $f(x)$
s.t. $g(x) \leq 0$
Analogy: Ball rolling down valley pinned by fence
Note: Balance of forces (∇f, ∇g_1)

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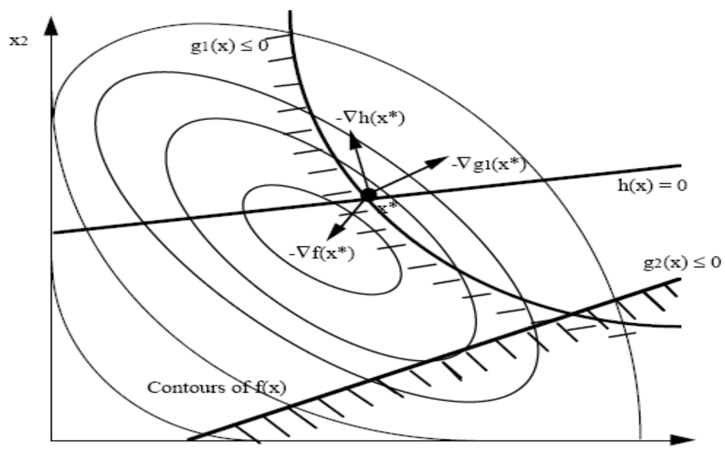
Optimal solution for general constrained problem



Problem: Min $f(x)$
s.t. $g(x) \leq 0$
$h(x) = 0$
Analogy: Ball rolling on rail pinned by fences
Balance of forces: ∇f, ∇g_1, ∇h

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Optimality conditions for local optimum

<u>Necessary First Order Karush Kuhn - Tucker Conditions</u>

$\nabla L(x^*, u, v) = \nabla f(x^*) + \nabla g(x^*)\, u + \nabla h(x^*)\, v = 0$
(Balance of Forces)
$u \geq 0$ (Inequalities act in only one direction)
$g(x^*) \leq 0,\ h(x^*) = 0$ (Feasibility)
$u_j\, g_j(x^*) = 0$ (Complementarity: either $g_j(x^*) = 0$ or $u_j = 0$)
u, v are "weights" for "forces," known as KKT multipliers, shadow prices, dual variables

"To guarantee that a local NLP solution satisfies KKT conditions, a constraint qualification is required. E.g., the *Linear Independence Constraint Qualification* (LICQ) requires active constraint gradients, $[\nabla g_A(x^*)\ \ \nabla h(x^*)]$, to be linearly independent. Also, under LICQ, KKT multipliers are uniquely determined."

<u>Necessary (Sufficient) Second Order Conditions</u>
- Positive curvature in "constraint" directions.
- $p^T \nabla^2 L(x^*)\, p \geq 0$ $(p^T \nabla^2 L(x^*)\, p > 0)$
  where p are the constrained directions: $\nabla h(x^*)^T p = 0$
  for $g_i(x^*)=0$, $\nabla g_i(x^*)^T p = 0$, for $u_i > 0$, $\nabla g_i(x^*)^T p \leq 0$, for $u_i = 0$

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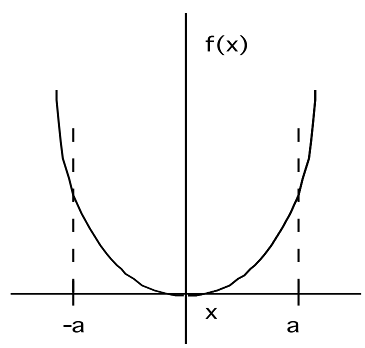
Single Variable Example of KKT Conditions

Min $(x)^2$ s.t. $-a \leq x \leq a,\ a > 0$
$x^* = 0$ is seen by inspection

<u>Lagrange function :</u>
$L(x, u) = x^2 + u_1(x-a) + u_2(-a-x)$

<u>First Order KKT conditions:</u>
$\nabla L(x, u) = 2x + u_1 - u_2 = 0$
$u_1\,(x-a) = 0$
$u_2\,(-a-x) = 0$
$-a \leq x \leq a$ $\qquad u_1, u_2 \geq 0$



<u>Consider three cases:</u>
- $u_1 \geq 0,\ u_2 = 0$ — Upper bound is active, $x = a$, $u_1 = -2a$, $u_2 = 0$
- $u_1 = 0,\ u_2 \geq 0$ — Lower bound is active, $x = -a$, $u_2 = -2a$, $u_1 = 0$
- $u_1 = u_2 = 0$ — Neither bound is active, $u_1 = 0$, $u_2 = 0$, $x = 0$

<u>Second order conditions</u> $(x^*, u_1, u_2 = 0)$
$$\nabla_{xx} L(x^*, u^*) = 2$$
$$p^T \nabla_{xx} L(x^*, u^*)\, p = 2\,(\Delta x)^2 > 0$$

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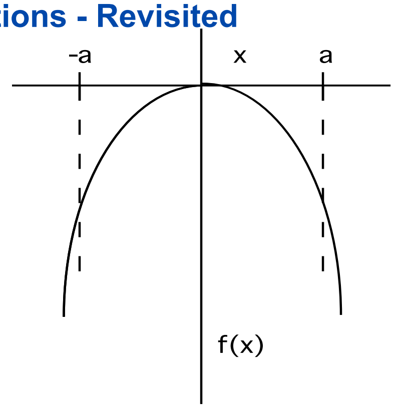
Single Variable Example of KKT Conditions - Revisited

Min $-(x)^2$ s.t. $-a \le x \le a,\ a > 0$
$x^* = \pm a$ is seen by inspection



Lagrange function :
$L(x, u) = -x^2 + u_1(x-a) + u_2(-a-x)$

First Order KKT conditions:
$\nabla L(x, u) = -2x + u_1 - u_2 = 0$
$u_1 (x-a) = 0$
$u_2 (-a-x) = 0$
$-a \le x \le a \qquad u_1, u_2 \ge 0$

Consider three cases:

- $u_1 \ge 0,\ u_2 = 0$ — Upper bound is active, $x = a,\ u_1 = 2a,\ u_2 = 0$
- $u_1 = 0,\ u_2 \ge 0$ — Lower bound is active, $x = -a,\ u_2 = 2a,\ u_1 = 0$
- $u_1 = u_2 = 0$ — Neither bound is active, $u_1 = 0,\ u_2 = 0,\ x = 0$

Second order conditions $(x^*, u_1, u_2 = 0)$

$$\nabla_{xx} L(x^*, u^*) = -2$$
$$p^T \nabla_{xx} L(x^*, u^*)\, p = -2(\Delta x)^2 < 0$$

Interpretation of Second Order Conditions

For $x = a$ or $x = -a$, we require the allowable direction to satisfy the active constraints exactly. Here, any point along the allowable direction, x^* must remain at its bound.

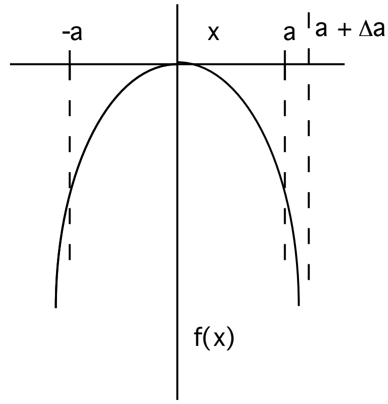
For this problem, however, there are no nonzero allowable directions that satisfy this condition. Consequently the solution x* is defined entirely by the active constraint. The condition:

$$p^T \nabla_{xx} L(x^*, u^*, v^*)\, p > 0$$

for the allowable directions, is *vacuously* satisfied - because there are *no* allowable directions that satisfy $\nabla g_A(x^*)^T p = 0$. Hence, *sufficient* second order conditions are satisfied.

As we will see, sufficient second order conditions are satisfied by linear programs as well.

Role of KKT Multipliers



Also known as:

- Shadow Prices
- Dual Variables
- Lagrange Multipliers

Suppose a in the constraint is increased to $a + \Delta a$

$$f(x^*) = -(a + \Delta a)^2$$

and

$$[f(x^*, a + \Delta a) - f(x^*, a)]/\Delta a = -2a - \Delta a$$

$$df(x^*)/da = -2a = -u_1$$

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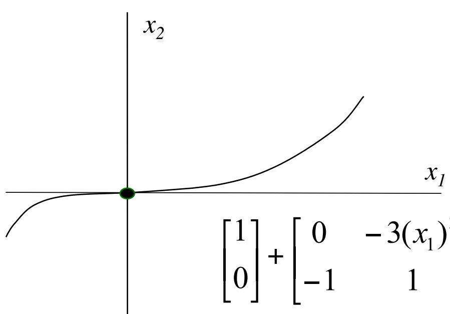
Another Example: Constraint Qualifications



$$\begin{aligned} &Min \;\; x_1 \\ &s.t. \;\; x_2 \geq 0 \\ &\qquad x_2 \leq (x_1)^3 \\ &\qquad x_1^* = x_2^* = 0 \end{aligned}$$

$$\begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & -3(x_1)^2 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \neq 0$$

$$-x_2 \leq 0, u_1 \geq 0, u_1 x_2 = 0$$

$$x_2 - (x_1)^3 \leq 0, u_2 \geq 0, u_2(x_2 - (x_1)^3) = 0$$

KKT conditions not satisfied at NLP solution

Because no CQ is satisfied (e.g., LICQ)

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Algorithms for Constrained Problems

Motivation: Build on unconstrained methods wherever possible.

Classification of Methods:

- Reduced Gradient Methods - (with Restoration) GRG2, CONOPT
- Reduced Gradient Methods - (without Restoration) MINOS
- Successive Quadratic Programming - generic implementations
- Penalty Functions - popular in 1970s, but fell into disfavor. Barrier Methods have been developed recently and are again popular.
- Successive Linear Programming - only useful for "mostly linear" problems

We will concentrate on algorithms for first four classes.

Evaluation: Compare performance on "typical problem," cite experience on process problems.

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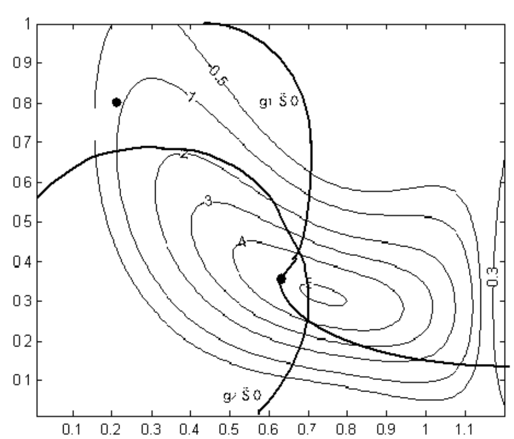
Representative Constrained Problem

(Hughes, 1981)



$$\text{Min } f(x_1, x_2) = \alpha \exp(-\beta)$$
$$g_1 = (x_2+0.1)^2[x_1^2+2(1-x_2)(1-2x_2)] - 0.16 \le 0$$
$$g_2 = (x_1 - 0.3)^2 + (x_2 - 0.3)^2 - 0.16 \le 0$$
$$x^* = [0.6335, 0.3465] \qquad f(x^*) = -4.8380$$

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Reduced Gradient Method with Restoration
(GRG2/CONOPT)

Min $f(x)$
s.t. $g(x) + s = 0$ *(add slack variable)*
$h(x) = 0$
$a \le x \le b,\ s \ge 0$

$\Rightarrow$

Min $f(z)$
s.t. $c(z) = 0$
$a \le z \le b$

Partition variables into:

- z_B - dependent or basic variables
- z_N - nonbasic variables, fixed at a bound
- z_S - independent or superbasic variables

Modified KKT Conditions

$$\nabla f(z) + \nabla c(z)\lambda - \nu_L + \nu_U = 0$$
$$c(z) = 0$$
$$z^{(i)} = z_U^{(i)} \quad or \quad z^{(i)} = z_L^{(i)}, \quad i \in N$$
$$\nu_U^{(i)},\ \nu_L^{(i)} = 0, \quad i \notin N$$

