Numerical Optimization

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Part I

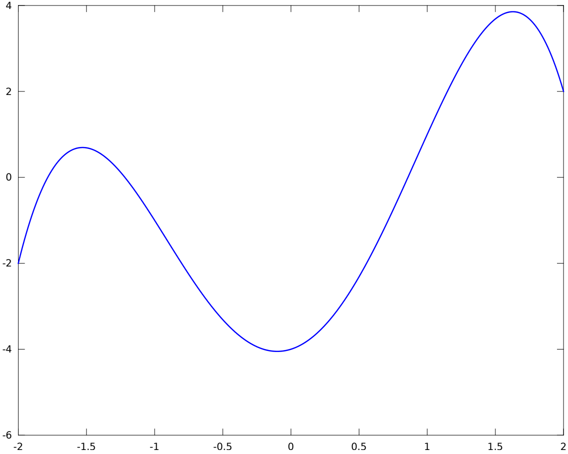
Introduction

Overview of Optimization

- One-dimensional unconstrained optimization
  - Characterization of critical points
  - Basic algorithms
- Nonlinear systems of equations
- Multi-dimensional unconstrained optimization
  - Critical points and their types
  - Computation of local minimizers
- Multi-dimensional constrained optimization
  - Critical points and Lagrange multipliers
  - Second-order sufficiency conditions
  - Globally-convergent algorithms
- Complementarity constraints
  - Stationarity concepts
  - Constraint qualifications
  - Numerical methods

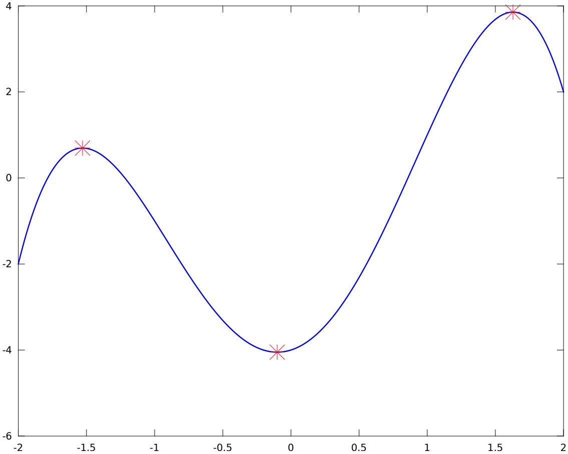
One-dimensional Unconstrained Optimization

$$\min_x f(x) = -x^4 + 5x^2 + x - 4$$



Critical Points

- Stationarity: $\nabla f(x) = -4x^3 + 10x + 1 = 0$
- Local maximizer: $\nabla^2 f(x) = -12x^2 + 10 < 0$
- Local minimizer: $\nabla^2 f(x) = -12x^2 + 10 > 0$



Locally Convergent Newton Method

- All good algorithms are variants of Newton's method
- Compute stationary points: $F(x) = \nabla f(x) = 0$
  - Form Taylor series approximation around x^k

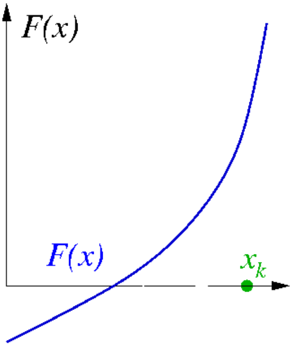
$$F(x) \approx \nabla F(x^k)(x - x^k) + F(x^k)$$

  - Solve for x and iterate

$$x^{k+1} = x^k - \frac{F(x^k)}{\nabla F(x^k)}$$

- Several possible outcomes
  - Convergence: $\lim_{k\to\infty} x^k = x^*$
  - Divergence: $\lim_{k\to\infty} \|(f(x^k), x^k)\| \to \infty$
  - Sequence cycles
    - Multiple convergent subsequences (limit points)
    - Limit points are not solutions