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Reduced Gradient Method with Restoration
(GRG2/CONOPT)

$$a)\quad \nabla_S f(z) + \nabla_S c(z)\lambda = 0$$
$$b)\quad \nabla_B f(z) + \nabla_B c(z)\lambda = 0$$
$$c)\quad \nabla_N f(z) + \nabla_N c(z)\lambda - \nu_L + \nu_U = 0$$
$$d)\quad z^{(i)} = z_U^{(i)} \quad or \quad z^{(i)} = z_L^{(i)}, \quad i \in N$$
$$e)\quad c(z) = 0 \Rightarrow z_B = z_B(z_S)$$

- Solve bound constrained problem in space of superbasic variables
  (apply gradient projection algorithm)
- Solve (e) to eliminate z_B
- Use (a) and (b) to calculate *reduced gradient* wrt z_S.
- Nonbasic variables z_N (temporarily) fixed (d)
- Repartition based on signs of ν, if z_s remain at bounds or if z_B violate bounds

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Definition of Reduced Gradient

$$\frac{df}{dz_S} = \frac{\partial f}{\partial z_S} + \frac{dz_B}{dz_S}\frac{\partial f}{\partial z_B}$$

Because $c(z) = 0$, we have :

$$dc = \left[\frac{\partial c}{\partial z_S}\right]^T dz_S + \left[\frac{\partial c}{\partial z_B}\right]^T dz_B = 0$$

$$\frac{dz_B}{dz_S} = -\left[\frac{\partial c}{\partial z_S}\right]\left[\frac{\partial c}{\partial z_B}\right]^{-1} = -\nabla_{z_S} c\left[\nabla_{z_B} c\right]^{-1}$$

This leads to :

$$\frac{df}{dz_S} = \nabla_S f(z) - \nabla_S c\left[\nabla_B c\right]^{-1}\nabla_B f(z) = \nabla_S f(z) + \nabla_S c(z)\lambda$$

- By remaining feasible always, $c(z) = 0$, $a \le z \le b$, one can apply an unconstrained algorithm (quasi-Newton) using (df/dz_S), using (b)

- Solve problem in reduced space of z_S variables, using (e).

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Example of Reduced Gradient

$$Min \quad x_1^2 - 2x_2$$

$$s.t. \quad 3x_1 + 4x_2 = 24$$

$$\nabla c^T = [3 \;\; 4], \;\; \nabla f^T = [2x_1 \;\; -2]$$

$$\text{Let } z_S = x_1, \; z_B = x_2$$

$$\frac{df}{dz_S} = \frac{\partial f}{\partial z_S} - \nabla_{z_S} c\left[\nabla_{z_B} c\right]^{-1}\frac{\partial f}{\partial z_B}$$

$$\frac{df}{dx_1} = 2x_1 - 3\left[4\right]^{-1}\left(-2\right) = 2x_1 + 3/2$$

If ∇c^T is (m x n); $\nabla z_S c^T$ is m x (n-m); $\nabla z_B c^T$ is (m x m)

(df/dz_S) is the change in f along constraint direction per unit change in z_S

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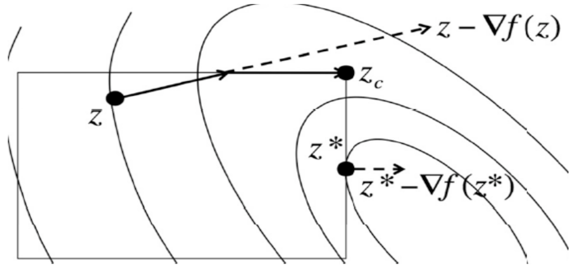
Gradient Projection Method
(superbasic → nonbasic variable partition)



Define the projection of an arbitrary point x onto box feasible region. ith component is given by:

$$\mathcal{P}(z) = \begin{cases} z_{(i)} & \text{if } z_{L,(i)} < z_{(i)} < z_{U,(i)}, \\ z_{L,(i)} & \text{if } z_{(i)} \le z_{L,(i)}, \\ z_{U,(i)} & \text{if } z_{U,(i)} \le z_{(i)}. \end{cases}$$

Piecewise linear path $z(\alpha)$ starting at the reference point z and obtained by projecting steepest descent (or any search) direction at z onto the box region given by:

$$z(\alpha) = \mathcal{P}(z - \alpha \nabla f(z))$$

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Sketch of GRG Algorithm

1. Initialize problem and obtain a feasible point at z^0
2. At feasible point z^k, partition variables z into z_N, z_B, z_S
3. Calculate reduced gradient, (df/dz_S)
4. Evaluate gradient projection search direction for z_S, with quasi-Newton extension
5. Perform a line search.
   - Find $\alpha \in (0,1]$ with $z_S(\alpha)$
   - Solve for $c(z_S(\alpha), z_B, z_N) = 0$
   - If $f(z_S(\alpha), z_B, z_N) < f(z_S^k, z_B, z_N)$, set $z_S^{k+1} = z_S(\alpha)$, $k := k+1$
6. If $\|(df/dz_S)\| < \varepsilon$, Stop. Else, go to 2.

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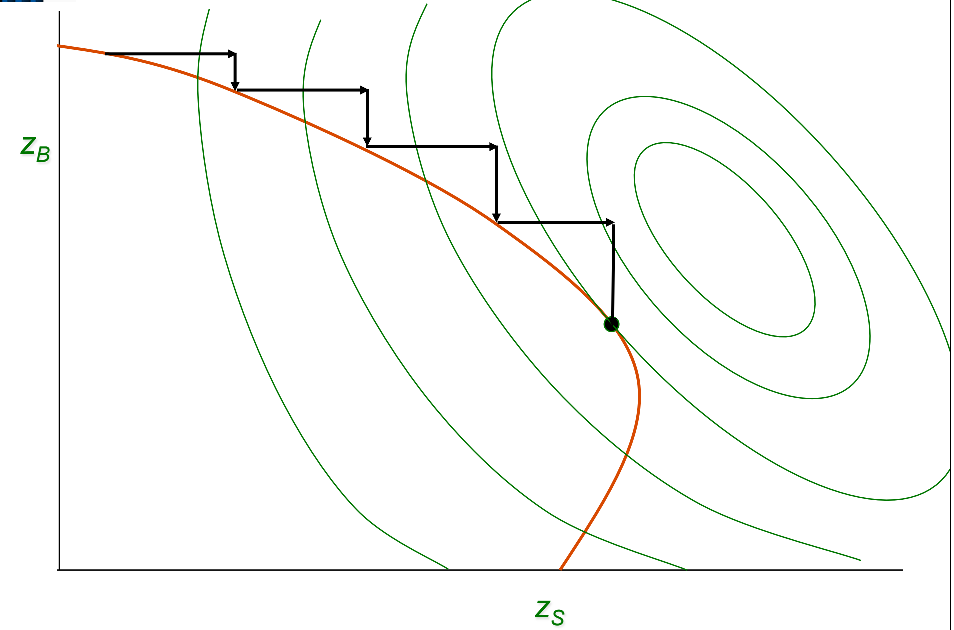
Reduced Gradient Method with Restoration



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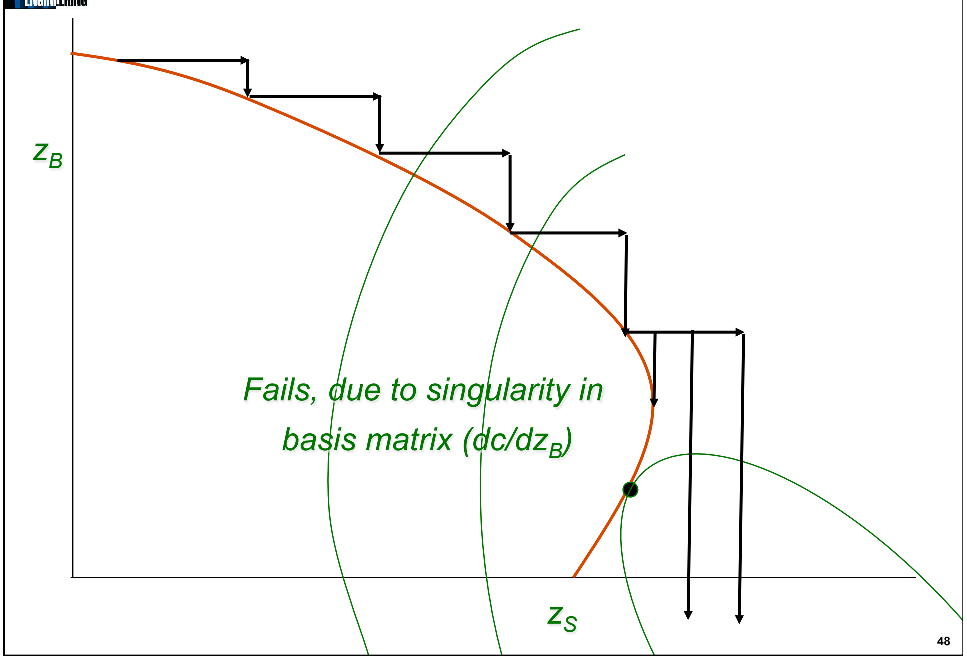
Reduced Gradient Method with Restoration



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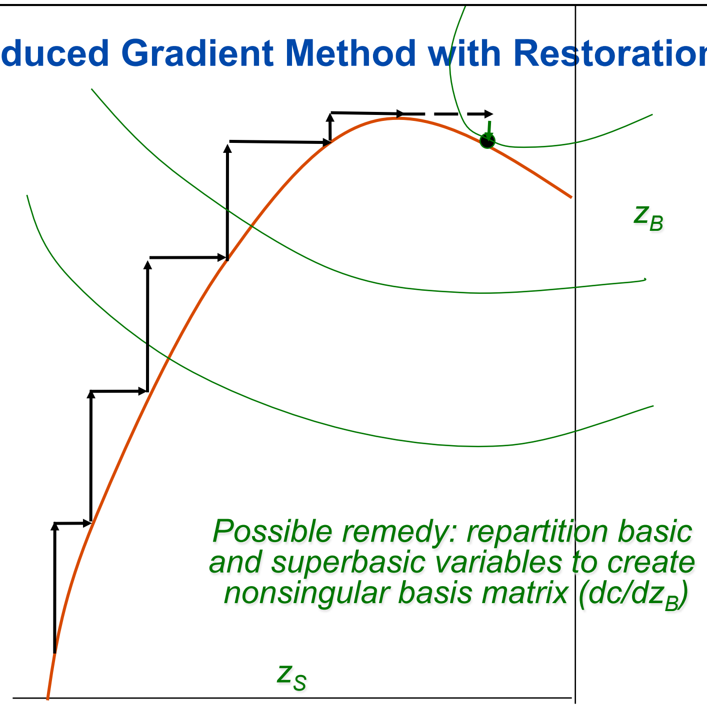
Reduced Gradient Method with Restoration



Possible remedy: repartition basic and superbasic variables to create nonsingular basis matrix (dc/dz_B)

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GRG Algorithm Properties

1. GRG2 has been implemented on PC's as GINO and is very reliable and robust. It is also the optimization solver in MS EXCEL.
2. CONOPT is implemented in GAMS, AIMMS and AMPL
3. GRG2 uses Q-N for small problems but can switch to conjugate gradients if problem gets large. CONOPT uses exact second derivatives.
4. Convergence of $c(z_S, z_B, z_N) = 0$ can get <u>very</u> expensive because $\nabla c(z)$ is calculated repeatedly.
5. Safeguards can be added so that restoration (step 5.) can be dropped and efficiency increases.

<u>Representative Constrained Problem</u> Starting Point [0.8, 0.2]

- GINO Results - 14 iterations to $||\nabla f(x^*)|| \leq 10^{-6}$
- CONOPT Results - 7 iterations to $||\nabla f(x^*)|| \leq 10^{-6}$ from feasible point.

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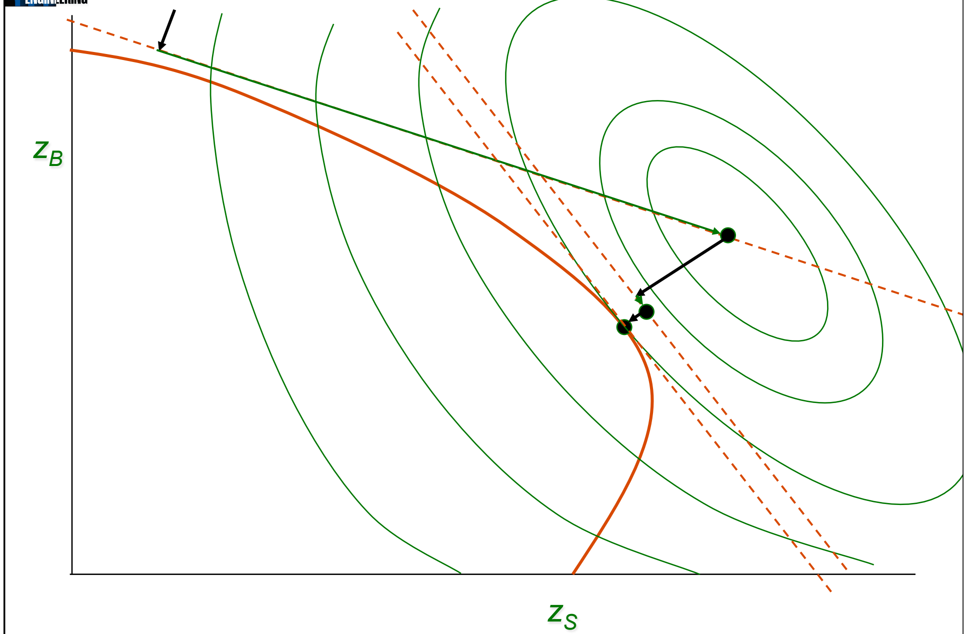
Reduced Gradient Method without Restoration



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Reduced Gradient Method without Restoration (MINOS/Augmented)

Motivation: Efficient algorithms are available that solve linearly constrained optimization problems (MINOS):

$$\begin{aligned} &Min \quad f(x) \\ &s.t.\ Ax \leq b \\ &\quad Cx = d \end{aligned}$$

Extend to nonlinear problems, through successive linearization

Develop major iterations (linearizations) and minor iterations (GRG solutions) .

Strategy: (Robinson, Murtagh & Saunders)

1. Partition variables into basic, nonbasic variables and superbasic variables..
2. Linearize active constraints at z^k
   $$D^k z = r^k$$
3. Let $\psi = f(z) + \lambda^T c(z) + \beta\, (c(z)^T c(z))$ (Augmented Lagrange),
4. Solve linearly constrained problem:
   $$\begin{aligned} &Min && \psi(z) \\ &s.t. && Dz = r \\ & && a \leq z \leq b \end{aligned}$$
   using reduced gradients to get z^{k+1}
5. Set $k=k+1$, go to 2.
6. Algorithm terminates when no movement between steps 2) and 4).

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MINOS/Augmented Notes

1. MINOS has been implemented very efficiently to take care of linearity. It becomes LP Simplex method if problem is totally linear. Also, very efficient matrix routines.
2. No restoration takes place, nonlinear constraints are reflected in $\psi(z)$ during step 3). MINOS is more efficient than GRG.
3. Major iterations (steps 3) - 4)) converge at a quadratic rate.
4. Reduced gradient methods are complicated, monolithic codes: hard to integrate efficiently into modeling software.

Representative Constrained Problem – Starting Point [0.8, 0.2]
MINOS Results: 4 major iterations, 11 function calls
to $\|\nabla f(x^*)\| \leq 10^{-6}$

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Successive Quadratic Programming (SQP)

Motivation:

- Take KKT conditions, expand in Taylor series about current point.
- Take Newton step (QP) to determine next point.

Derivation – KKT Conditions

$$\nabla_x L\,(x^*, u^*, v^*) = \nabla f(x^*) + \nabla g_A(x^*)\, u^* + \nabla h(x^*)\, v^* = 0$$

$$h(x^*) = 0$$

$$g_A(x^*) = 0,$$ where g_A are the active constraints.

Newton - Step

$$\begin{bmatrix} \nabla_{xx} L & \nabla g_A & \nabla h \\ \nabla g_A^T & 0 & 0 \\ \nabla h^T & 0 & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta u \\ \Delta v \end{bmatrix} = - \begin{bmatrix} \nabla_x L\left(x^k, u^k, v^k\right) \\ g_A\left(x^k\right) \\ h\left(x^k\right) \end{bmatrix}$$

Requirements:

- $\nabla_{xx} L$ must be calculated and should be 'regular'
- correct active set g_A
- good estimates of u^k, v^k

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SQP Chronology

1. *Wilson (1963)*
 - active set can be determined by solving QP:

$$\min_{d} \quad \nabla f(x_k)^T d + 1/2\, d^T\, \nabla_{xx} L(x_k, u_k, v_k)\, d$$
$$s.t. \quad g(x_k) + \nabla g(x_k)^T d \le 0$$
$$h(x_k) + \nabla h(x_k)^T d = 0$$

2. *Han (1976), (1977), Powell (1977), (1978)*
 - approximate $\nabla_{xx}L$ using a positive definite quasi-Newton update (BFGS)
 - use a line search to converge from poor starting points.

<u>Notes</u>:
 - Similar methods were derived using penalty (not Lagrange) functions.
 - Method converges quickly; very few function evaluations.
 - Not well suited to large problems (full space update used).
 For n > 100, say, use reduced space methods (e.g. MINOS).

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Elements of SQP – Hessian Approximation

What about $\nabla_{xx}L$?

- need to get second derivatives for $f(x)$, $g(x)$, $h(x)$.
- need to estimate multipliers, u^k, v^k; $\nabla_{xx}L$ may not be positive semidefinite

$\Rightarrow$Approximate $\nabla_{xx}L\,(x^k, u^k, v^k)$ by B^k, a symmetric positive definite matrix.

$$B^{k+1} = B^k + \frac{yy^T}{s^T y} - \frac{B^k s\, s^T B^k}{s\, B^k s}$$

<u>BFGS Formula</u> $\quad s = x^{k+1} - x^k$

$$y = \nabla L(x^{k+1}, u^{k+1}, v^{k+1}) - \nabla L(x^k, u^{k+1}, v^{k+1})$$

- second derivatives approximated by change in gradients
- positive definite B^k ensures *unique* QP solution

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Elements of SQP – Search Directions

How do we obtain search directions?

- Form QP and let QP determine constraint activity
- At each iteration, k, solve:

$$\min_{d} \quad \nabla f(x^k)^T d + 1/2\, d^T B^k d$$
$$s.t. \quad g(x^k) + \nabla g(x^k)^T d \le 0$$
$$h(x^k) + \nabla h(x^k)^T d = 0$$

Convergence from poor starting points

- As with Newton's method, choose α (stepsize) to ensure progress toward optimum: $x^{k+1} = x^k + \alpha\, d$.
- α is chosen by making sure a *merit function* is decreased at each iteration.

Exact Penalty Function

$$\psi(x) = f(x) + \mu\, [\Sigma \max(0, g_j(x)) + \Sigma\, |h_j(x)|]$$
$$\mu > \max_j \{|u_j|, |v_j|\}$$

Augmented Lagrange Function

$$\psi(x) = f(x) + u^T g(x) + v^T h(x) + \eta/2\, \{\Sigma (h_j(x))^2 + \Sigma \max(0, g_j(x))^2\}$$

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Newton-Like Properties for SQP

Fast Local Convergence	
$B = \nabla_{xx}L$	Quadratic
$\nabla_{xx}L$ is p.d and B is Q-N	1 step Superlinear
B is Q-N update, $\nabla_{xx}L$ not p.d	2 step Superlinear

Enforce Global Convergence

Ensure decrease of merit function by taking $\alpha \le 1$

Trust region adaptations provide a stronger guarantee of global convergence - but harder to implement.

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Basic SQP Algorithm

0. Guess x^0, Set $B^0 = I$ (Identity). Evaluate $f(x^0)$, $g(x^0)$ and $h(x^0)$.
1. At x^k, evaluate $\nabla f(x^k)$, $\nabla g(x^k)$, $\nabla h(x^k)$.
2. If k > 0, update B^k using the BFGS Formula.
3. Solve: $Min_d \ \nabla f(x^k)^T d + 1/2\, d^T B^k d$

   s.t. $g(x^k) + \nabla g(x^k)^T d \le 0$

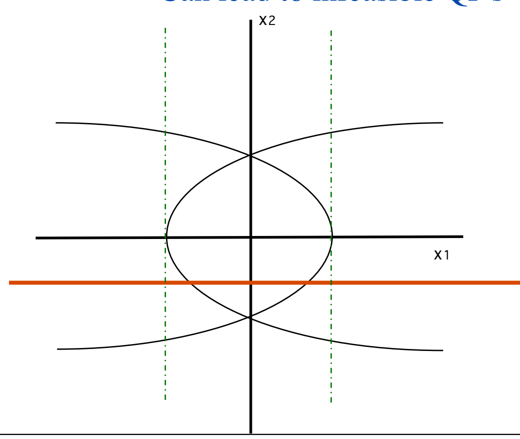
   $h(x^k) + \nabla h(x^k)^T d = 0$

   If KKT error less than tolerance: $\|\nabla L(x^*)\| \le \varepsilon$, $\|h(x^*)\| \le \varepsilon$, $\|g(x^*)_+\| \le \varepsilon$. STOP, else go to 4.
4. Find α so that $0 < \alpha \le 1$ and $\psi(x^k + \alpha d) < \psi(x^k)$ sufficiently

   (Each trial requires evaluation of $f(x)$, $g(x)$ and $h(x)$).
5. $x^{k+1} = x^k + \alpha\, d$. Set k = k + 1 Go to 2.

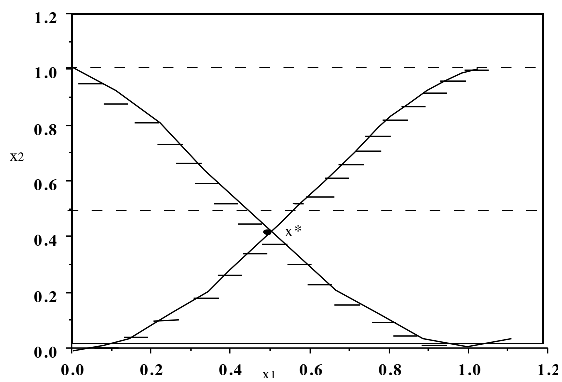
Problems with SQP

Nonsmooth Functions - Reformulate
Ill-conditioning - Proper scaling
Poor Starting Points – Trust Regions can help
Inconsistent Constraint Linearizations
- Can lead to infeasible QP's



$$
\begin{aligned}
&Min \ x_2 \\
&s.t. \ \ 1 + x_1 - (x_2)^2 \le 0 \\
&\quad\ \ 1 - x_1 - (x_2)^2 \le 0 \\
&\quad\ \ x_2 \ge -1/2
\end{aligned}
$$

SQP Test Problem



Min x_2

s.t. $-x_2 + 2\,x_1^2 - x_1^3 \le 0$

$-x_2 + 2\,(1-x_1)^2 - (1-x_1)^3 \le 0$

$x^* = [0.5, 0.375]$.

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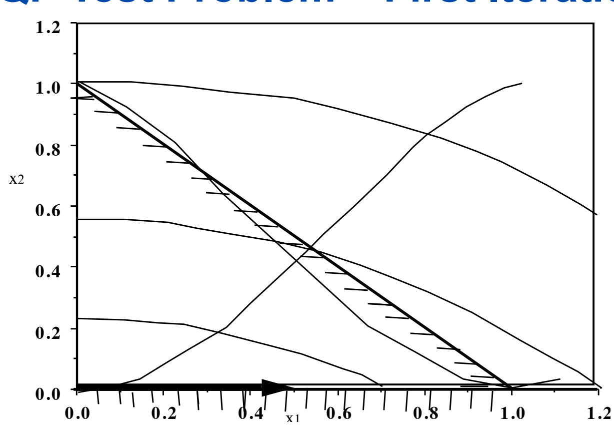
SQP Test Problem – First Iteration



Start from the origin ($x_0 = [0, 0]^T$) with $B^0 = I$, form:

Min $d_2 + 1/2\,(d_1^2 + d_2^2)$

s.t. $d_2 \ge 0$

$d_1 + d_2 \ge 1$

$d = [1, 0]^T$. with $\mu_1 = 0$ and $\mu_2 = 1$.