Illustration of Newton's Method



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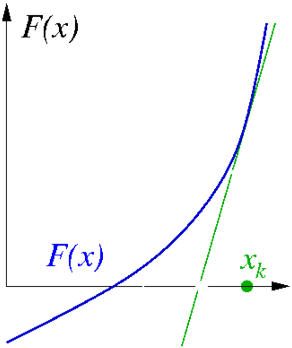

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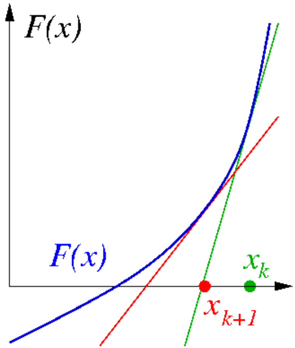

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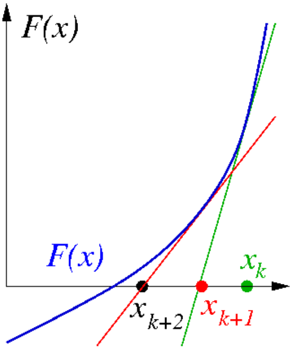


Illustration of Divergence

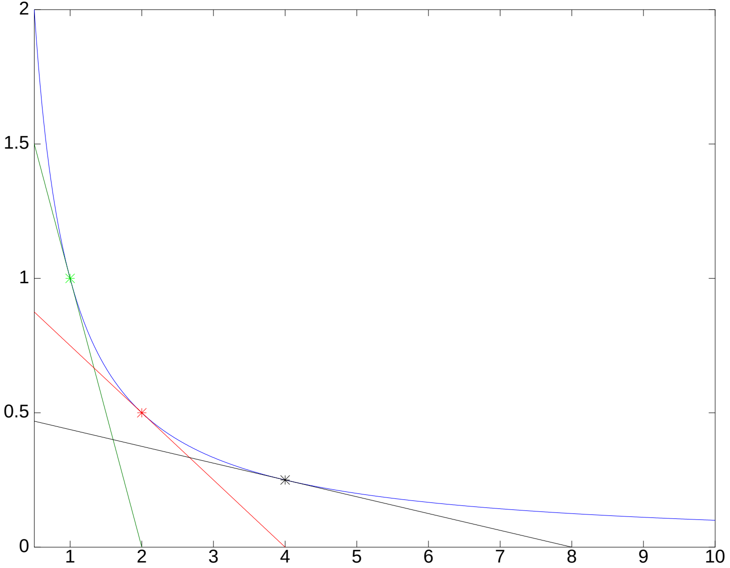
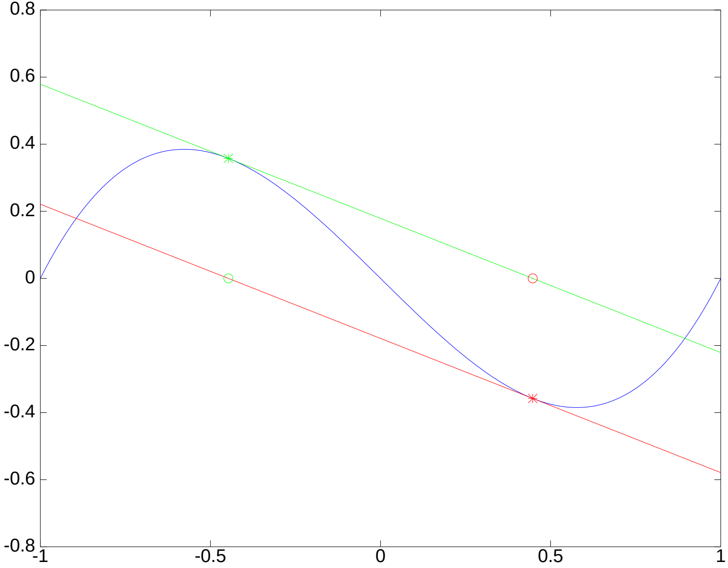