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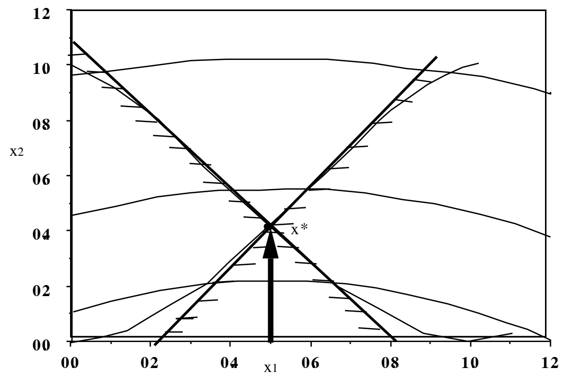
SQP Test Problem – Second Iteration



From $x_1 = [0.5, 0]^T$ with $B^1 = I$
(no update from BFGS possible), form:

$$
\begin{aligned}
&Min \quad d_2 + 1/2\,(d_1^2 + d_2^2)\\
&s.t. \quad -1.25\, d_1 - d_2 + 0.375 \le 0\\
&\qquad\;\; 1.25\, d_1 - d_2 + 0.375 \le 0
\end{aligned}
$$

$d = [0, 0.375]^T$ with $\mu_1 = 0.5$ and $\mu_2 = 0.5$

$x^* = [0.5, 0.375]^T$ is optimal

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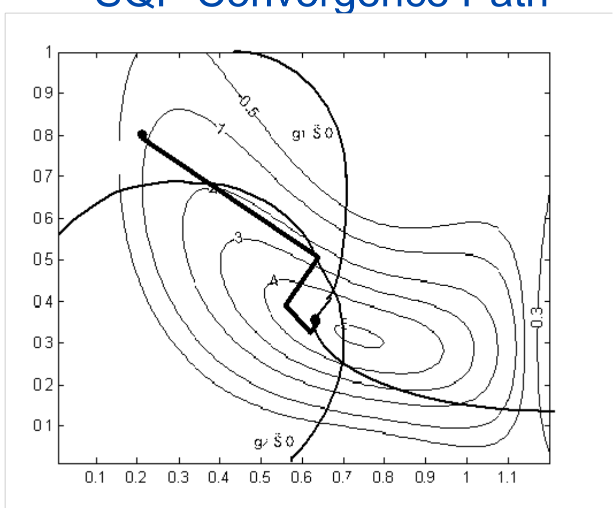
Representative Constrained Problem SQP Convergence Path



Starting Point [0.8, 0.2] - starting from $B^0 = I$ and staying in bounds and linearized constraints; converges in 8 iterations to $||\nabla f(x^*)|| \le 10^{-6}$

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Barrier Methods for Large-Scale Nonlinear Programming

Original Formulation

$$\min_{x \in \Re^n} f(x)$$
$$\text{s.t} \quad c(x) = 0$$
$$x \geq 0$$

Can generalize for $a \leq x \leq b$

Barrier Approach

$$\min_{x \in \Re^n} \varphi_\mu(x) = f(x) - \mu \sum_{i=1}^{n} \ln x_i$$
$$\text{s.t} \quad c(x) = 0$$

⇒As μ ➔ 0, $x^*(\mu)$ ➔ x^* Fiacco and McCormick (1968)

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Solution of the Barrier Problem

⇒**Newton Directions (KKT System)**

$$\begin{aligned} \nabla f(x) + A(x)\lambda - v &= 0 \\ Xv - \mu e &= 0 \\ c(x) &= 0 \end{aligned}$$

$e^T = [1, 1, 1 \ldots], \; X = diag(x)$

$A = \nabla c(x), \; W = \nabla_{xx} L(x, \lambda, \nu)$

⇒ **Reducing the System**

$$d_v = \mu X^{-1} e - v - X^{-1} V d_x$$

$$\begin{bmatrix} W + \Sigma & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d_x \\ \lambda^+ \end{bmatrix} = - \begin{bmatrix} \nabla \varphi_\mu \\ c \end{bmatrix} \qquad \Sigma = X^{-1} V$$

IPOPT Code – www.coin-or.org

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Global Convergence of Newton-based Barrier Solvers

Merit Function

Exact Penalty: $P(x, \eta) = f(x) + \eta \, ||c(x)||$

Aug'd Lagrangian: $L^*(x, \lambda, \eta) = f(x) + \lambda^T c(x) + \eta \, ||c(x)||^2$

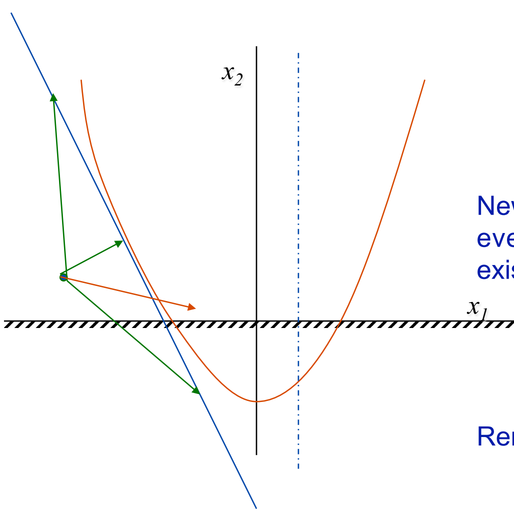
Assess Search Direction (e.g., from IPOPT)

Line Search – choose *stepsize* α to give sufficient decrease of merit function using a 'step to the boundary' rule with τ ~0.99.

$$\text{for } \alpha \in (0, \bar{\alpha}],\ x_{k+1} = x_k + \alpha \, d_x$$
$$x_k + \bar{\alpha} \, d_x \geq (1-\tau) x_k > 0$$
$$v_{k+1} = v_k + \bar{\alpha} \, d_v \geq (1-\tau) v_k > 0$$
$$\lambda_{k+1} = \lambda_k + \alpha \, (\lambda_+ - \lambda_k)$$

- How do we balance $\phi(x)$ and $c(x)$ with η?
- Is this approach globally convergent? Will it still be fast?

Global Convergence Failure
(Wächter and B., 2000)



$$Min \ f(x)$$
$$s.t. \ x_1 - x_3 - \frac{1}{2} = 0$$
$$(x_1)^2 - x_2 - 1 = 0$$
$$x_2, x_3 \geq 0$$

Newton-type line search 'stalls' even though descent directions exist

$$A(x^k)^T d_x + c(x^k) = 0$$
$$x^k + \alpha \, d_x > 0$$

Remedies:

- •Composite Step Trust Region (Byrd et al.)
- •Filter Line Search Methods

Line Search Filter Method

Store (ϕ_k, θ_k) at allowed iterates

Allow progress if trial point is acceptable to filter with θ margin

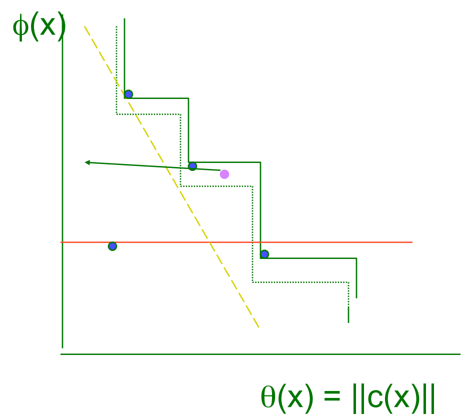
If switching condition

$$\alpha[-\nabla\phi_k^T d]^a \geq \delta[\theta_k]^b, a > 2b > 2$$

is satisfied, only an Armijo line search is required on ϕ_k

If insufficient progress on stepsize, evoke restoration phase to reduce θ.

Global convergence and superlinear local convergence proved (with second order correction)



Implementation Details

Modify KKT (full space) matrix if singular

$$\begin{bmatrix} W_k + \Sigma_k + \delta_1 & A_k \\ A_k^T & -\delta_2 I \end{bmatrix}$$

- δ_1 - Correct inertia to guarantee descent direction
- δ_2 - Deal with rank deficient A_k

KKT matrix factored by MA27

Feasibility restoration phase

$$Min \| c(x) \|_1 + \| x - x_k \|_Q^2$$

$$x_l \leq x_k \leq x_u$$

Apply Exact Penalty Formulation

Exploit same structure/algorithm to reduce infeasibility

IPOPT Algorithm – Features

Line Search Strategies for Globalization

- ℓ_2 exact penalty merit function
- augmented Lagrangian merit function
- **Filter method (adapted and extended from Fletcher and Leyffer)**

Hessian Calculation

- BFGS (full/LM and reduced space)
- SR1 (full/LM and reduced space)
- **Exact full Hessian (direct)**
- Exact reduced Hessian (direct)
- Preconditioned CG

Algorithmic Properties

Globally, superlinearly convergent (Wächter and B., 2005)

Easily tailored to different problem structures

Freely Available

CPL License and COIN-OR distribution: **http://www.coin-or.org**

IPOPT 3.1 recently rewritten in C++

Solved on thousands of test problems and applications

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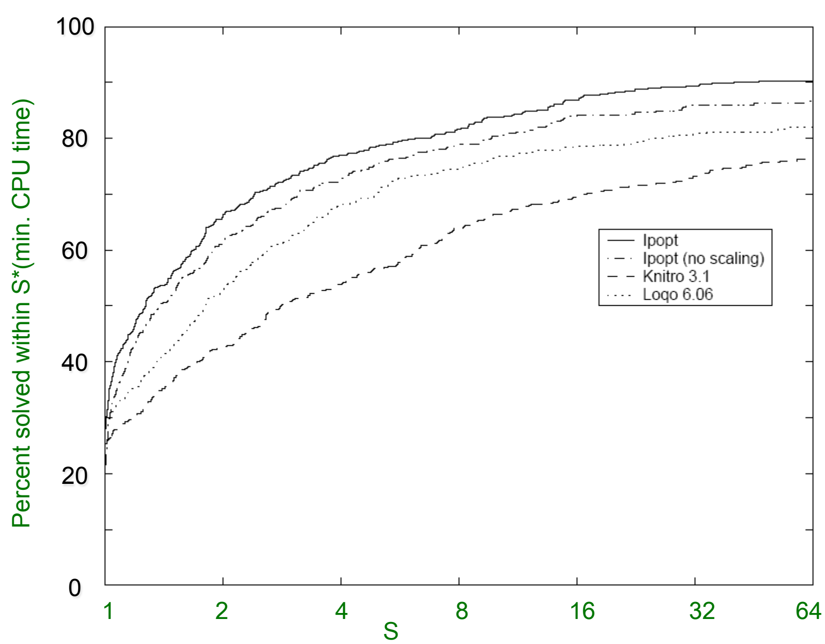
IPOPT Comparison on 954 Test Problems



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Recommendations for Constrained Optimization

1. Best current algorithms
   - GRG 2/CONOPT
   - MINOS
   - SQP
   - IPOPT
2. GRG 2 (or CONOPT) is generally slower, but is robust. Use with highly nonlinear functions. Solver in Excel!
3. For small problems ($n \leq 100$) with nonlinear constraints, use SQP.
4. For large problems ($n \geq 100$) with mostly linear constraints, use MINOS.
   ==> Difficulty with many nonlinearities

Fewer Function Evaluations ⟷ Tailored Linear Algebra

Small, Nonlinear Problems - SQP solves QP's, not LCNLP's, fewer function calls.
Large, Mostly Linear Problems - MINOS performs sparse constraint decomposition. Works efficiently in reduced space if function calls are cheap!
Exploit Both Features – IPOPT takes advantages of few function evaluations and large-scale linear algebra, but requires exact second derivatives

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Available Software for Constrained Optimization

SQP Routines
HSL, NaG and IMSL (NLPQL) Routines
NPSOL – Stanford Systems Optimization Lab
SNOPT – Stanford Systems Optimization Lab (rSQP discussed later)
IPOPT – http://www.coin-or.org

GAMS Programs
CONOPT - Generalized Reduced Gradient method with restoration
MINOS - Generalized Reduced Gradient method without restoration
NPSOL – Stanford Systems Optimization Lab
SNOPT – Stanford Systems Optimization Lab (rSQP discussed later)
IPOPT – barrier NLP, COIN-OR, open source
KNITRO – barrier NLP

MS Excel
Solver uses Generalized Reduced Gradient method with restoration

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Rules for Formulating Nonlinear Programs

1) Avoid overflows and undefined terms, (do not divide, take logs, etc.)
   e.g. $x + y - \ln z = 0 \rightarrow x + y - u = 0$
   $\exp u - z = 0$
2) If constraints must <u>always</u> be enforced, make sure they are linear or bounds.
   e.g. $v(xy - z^2)^{1/2} = 3 \rightarrow vu = 3$
   $u^2 - (xy - z^2) = 0,\ u \geq 0$
3) Exploit linear constraints as much as possible, e.g. mass balance
   $$x_i L + y_i V = F z_i \rightarrow l_i + v_i = f_i$$
   $$L - \sum l_i = 0$$
4) Use bounds and constraints to enforce characteristic solutions.
   e.g. $a \leq x \leq b,\ \ g(x) \leq 0$
   to isolate correct root of $h(x) = 0$.
5) Exploit <u>global</u> properties when possibility exists. Convex (linear equations?) Linear Program? Quadratic Program? Geometric Program?
6) Exploit problem structure when possible.
   e.g. $Min\ \ [Tx - 3Ty]$
   $s.t.\ \ xT + y - T^2 y = 5$
   $4x - 5Ty + Tx = 7$
   $0 \leq T \leq 1$
   (If T is fixed $\Rightarrow$ solve LP) $\Rightarrow$ put T in outer optimization loop.

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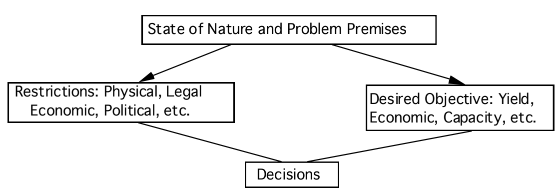
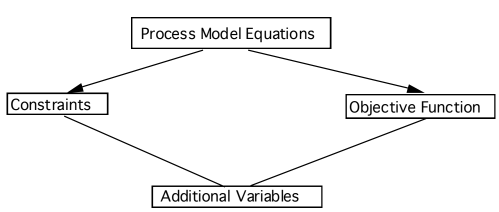
Process Optimization
Problem Definition and Formulation



Mathematical Modeling and Algorithmic Solution



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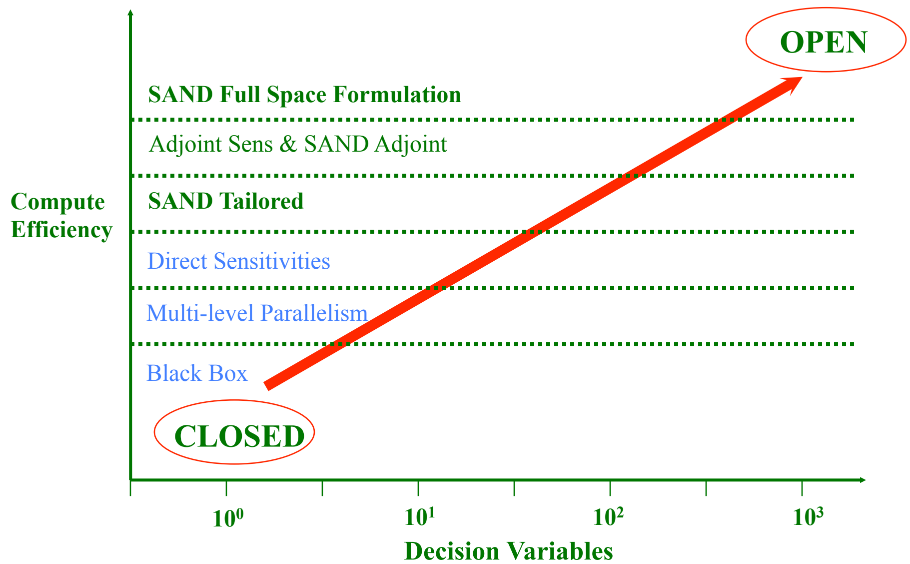
Hierarchy of Nonlinear Programming Formulations and Model Intrusion



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Large Scale NLP Algorithms

Motivation: Improvement of Successive Quadratic Programming as Cornerstone Algorithm

➔ ***process optimization for design, control and operations***

Evolution of NLP Solvers:

SQP ⟶ rSQP ⟶ IPOPT

rSQP ↓ rSQP++

IPOPT ↓ IPOPT 3.x

2000 - : Simultaneous dynamic optimization over 1 000 000 variables and constraints

Current: Tailor structure, architecture and problems

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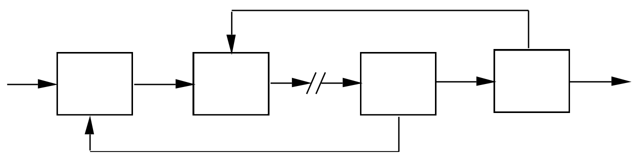
Flowsheet Optimization Problems - Introduction

Modular Simulation Mode

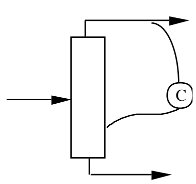
Physical Relation to Process

- Intuitive to Process Engineer
- Unit equations solved internally
- tailor-made procedures.

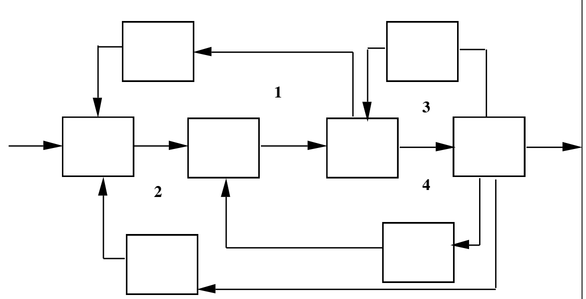


•Convergence Procedures - for simple flowsheets, often identified from flowsheet structure
•Convergence "mimics" startup.
•Debugging flowsheets on "physical" grounds

Flowsheet Optimization Problems - Features



Design Specifications
Specify # trays reflux ratio, but would like to specify overhead comp. ==> Control loop -Solve Iteratively



Nested Recycles Hard to Handle
Best Convergence Procedure?

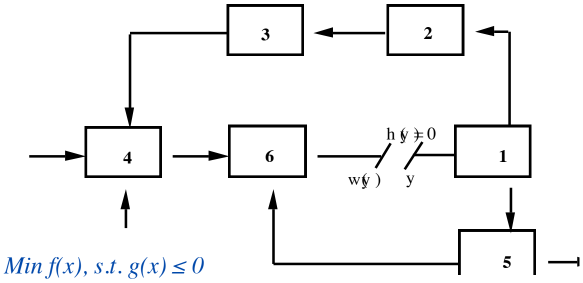
•Frequent block evaluation can be expensive
•Slow algorithms applied to flowsheet loops.
•NLP methods are good at breaking loops

Chronology in Process Optimization

	Sim. Time Equiv.
1. Early Work - Black Box Approaches	
Friedman and Pinder (1972)	75-150
Gaddy and co-workers (1977)	300
2. Transition - more accurate gradients	
Parker and Hughes (1981)	64
Biegler and Hughes (1981)	13
3. Infeasible Path Strategy for Modular Simulators	
Biegler and Hughes (1982)	<10
Chen and Stadtherr (1985)	
Kaijaluoto et al. (1985)	
and many more	
4. Equation Based Process Optimization	
Westerberg et al. (1983)	<5
Shewchuk (1985)	2
DMO, NOVA, RTOPT, etc. (1990s)	1-2

Process optimization should be as cheap and easy as process simulation

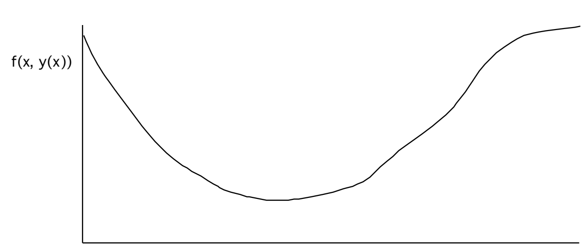
Simulation and Optimization of Flowsheets



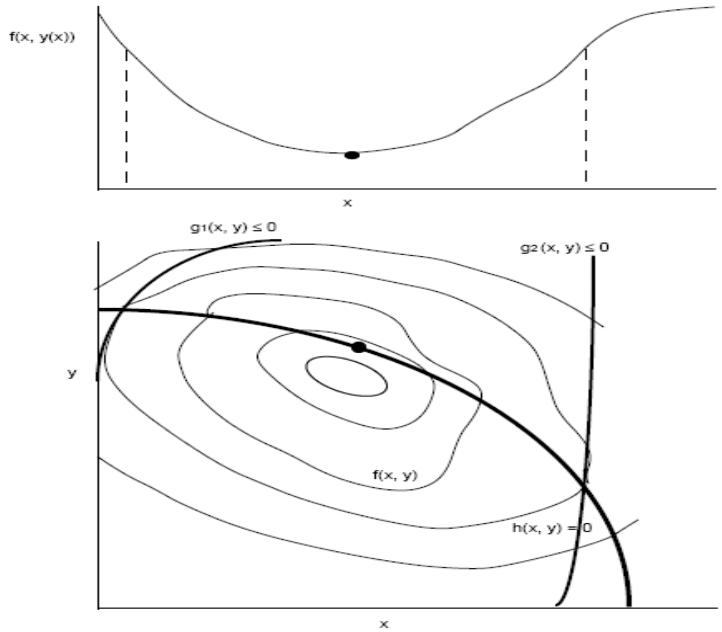
Min f(x), s.t. g(x) $\leq$ *0*

For single degree of freedom:

- work in space defined by curve below.
- requires repeated (expensive) recycle convergence



Expanded Region with Feasible Path



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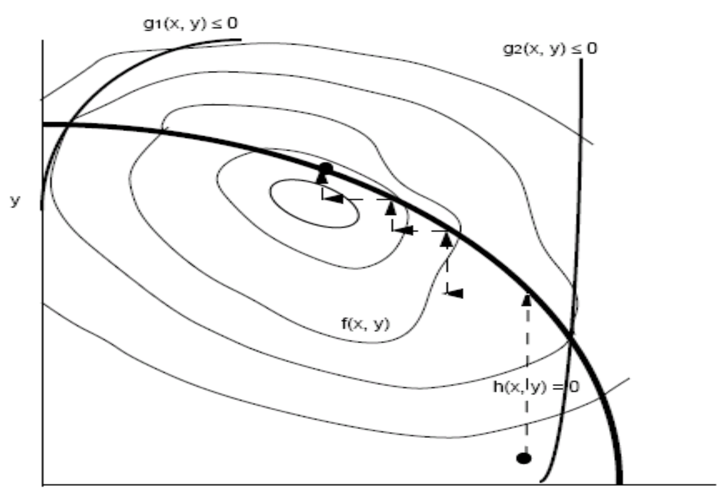

"Black Box" Optimization Approach

- Vertical steps are expensive (flowsheet convergence)
- Generally no connection between x and y.
- Can have "noisy" derivatives for gradient optimization.