Illustration of Cycling



Globally Convergent Newton Method

- Use Newton method to compute a direction

$$s^k = -\frac{F(x^k)}{\nabla F(x^k)}$$

- Check direction for descent using objective function

$$\nabla f(x^k) s^k < 0$$

- Determine an appropriate stepsize
  - Line search to minimize the objective function

$$f(x^k + ts^k) \leq f(x^k) + \sigma t \nabla f(x^k) s^k$$

  - Trust region around the approximation
- Iterate until convergence
- Two possible outcomes
  - Convergence: $\lim_{k \to \infty} x^k \to x^*$
  - Divergence: $\lim_{k \to \infty} \|(f(x^k), x^k)\| \to \infty$

Newton Method for Square Systems of Equations

- Given $F : \Re^n \to \Re^n$, compute x such that

$$F(x) = 0$$

- First-order Taylor series approximation

$$\nabla F(x^k)(x - x^k) + F(x^k) = 0$$

- Solve linear system of equations

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

  - Direct method – compute factorization
  - Iterative method – use Krylov subspace
- Method has local (fast) convergence under suitable conditions
  - If x^k is near a solution, method converges to a solution x^*
  - The distance to the solution decreases quickly; ideally,

$$\|x^{k+1} - x^*\| \le c\|x^k - x^*\|^2$$

Globally Convergent Newton Method

- Solve linear system of equations

$$\nabla F(x^k) s_k = -F(x^k)$$

- Determine step length by minimizing merit function

$$t_k \in \arg \min_{t \in (0,1]} \|F(x^k + t s_k)\|_2^2$$

- Update iterate

$$x^{k+1} = x^k + t_k s_k$$

Globalized Newton Method with Proximal Perturbation

- Solve linear system of equations

$$(\nabla F(x^k) + \lambda_k I)s_k = -F(x^k)$$

- Check step and possibly use steepest descent direction
- Determine step length

$$t_k \in \arg\min_{t\in(0,1]} \|F(x^k + ts_k)\|_2^2$$

- Update iterate

$$x^{k+1} = x^k + t_k s_k$$

- Update perturbation

Nonsquare Nonlinear Systems of Equations

- Given $F : \Re^n \to \Re^m$, compute x such that

$$F(x) = 0$$

- System is underdetermined if $m < n$
  - More variables than constraints
  - Solution typically not unique
  - Need to select one solution

$$\min_x \; \|x\|_2 \text{ subject to } F(x) = 0$$

- System is overdetermined if $m > n$
  - More constraints than variables
  - Solution typically does not exist
  - Need to select approximate solution

$$\min_x \; \|F(x)\|_2$$

- System is square if $m = n$
  - Jacobian has full rank then solution is unique
  - If Jacobian is rank deficient then
    - Underdetermined when compatible
    - Overdetermined when incompatible

Part II

Unconstrained Optimization

Model Formulation

- Classify m people into two groups using v variables
  - $c \in \{0, 1\}^m$ is the known classification
  - $d \in \Re^{m \times v}$ are the observations
  - $\beta \in \Re^{v+1}$ defines the separator
  - logit distribution function
- Maximum likelihood problem

$$\max_{\beta} \quad \sum_{i=1}^{m} c_i \log(f(\beta, d_{i,\cdot})) + (1 - c_i) \log(1 - f(\beta, d_{i,\cdot}))$$

where

$$f(\beta, x) = \frac{\exp\left(\beta_0 + \sum_{j=1}^{v} \beta_j x_j\right)}{1 + \exp\left(\beta_0 + \sum_{j=1}^{v} \beta_j x_j\right)}$$

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$$\min_{\beta} \quad -\left(\sum_{i=1}^{m} c_i \log(f(\beta, d_{i,\cdot})) + (1-c_i)\log(1 - f(\beta, d_{i,\cdot})) \right)$$

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Basic Theory

$$\min_x f(x)$$

- Convex functions – local minimizers are global minimizers
- Nonconvex functions
  - Stationarity: $\nabla f(x) = 0$
  - Local minimizer: $\nabla^2 f(x)$ is positive definite (min eig positive)
  - Local maximizer: $\nabla^2 f(x)$ is negative definite (max eig negative)

Solution Techniques

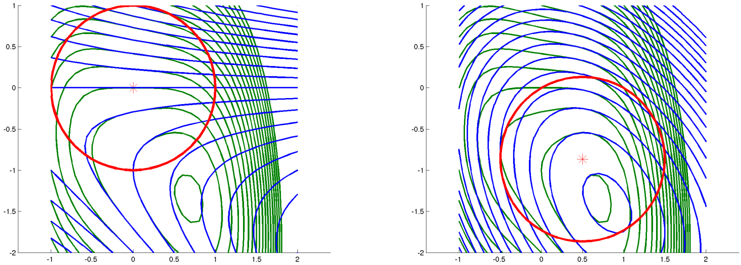
$$\min_x f(x)$$

Main ingredients of solution approaches:

- Local method: given x_k (solution guess) compute a step s^k
  - Gradient Descent
  - Quasi-Newton Approximation
  - Sequential Quadratic Programming
- Globalization strategy: converge from any starting point
  - Trust region
  - Line search

Trust-Region Method

$$
\begin{array}{ll}
\min\limits_{s} & f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T H(x_k) s \\
\text{subject to} & \|s\|_2 \leq \Delta_k
\end{array}
$$



Trust-Region Method

1. Initialize trust-region radius
2. Compute a new iterate
   2.1 Solve trust-region subproblem

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   2.2 Accept or reject iterate

   2.3 Update trust-region radius

   - Increase if actual reduction more than predicted
   - Decrease if actual reduction less than predicted

3. Check convergence

Solving a Convex Quadratic Program

- Assume the quadratic program is strictly convex

$$\min_s \quad \frac{1}{2} s^T H s + c^T s$$

  - H is symmetric and positive definite
  - H^{-1} exists
- Stationary points are necessary and sufficient

$$Hs = -c$$

  - Cholesky factorization
    - Compute (sparse) lower triangular matrix with $H = LL^T$
    - Solve $s = L^{-T}(L^{-1}c)$ exploiting lower triangular property
  - Conjugate gradient method
    - Iteratively compute a set of H conjugate directions
    - Analytically minimize quadratic along the directions
    - Objective function decreases monotonically
    - Guaranteed convergence in n steps

Solving a Nonconvex Quadratic Program

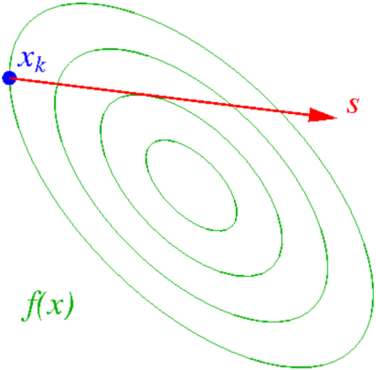
- No assumptions on the quadratic program

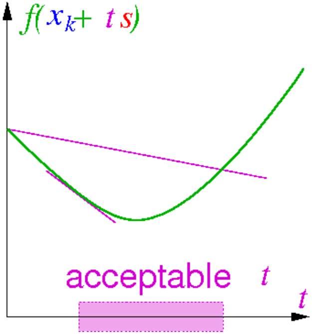
$$\begin{array}{ll} \min\limits_{s} & \frac{1}{2} s^T H s + c^T s \\ \text{subject to} & \|s\|_2 \leq \Delta_k \end{array}$$

  - Trust region bounds objective function
  - No unbounded solutions
- Can detect inertia with a LDL^T factorization and use direct method
- Global solutions computed with Moré-Sorensen method
  - Requires repeated factorization of a matrix
  - Can be expensive to calculate
  - Little benefit
- Conjugate gradient method with a trust region
  - Iteratively compute a set of H conjugate directions
  - Analytically minimize quadratic along the directions
  - Stop when trust region boundary is encountered
  - Objective function decreases monotonically

Line-Search Method

$$\min_{s} \quad f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T (H(x_k) + \lambda_k I) s$$