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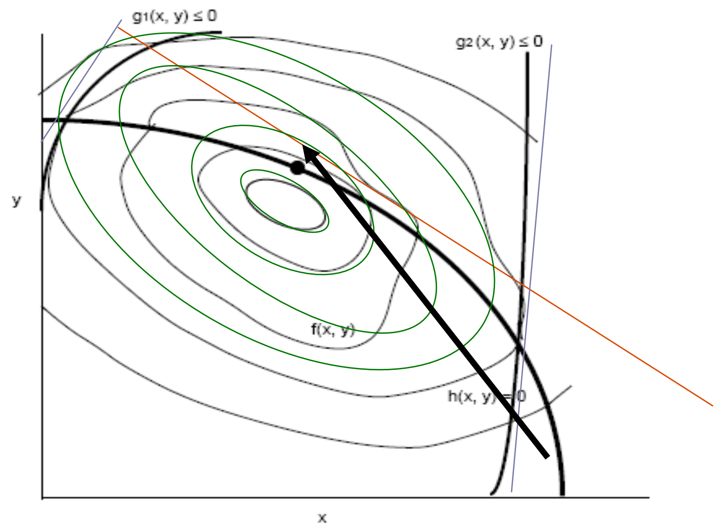

SQP - Infeasible Path Approach
- solve and optimize simultaneously in x and y
- extended Newton method

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Optimization Capability for Modular Simulators
(FLOWTRAN, Aspen/Plus, Pro/II, HySys)

Architecture
- Replace convergence with optimization block
- Problem definition needed (in-line FORTRAN)
- Executive, preprocessor, modules intact.

Examples
1. Single Unit and Acyclic Optimization
   - Distillation columns & sequences

2. "Conventional" Process Optimization
   - Monochlorobenzene process
   - NH3 synthesis

3. Complicated Recycles & Control Loops
   - Cavett problem
   - Variations of above

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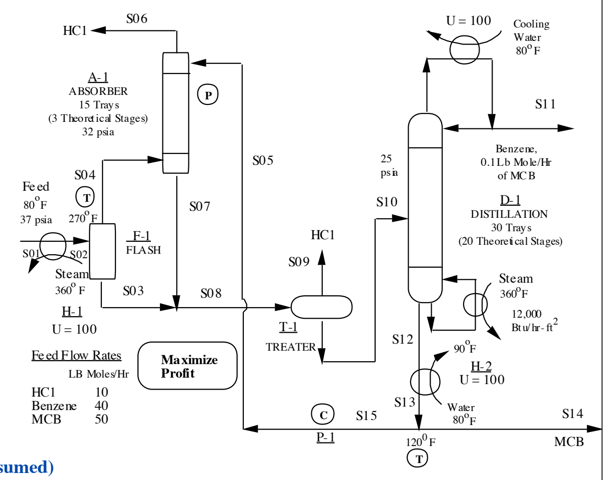
Optimization of Monochlorobenzene Process



PHYSICAL PROPERTY OPTIONS
Cavett Vapor Pressure
Redlich-Kwong Vapor Fugacity
Corrected Liquid Fugacity
Ideal Solution Activity Coefficient
OPT (SCOPT) OPTIMIZER
Optimal Solution Found After 4 Iterations
Kuhn-Tucker Error 0.29616E-05
Allowable Kuhn-Tucker Error 0.19826E-04
Objective Function -0.98259

Optimization Variables
32.006 0.38578 200.00 120.00
Tear Variables
0.10601E-19 13.064 79.229 120.00 50.000
Tear Variable Errors (Calculated Minus Assumed)
-0.10601E-19 0.72209E-06
-0.36563E-04 0.00000E+00 0.00000E+00
-Results of infeasible path optimization
-Simultaneous optimization and convergence of tear streams.

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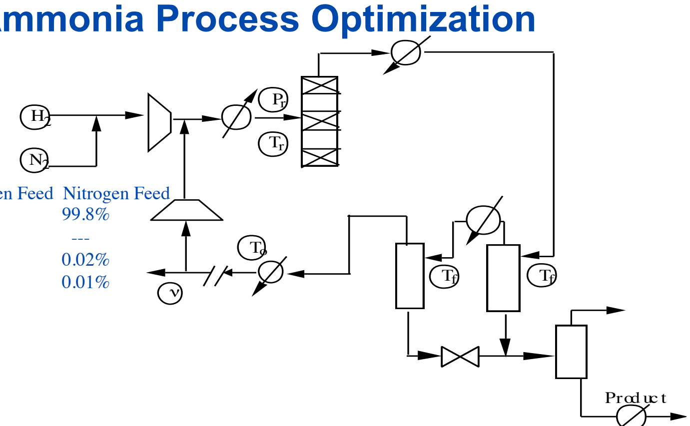
Ammonia Process Optimization



	Hydrogen Feed	Nitrogen Feed
N2	5.2%	99.8%
H2	94.0%	---
CH4	0.79 %	0.02%
Ar	---	0.01%

Hydrogen and Nitrogen feed are mixed, compressed, and combined with a recycle stream and heated to reactor temperature. Reaction occurs in a multibed reactor (modeled here as an equilibrium reactor) to partially convert the stream to ammonia. The reactor effluent is cooled and product is separated using two flash tanks with intercooling. Liquid from the second stage is flashed at low pressure to yield high purity NH_3 product. Vapor from the two stage flash forms the recycle and is recompressed.

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Ammonia Process Optimization

Optimization Problem

Max {Total Profit @ 15% over five years}

s.t.
- 10^5 tons NH3/yr.
- Pressure Balance
- No Liquid in Compressors
- $1.8 \leq$ H2/N2 ≤ 3.5
- Treact $\leq 1000^o$ F
- NH3 purged ≤ 4.5 lb mol/hr
- NH3 Product Purity ≥ 99.9 %
- Tear Equations

Performance Characterstics

- 5 SQP iterations.
- 2.2 base point simulations.
- objective function improves by $20.66 x 10^6 to $24.93 x 10^6.
- difficult to converge flowsheet at starting point

Item	Optimum	Starting point
Objective Function($\$10^6$)	24.9286	20.659
1. Inlet temp. reactor (°F)	400	400
2. Inlet temp. 1st flash (°F)	65	65
3. Inlet temp. 2nd flash (°F)	35	35
4. Inlet temp. rec. comp. (°F)	80.52	107
5. Purge fraction (%)	0.0085	0.01
6. Reactor Press. (psia)	2163.5	2000
7. Feed 1 (lb mol/hr)	2629.7	2632.0
8. Feed 2 (lb mol/hr)	691.78	691.4

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How accurate should gradients be for optimization?

Recognizing True Solution
- KKT conditions and Reduced Gradients determine true solution
- Derivative Errors will lead to wrong solutions!

Performance of Algorithms

Constrained NLP algorithms are gradient based
(SQP, Conopt, GRG2, MINOS, etc.)

Global and Superlinear convergence theory assumes accurate gradients

Worst Case Example (Carter, 1991)

Newton's Method generates an *ascent direction* and fails *for any* ε !

$$Min\ f(x) = x^T Ax$$

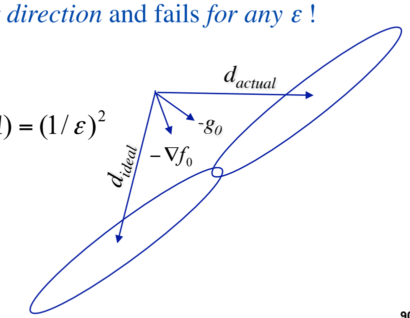
$$A = \begin{bmatrix} \varepsilon + 1/\varepsilon & \varepsilon - 1/\varepsilon \\ \varepsilon - 1/\varepsilon & \varepsilon + 1/\varepsilon \end{bmatrix}$$

$$\kappa(A) = (1/\varepsilon)^2$$

$$x_0 = [1 \quad 1]^T \quad \nabla f(x_0) = \varepsilon\, x_0$$

$$g(x_0) = \nabla f(x_0) + O(\varepsilon)$$

$$d = -A^{-1} g(x_0)$$



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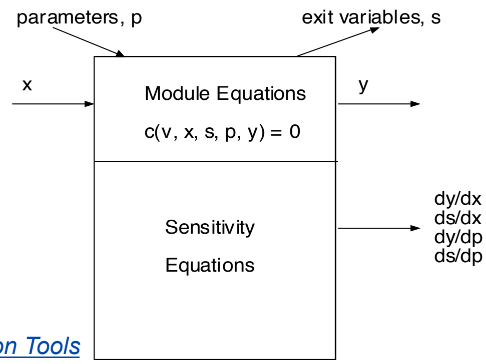
Implementation of Analytic Derivatives



Automatic Differentiation Tools

JAKE-F, limited to a subset of FORTRAN (Hillstrom, 1982)
DAPRE, which has been developed for use with the NAG library (Pryce, Davis, 1987)
ADOL-C, implemented using operator overloading features of C++ (Griewank, 1990)
ADIFOR, (Bischof et al, 1992) uses source transformation approach FORTRAN code .
TAPENADE, web-based source transformation for FORTRAN code

Relative effort needed to calculate gradients is not n+1 but about 3 to 5 (Wolfe, Griewank)

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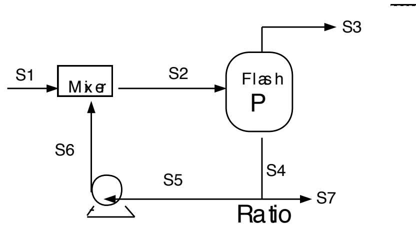
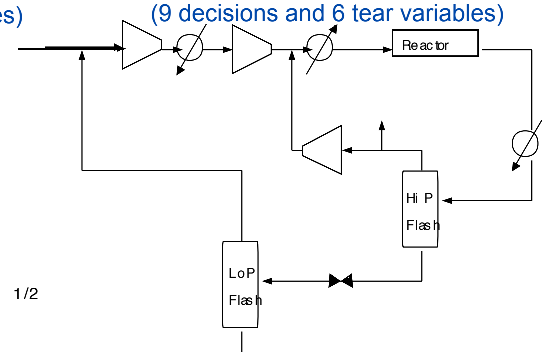
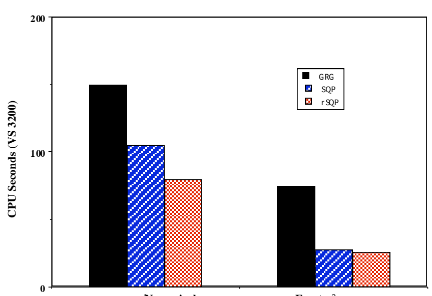
Flash Recycle Optimization
(2 decisions + 7 tear variables)

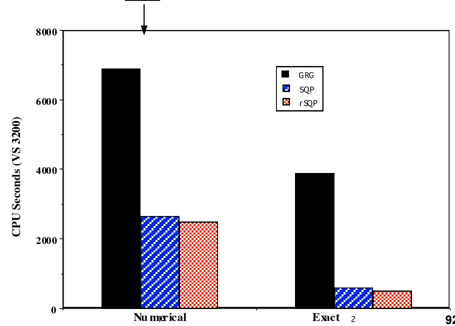


$\text{Max } S3(A)^2 * S3(B) - S3(A)^2 - S3(C) + S3(D)^3 - (S3(E))^{1/2}$

Ammonia Process Optimization
(9 decisions and 6 tear variables)







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Large-Scale SQP

$$\begin{array}{llcll} Min & f(z) & \qquad & Min & \nabla f(z^k)^T d + 1/2\, d^T W^k d \\ s.t. & c(z)=0 & & s.t. & c(z^k) + (A^k)^T d = 0 \\ & z_L \le z \le z_U & & & z_L \le z^k + d \le z_U \end{array}$$

Characteristics

- Many equations and variables (≥ 100 000)
- Many bounds and inequalities (≥ 100 000)

Few degrees of freedom (10 - 100)
Steady state flowsheet optimization
Real-time optimization
Parameter estimation

Many degrees of freedom (≥ 1000)
Dynamic optimization (optimal control, MPC)
State estimation and data reconciliation

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Few degrees of freedom => reduced space SQP (rSQP)

- Take advantage of sparsity of $A = \nabla c(x)$
- project W into space of active (or equality constraints)
- curvature (second derivative) information only needed in space of degrees of freedom
- second derivatives can be applied or approximated with positive curvature (e.g., BFGS)
- use dual space QP solvers

\+ easy to implement with existing sparse solvers, QP methods and line search techniques
\+ exploits 'natural assignment' of dependent and decision variables (some decomposition steps are 'free')
\+ does not require second derivatives