Line-Search Method

1. Initialize perturbation to zero
2. Solve perturbed quadratic model

$$\min_{s} \quad f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T (H(x_k) + \lambda_k I) s$$

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   3.1 Search along Newton direction
   3.2 Search along gradient-based direction

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3. Find new iterate
   3.1 Search along Newton direction
   3.2 Search along gradient-based direction
4. Update perturbation
   - Decrease perturbation if the following hold
     - Iterative method succeeds
     - Search along Newton direction succeeds
   - Otherwise increase perturbation
5. Check convergence

Solving the Subproblem

- Use LDL^T to determine inertia and update perturbation
- Apply conjugate gradient method and stop on unbounded directions

Solving the Subproblem

- Use LDL^T to determine inertia and update perturbation
- Apply conjugate gradient method and stop on unbounded directions
- Conjugate gradient method with trust region
  - Initialize radius
  - Update radius

Performing the Line Search

- Backtracking Armijo line search
  - Find t to satisfy sufficient decrease condition

$$f(x_k + ts) \leq f(x_k) + \sigma t \nabla f(x_k)^T s$$

  - Try $t = 1, \beta, \beta^2, \ldots$ for $0 < \beta < 1$
- More-Thuente line search
  - Find t to satisfy strong Wolfe conditions

$$\begin{aligned} f(x_k + ts) &\leq f(x_k) + \sigma t \nabla f(x_k)^T s \\ |\nabla f(x_k + ts)^T s| &\leq \delta |\nabla f(x_k)^T s| \end{aligned}$$

  - Construct cubic interpolant
  - Compute t to minimize interpolant
  - Refine interpolant

Updating the Perturbation

1. If increasing and $\lambda_k = 0$
$$\lambda_{k+1} = \mathrm{Proj}_{[\ell_0, u_0]} \left(\alpha_0 \|\nabla f(x^k)\| \right)$$
2. If increasing and $\lambda_k > 0$
$$\lambda_{k+1} = \mathrm{Proj}_{[\ell_i, u_i]} \left(\max \left(\alpha_i \|\nabla f(x^k)\|, \beta_i \lambda_k \right) \right)$$
3. If decreasing
$$\lambda_{k+1} = \min \left(\alpha_d \|\nabla f(x^k)\|, \beta_d \lambda_k \right)$$
4. If $\lambda_{k+1} < \ell_d$, then $\lambda_{k+1} = 0$

Trust-Region Line-Search Method

1. Initialize trust-region radius
2. Compute a new iterate
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$$\begin{array}{ll} \min_s & f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T H(x_k) s \\ \text{subject to} & \|s\| \leq \Delta_k \end{array}$$

   2.2 Search along direction
   2.3 Update trust-region radius
3. Check convergence

Iterative Methods

- Conjugate gradient method
  - Stop if negative curvature encountered
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Iterative Methods

- Conjugate gradient method
  - Stop if negative curvature encountered
  - Stop if residual norm is small
- Conjugate gradient method with trust region
  - Nash
    - Follow direction to boundary if first iteration
    - Stop at base of direction otherwise
  - Steihaug-Toint
    - Follow direction to boundary
  - Generalized Lanczos
    - Compute tridiagonal approximation
    - Find global solution to approximate problem on boundary
    - Initialize perturbation with approximate minimum eigenvalue

Preconditioners to Improve Performance

- Modify system of equations solved

$$AHs = -Ac$$

  - A is symmetric positive definite
  - A^{-1} can be easily applied to vector
  - AH is well conditioned or has clustered eigenvalues
  - Corresponds to changing to an elliptic trust region

$$\begin{array}{ll} \min_s & \frac{1}{2} s^T H s + c^T s \\ \text{subject to} & \|s\|_A \leq \Delta_k \end{array}$$

- Preconditioners are problem specific
- Many possibly preconditioners
  - No preconditioner – $A = I$
  - Diagonal of Hessian – $A = |\text{diag}(H(x_k))|$
  - Diagonal of perturbed Hessian – $A = |\text{diag}(H(x_k) + \lambda_k I)|$
  - Quasi-newton approximation to Hessian matrix
  - Incomplete Cholesky factorization of Hessian
  - Block Jacobi with Cholesky factorization of blocks