\- reduced space matrices are dense
\- may be dependent on variable partitioning
\- can be very expensive for many degrees of freedom
\- can be expensive if many QP bounds

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Reduced space SQP (rSQP)
Range and Null Space Decomposition

Assume no active bounds, QP problem with n variables and m constraints becomes:

$$\begin{bmatrix} W^k & A^k \\ A^{kT} & 0 \end{bmatrix} \begin{bmatrix} d \\ \lambda_+ \end{bmatrix} = -\begin{bmatrix} \nabla f(x^k) \\ c(x^k) \end{bmatrix}$$

- Define reduced space basis, $Z^k \in \Re^{n \times (n-m)}$ with $(A^k)^T Z^k = 0$
- Define basis for remaining space $Y^k \in \Re^{n \times m}$, $[Y^k\ Z^k] \in \Re^{n \times n}$ is nonsingular.
- Let $d = Y^k d_Y + Z^k d_Z$ to rewrite:

$$\begin{bmatrix} [Y^k\ Z^k]^T & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} W^k & A^k \\ A^{kT} & 0 \end{bmatrix} \begin{bmatrix} [Y^k\ Z^k] & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} d_Y \\ d_Z \\ \lambda_+ \end{bmatrix} = -\begin{bmatrix} [Y^k\ Z^k]^T & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} \nabla f(x^k) \\ c(x^k) \end{bmatrix}$$

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Reduced space SQP (rSQP)
Range and Null Space Decomposition

$$\begin{bmatrix} \cancelto{0}{Y^{kT} W^k Y^k} & \cancelto{0}{Y^{kT} W^k Z^k} & Y^{kT} A^k \\ Z^{kT} W^k Y^k & Z^{kT} W^k Z^k & 0 \\ A^{kT} Y^k & 0 & 0 \end{bmatrix} \begin{bmatrix} d_Y \\ d_Z \\ \lambda_+ \end{bmatrix} = -\begin{bmatrix} Y^{kT} \nabla f(x^k) \\ Z^{kT} \nabla f(x^k) \\ c(x^k) \end{bmatrix}$$

- $\boldsymbol{(A^T Y)\, d_Y = -c(x^k)}$ is square, d_Y determined from bottom row.
- Cancel $Y^T W Y$ and $Y^T W Z$; (unimportant as $d_Z, d_Y \to 0$)
- $\boldsymbol{(Y^T A)\, \lambda = -Y^T \nabla f(x^k)}$, λ can be determined by first order estimate
- Calculate or approximate $w = Z^T W Y d_Y$, solve $\boldsymbol{Z^T W Z\, d_Z = -Z^T \nabla f(x^k) - w}$
- Compute total step: $\boldsymbol{d = Y d_Y + Z d_Z}$

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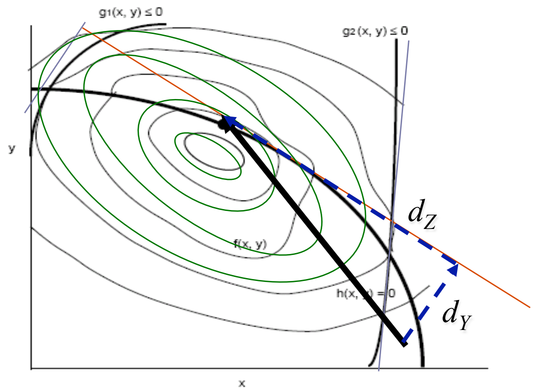
Reduced space SQP (rSQP) Interpretation



Range and Null Space Decomposition

- SQP step (d) operates in a higher dimension
- Satisfy constraints using range space to get d_Y
- Solve small QP in null space to get d_Z
- In general, same convergence properties as SQP.

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Choice of Decomposition Bases

1. Apply *QR* factorization to *A*. Leads to dense but well-conditioned *Y* and *Z*.

$$A = Q\begin{bmatrix} R \\ 0 \end{bmatrix} = \begin{bmatrix} Y & Z \end{bmatrix}\begin{bmatrix} R \\ 0 \end{bmatrix}$$

2. Partition variables into decisions *u* and dependents *v*. Create orthogonal *Y* and *Z* with embedded identity matrices ($A^TZ = 0,\ Y^TZ=0$).

$$A^T = \begin{bmatrix} \nabla_u c^T & \nabla_v c^T \end{bmatrix} = \begin{bmatrix} N & C \end{bmatrix}$$

$$Z = \begin{bmatrix} I \\ -C^{-1}N \end{bmatrix} \quad Y = \begin{bmatrix} N^T C^{-T} \\ I \end{bmatrix}$$

3. Coordinate Basis - same *Z* as above, $Y^T = [\ 0 \quad I\ ]$

- Bases use gradient information already calculated.
- Adapt decomposition to QP step
- Theoretically same rate of convergence as original SQP.
- Coordinate basis can be sensitive to choice of *u* and *v*. Orthogonal is not.
- Need consistent initial point and nonsingular *C*; automatic generation

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rSQP Algorithm

1. Choose starting point x^0.
2. At iteration k, evaluate functions $f(x^k)$, $c(x^k)$ and their gradients.
3. Calculate bases Y and Z.
4. Solve for step d_Y in Range space from
   $(A^T Y)\ d_Y = -c(x^k)$
5. Update projected Hessian $B^k \sim Z^T W Z$ (e.g. with BFGS), w_k (e.g., zero)
6. Solve small QP for step d_Z in Null space.

$$Min \quad (Z^T \nabla f(x^k) + w^k)^T d_Z + 1/2 d_Z^{\ T} B^k d_Z$$
$$s.t. \quad x_L \le x^k + Y d_Y + Z d_Z \le x_U$$

7. If error is less than tolerance stop. Else
8. Solve for multipliers using $(Y^T A)\ \lambda = -Y^T \nabla f(x^k)$
9. Calculate total step $d = Y\, d_Y + Z\, d_Z$.
10. Find step size α and calculate new point, $x_{k+1} = x_k + \alpha\, d$
13. Continue from step 2 with $k = k+1$.

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rSQP Results: Computational Results for General Nonlinear Problems

Vasantharajan et al (1990)

Problem	Specifications			MINOS (5.2)		Reduced SQP	
	N	M	MEQ	TIME*	FUNC	TIME* RND/LP	FUNC
Ramsey	34	23	10	1.4	46	1.7 1.0/0.7	8
Chenery	44	39	20	2.6	81	4.6 2.1/2.5	18
Korcge	100	96	78	3.9	9	3.7 1.4/2.3	3
Camcge	280	243	243	23.6	14	24.4 10.3/14.1	3
Ganges	357	274	274	22.7	14	59.7 35.7/24.0	4

* CPU Seconds - VAX 6320

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rSQP Results: Computational Results for Process Problems

Vasantharajan et al (1990)

Prob.	Specifications			MINOS (5.2)		Reduced SQP	
	N	M	MEQ	TIME*	FUNC	TIME* (rSQP/LP)	FUN.
Absorber	50	42	42				
(a)				4.4	144	3.2 (2.1/1.1)	23
(b)				4.7	157	2.8 (1.6/1.2)	13
Distill'n Ideal	228	227	227				
(a)				28.5	24	38.6 (9.6/29.0)	7
(b)				33.5	58	69.8 (17.2/52.6)	14
Distill'n Nonideal (1)	569	567	567				
(a)				172.1	34	130.1 (47.6/82.5)	14
(b)				432.1	362	144.9 (132.6/12.3)	47
(c)				855.3	745	211.5 (147.3/64.2)	49
Distill'n Nonideal (2)	977	975	975				
(a)				(F)	(F)	230.6 (83.1/147.5)	9
(b)				520.0+	162	322.1 (296.4/25.7)	26
(c)				(F)	(F)	466.7 (323/143.7)	34

* CPU Seconds - VAX 6320 (F) Failed
\+ MINOS (5.1)

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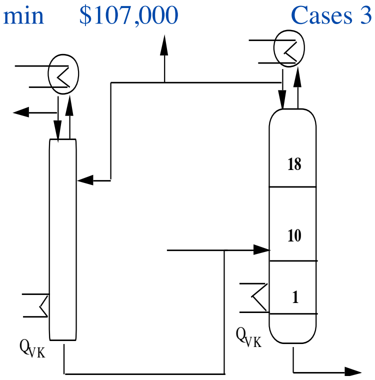
Comparison of SQP and rSQP

Coupled Distillation Example - 5000 Equations
Decision Variables - boilup rate, reflux ratio

	Method	CPU Time	Annual Savings	Comments
1.	SQP*	2 hr	negligible	Base Case
2.	rSQP	15 min.	\$ 42,000	Base Case
3.	rSQP	15 min.	\$ 84,000	Higher Feed Tray Location
4.	rSQP	15 min.	\$ 84,000	Column 2 Overhead to Storage
5.	rSQP	15 min	\$107,000	Cases 3 and 4 together



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Nonlinear Optimization Engines

Evolution of NLP Solvers:

➔ ***process optimization for design, control and operations***

SQP ⟶ rSQP ⟶ IPOPT

'00s: Simultaneous dynamic optimization
over 1 000 000 variables and constraints

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Many degrees of freedom => full space IPOPT

$$\begin{bmatrix} W^k + \Sigma & A^k \\ A^{kT} & 0 \end{bmatrix} \begin{bmatrix} d \\ \lambda_+ \end{bmatrix} = - \begin{bmatrix} \nabla \varphi(x^k) \\ c(x^k) \end{bmatrix}$$

- work in full space of all variables
- second derivatives useful for objective and constraints
- use specialized large-scale Newton solver

+ $W = \nabla_{xx} L(x,\lambda)$ and $A = \nabla c(x)$ sparse, often structured
+ fast if many degrees of freedom present
+ no variable partitioning required

- second derivatives strongly desired
- W is indefinite, requires complex stabilization
- requires specialized large-scale linear algebra

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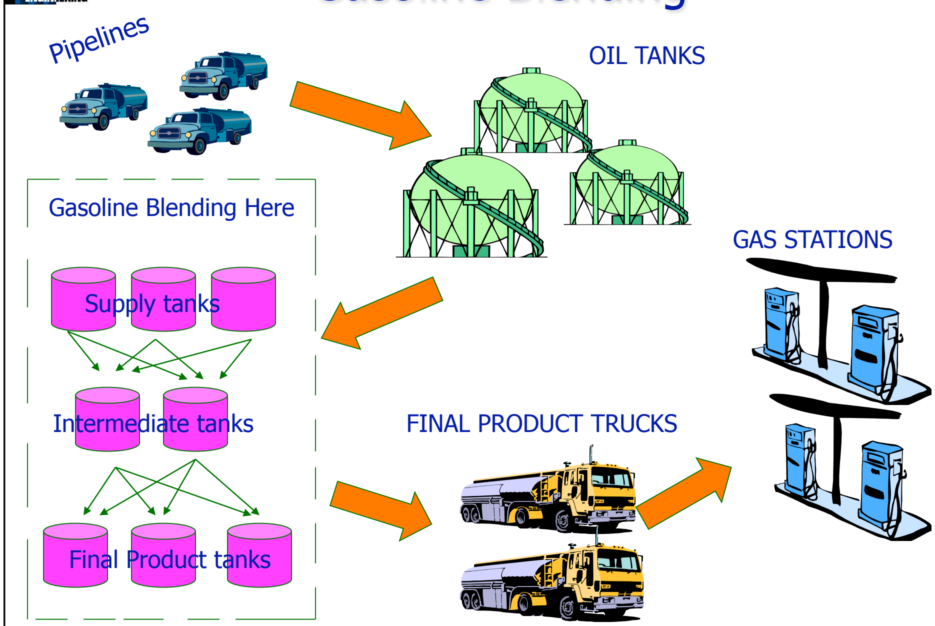
Gasoline Blending