Termination

- Typical convergence criteria
  - Absolute residual $\|\nabla f(x_k)\| < \tau_a$
  - Relative residual $\frac{\|\nabla f(x_k)\|}{\|\nabla f(x_0)\|} < \tau_r$
  - Unbounded objective $f(x_k) < \kappa$
  - Slow progress $|f(x_k) - f(x_{k-1})| < \epsilon$
  - Iteration limit
  - Time limit
- Check the solver status

Convergence Issues

- Quadratic convergence – best outcome
- Linear convergence
  - Far from a solution – $\|\nabla f(x_k)\|$ is large
  - Hessian is incorrect – disrupts quadratic convergence
  - Hessian is rank deficient – $\|\nabla f(x_k)\|$ is small
  - Limits of finite precision arithmetic
    1. $\|\nabla f(x_k)\|$ converges quadratically to small number
    2. $\|\nabla f(x_k)\|$ hovers around that number with no progress
- Domain violations such as $\frac{1}{x}$ when $x = 0$
  - Make implicit constraints explicit
- Nonglobal solution
  - Apply a multistart heuristic
  - Use global optimization solver

Some Available Software

- TRON – Newton method with trust-region
- LBFGS – Limited-memory quasi-Newton method with line search
- TAO – Toolkit for Advanced Optimization
  - NLS – Newton line-search method
  - NTR – Newton trust-region method
  - NTL – Newton line-search/trust-region method
  - LMVM – Limited-memory quasi-Newton method
  - CG – Nonlinear conjugate gradient methods

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    - Increase size of the simplex
    - Reduce size of the simplex
    - Reflection of the simplex
  - Convergent methods can be constructed
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- Pattern search methods
  - Evaluate objective along coordinate directions
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  - Show convergence
- Model based methods
  - Sample the objective at various points
  - Construct a model based on the samples
  - Compute optimal solution for the model
  - Update the set of sample points
  - Show convergence

Part III

Constrained Optimization

Social Planning Model

- Economy with n agents and m commodities
  - $e \in \Re^{n \times m}$ are the endowments
  - $\alpha \in \Re^{n \times m}$ and $\beta \in \Re^{n \times m}$ are the utility parameters
  - $\lambda \in \Re^{n}$ are the social weights
- Social planning problem

$$
\begin{array}{lll}
\max\limits_{x \geq 0} & \displaystyle\sum_{i=1}^{n} \lambda_i \left(\sum_{k=1}^{m} \frac{\alpha_{i,k} (1 + x_{i,k})^{1-\beta_{i,k}}}{1 - \beta_{i,k}} \right) & \\
\text{subject to} & \displaystyle\sum_{i=1}^{n} x_{i,k} \leq \sum_{i=1}^{n} e_{i,k} & \forall k = 1, \ldots, m
\end{array}
$$

Life-Cycle Saving Model

- Maximize discounted utility
  - $u(\cdot)$ is the utility function
  - R is the retirement age
  - T is the terminal age
  - w is the wage
  - β is the discount factor
  - r is the interest rate
- Optimization problem

$$
\begin{array}{lll}
\max\limits_{s,c} & \sum\limits_{t=0}^{T} \beta^t u(c_t) & \\
\text{subject to} & s_{t+1} = (1+r)s_t + w - c_t & t = 0, \ldots, R-1 \\
 & s_{t+1} = (1+r)s_t - c_t & t = R, \ldots, T \\
 & s_0 = s_{T+1} = 0 &
\end{array}
$$