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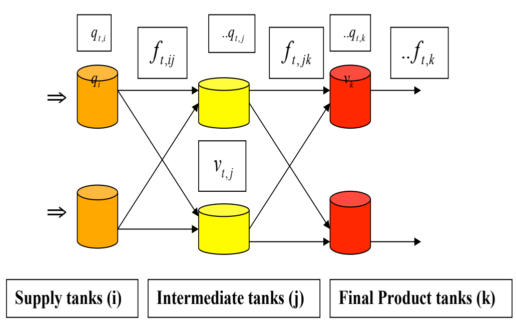
Blending Problem & Model Formulation



$$\max \sum_{t} \Big(\sum_{k} c_k f_{t,k} - \sum_{i} c_i f_{t,i}\Big)$$

$$\text{s.t.} \quad \sum_{k} f_{t,jk} - \sum_{i} f_{t,ij} + v_{t+1,j} = v_{t,j}$$

$$f_{t,k} - \sum_{j} f_{t,jk} = 0$$

$$\sum_{k} q_{t,j} f_{t,jk} - \sum_{i} q_{t,i} f_{t,ij} + q_{t+1,j} v_{t+1,j} = q_{t,j} v_{t,j}$$

$$q_{t,k} f_{t,k} - \sum_{j} q_{t,j} f_{t,jk} = 0$$

$$q_{k_{\min}} \le q_{t,k} \le q_{k_{\max}}$$

$$v_{j_{\min}} \le v_{t,j} \le v_{j_{\max}}$$

f, v ------ flowrates and tank volumes

q ------ tank qualities

Model Formulation in AMPL

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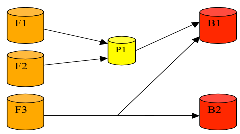
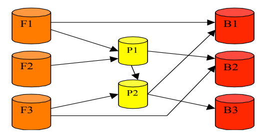
Small Multi-day Blending Models

Single Qualities

Haverly, C. 1978 (HM)



Audet & Hansen 1998 (AHM)



	no. of iterations	objective	CPU (s)	normalized CPU (s)
HM Day 1 ($N = 13$, $M = 8$, $S = 8$)				
LANCELOT	62	100	0.10	0.05
MINOS	15	400	0.04	0.13
SNOPT	36	400	0.02	0.01
KNITRO	38	100	0.14	0.06
LOQO	30	400	0.10	0.08
IPOPT, exact	31	400	0.01	0.01
IPOPT, L-BFGS	199	400	0.08	0.08
AHM Day 1 ($N = 21$, $M = 14$, $S = 14$)				
LANCELOT	112	49.2	0.32	0.14
MINOS	29	0.00	0.01	0.03
SNOPT	60	49.2	0.01	<0.01
KNITRO	44	31.6	0.15	0.07
LOQO	28	49.2	0.10	0.08
IPOPT, exact	28	49.2	0.01	0.01
IPOPT, L-BFGS	44	49.2	0.02	0.02

	no. of iterations	objective	CPU (s)	normalized CPU (s)
HM Day 25 ($N = 325$, $M = 200$, $S = 200$)				
LANCELOT	67	1.00×10^4	6.75	3.04
MINOS	801	6.40×10^3	1.21	3.83
SNOPT	739	1.00×10^4	0.59	0.27
KNITRO	>1000	*a*	*a*	*a*
LOQO	31	1.00×10^4	0.44	0.33
IPOPT, exact	47	1.00×10^4	0.24	0.24
IPOPT, L-BFGS	344	1.00×10^4	1.99	1.99
AHM Day 25 ($N = 525$, $M = 300$, $S = 350$)				
LANCELOT	149	8.13×10^2	26.8	12.1
MINOS	940	3.75×10^2	2.92	9.23
SNOPT	1473	1.23×10^3	1.47	0.66
KNITRO	316	1.13×10^3	17.5	7.88
LOQO	30	1.23×10^3	0.80	0.60
IPOPT, exact	44	1.23×10^3	0.25	0.25
IPOPT, L-BFGS	76	1.23×10^3	0.98	0.98

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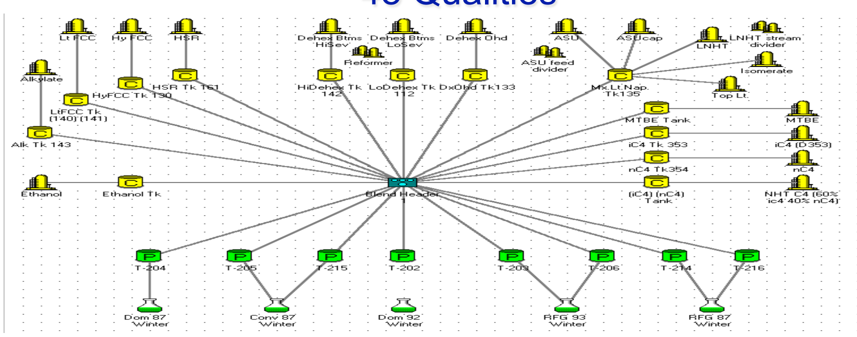
Honeywell Blending Model – Multiple Days

48 Qualities



	no. of iterations	objective	CPU (s)	normalized CPU (s)
IHM Day 1 ($N = 2003$, $M = 1595$, $S = 1449$)				
LANCELOT	388	6.14×10^1	1.17×10^5	5.28×10^3
MINOS	2238	6.14×10^1	5.24×10^1	1.66×10^2
SNOPT	*a*	*a*	*a*	*a*
KNITRO	37	1.00×10^2	1.58×10^2	7.11×10^1
LOQO	*b*	*b*	*b*	*b*
IPOPT, exact	21	6.14×10^1	2.60	2.60
IPOPT, L-BFGS	52	6.14×10^1	8.89	8.89
IHM Day 5 ($N = 10\,134$, $M = 8073$, $S = 7339$)				
LANCELOT	*c*	*c*	*c*	*c*
MINOS	8075	1.39×10^5	3.08×10^2	9.74×10^2
SNOPT	*a*	*a*	*a*	*a*
KNITRO	*a*	*a*	*a*	*a*
LOQO	*b*	*b*	*b*	*b*
IPOPT, exact	39	1.39×10^5	1.06×10^3	1.06×10^3
IPOPT. L-BFGS	1000	1.39×10^5	2.91×10^5	2.91×10^5

	no. of iterations	objective	CPU (s)	normalized CPU (s)
IHM Day 10 ($N = 20\,826$, $M = 16\,074$, $S = 15\,206$)				
LANCELOT	*c*	*c*	*c*	*c*
MINOS	*a*	*a*	*a*	*a*
SNOPT	*a*	*a*	*a*	*a*
KNITRO	*a*	*a*	*a*	*a*
LOQO	*b*	*b*	*b*	*b*
IPOPT, exact	65	2.64×10^4	1.12×10^4	1.12×10^4
IHM Day 15 ($N = 31\,743$, $M = 25\,560$, $S = 23\,073$)				
LANCELOT	*c*	*c*	*c*	*c*
MINOS	*a*	*a*	*a*	*a*
SNOPT	*a*	*a*	*a*	*a*
KNITRO	*a*	*a*	*a*	*a*
LOQO	*b*	*b*	*b*	*b*
IPOPT, exact	110	4.15×10^4	7.25×10^4	7.25×10^4

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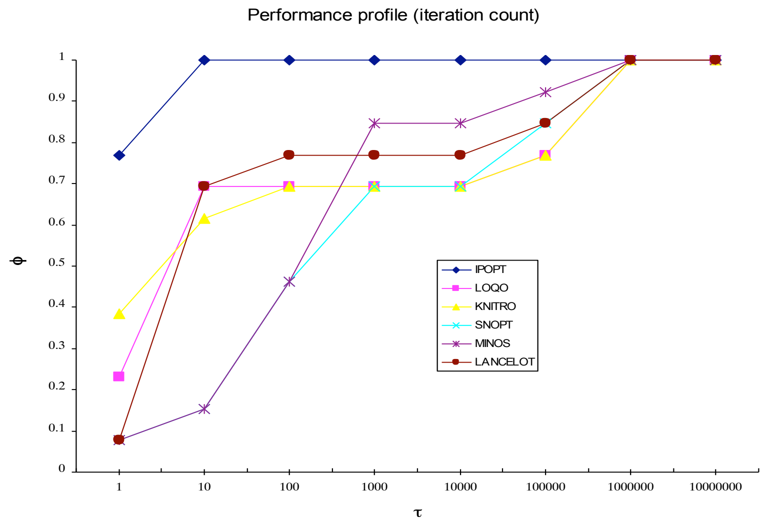
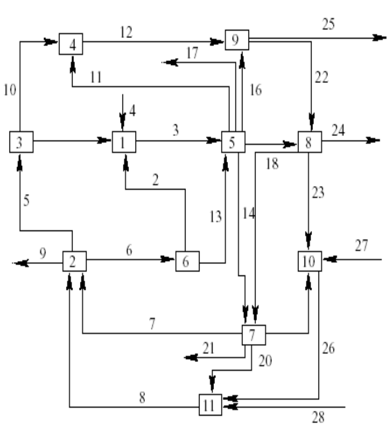
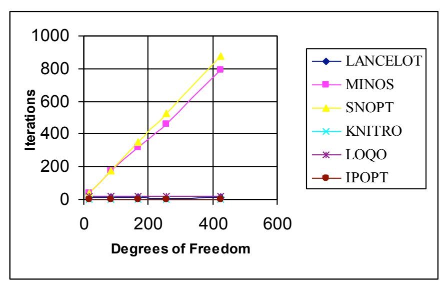
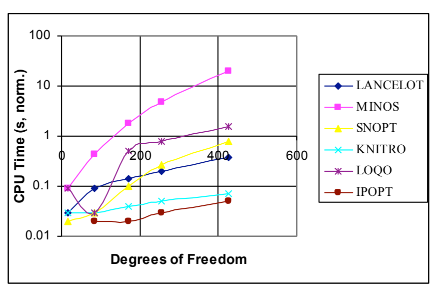
Summary of Results – Dolan-Moré plot



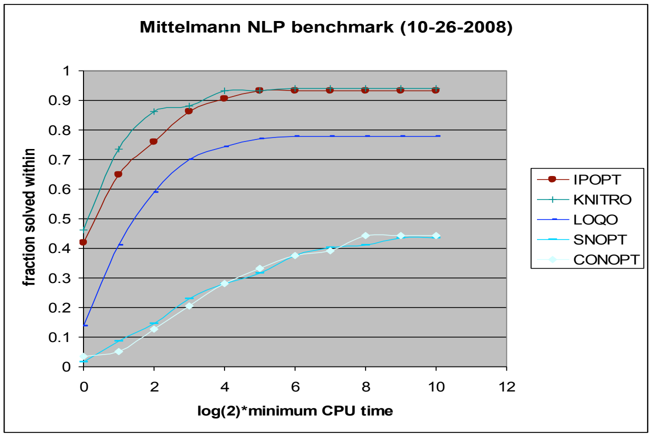
Comparison of NLP Solvers: Data Reconciliation







Comparison of NLP solvers
(latest Mittelmann study)



	Limits	Fail
IPOPT	7	2
KNITRO	7	0
LOQO	23	4
SNOPT	56	11
CONOPT	55	11

117 Large-scale Test Problems

500 - 250 000 variables, 0 – 250 000 constraints

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Typical NLP algorithms and software

SQP - NPSOL, VF02AD, NLPQL, fmincon

reduced SQP - SNOPT, rSQP, MUSCOD, DMO, LSSOL…

Reduced Grad. rest. - GRG2, GINO, SOLVER, CONOPT

Reduced Grad no rest. - MINOS

Second derivatives and barrier - IPOPT, KNITRO, LOQO

Interesting hybrids -

•FSQP/cFSQP - SQP and constraint elimination

•LANCELOT (Augmented Lagrangian w/ Gradient Projection)

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Summary and Conclusions

Optimization Algorithms
-Unconstrained Newton and Quasi Newton Methods
-KKT Conditions and Specialized Methods
-Reduced Gradient Methods (GRG2, MINOS)
-Successive Quadratic Programming (SQP)
-Reduced Hessian SQP
-Interior Point NLP (IPOPT)

Process Optimization Applications
-Modular Flowsheet Optimization
-Equation Oriented Models and Optimization
-Realtime Process Optimization
-Blending with many degrees of freedom

Further Applications
-Sensitivity Analysis for NLP Solutions
-Multi-Scenario Optimization Problems