Theory Revisited

- Strict descent direction d

$$\nabla f(x)^T d < 0$$

- Stationarity conditions (first-order conditions)
  - No feasible, strict descent directions
  - For all feasible directions d

$$\nabla f(x)^T d \geq 0$$

  - Unconstrained case, $d \in \Re^n$ and

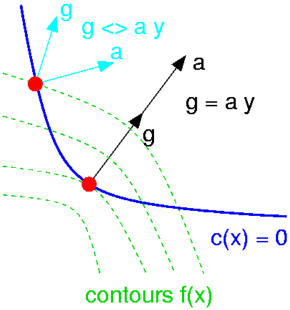
$$\nabla f(x) = 0$$

  - Constrained cases
    - Characterize superset of feasible directions
    - Requires constraint qualification

Convergence Criteria

$$\begin{array}{ll} \min\limits_{x} & f(x) \\ \text{subject to} & c(x) \geq 0 \end{array}$$

- Feasible and no strict descent directions
  - Constraint qualification – LICQ, MFCQ
  - Linearized active constraints characterize directions
  - Objective gradient is a linear combination of constraint gradients



Optimality Conditions

- If x^* is a local minimizer and a constraint qualification holds, then there exist multipliers $\lambda^* \geq 0$ such that

$$\nabla f(x^*) - \nabla c_{\mathcal{A}}(x^*)^T \lambda^*_{\mathcal{A}} = 0$$

  - Lagrangian function $\mathcal{L}(x, \lambda) := f(x) - \lambda^T c(x)$
- Optimality conditions can be written as

$$\begin{aligned} &\nabla f(x) - \nabla c(x)^T \lambda = 0 \\ &0 \leq \lambda \quad \perp \quad c(x) \geq 0 \end{aligned}$$

  - Complementarity problem

Solving Constrained Optimization Problems

Main ingredients of solution approaches:

- Local method: given x_k (solution guess) find a step s.
  - Sequential Quadratic Programming (SQP)
  - Sequential Linear/Quadratic Programming (SLQP)
  - Interior-Point Method (IPM)
- Globalization strategy: converge from any starting point.
  - Trust region
  - Line search
- Acceptance criteria: filter or penalty function.

Sequential Linear Programming

1. Initialize trust-region radius
2. Compute a new iterate

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    2.1 Solve linear program

$$\begin{array}{ll} \min\limits_{s} & f(x_k) + s^T \nabla f(x_k) \\ \text{subject to} & c(x_k) + \nabla c(x_k)^T s \geq 0 \\ & \|s\| \leq \Delta_k \end{array}$$

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   2.2 Accept or reject iterate
   2.3 Update trust-region radius
3. Check convergence

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$$\begin{array}{ll} \min\limits_{s} & f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T W(x_k) s \\ \text{subject to} & c(x_k) + \nabla c(x_k)^T s \geq 0 \\ & \|s\| \leq \Delta_k \end{array}$$

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Sequential Linear Quadratic Programming

1. Initialize trust-region radius
2. Compute a new iterate

Sequential Linear Quadratic Programming

1. Initialize trust-region radius
2. Compute a new iterate
    2.1 Solve linear program to predict active set

$$
\begin{array}{ll}
\min\limits_{d} & f(x_k) + d^T \nabla f(x_k) \\
\text{subject to} & c(x_k) + \nabla c(x_k)^T d \geq 0 \\
 & \|d\| \leq \Delta_k
\end{array}
$$

Sequential Linear Quadratic Programming

1. Initialize trust-region radius
2. Compute a new iterate
   2.1 Solve linear program to predict active set

$$\begin{array}{ll} \min\limits_{d} & f(x_k) + d^T \nabla f(x_k) \\ \text{subject to} & c(x_k) + \nabla c(x_k)^T d \geq 0 \\ & \|d\| \leq \Delta_k \end{array}$$

   2.2 Solve equality constrained quadratic program

$$\begin{array}{ll} \min\limits_{s} & f(x_k) + s^T \nabla f(x_k) + \frac{1}{2} s^T W(x_k) s \\ \text{subject to} & c_{\mathcal{A}}(x_k) + \nabla c_{\mathcal{A}}(x_k)^T s = 0 \end{array}$$

   2.3 Accept or reject iterate
   2.4 Update trust-region radius
3. Check convergence

Acceptance Criteria

- Decrease objective function value: $f(x_k + s) \leq f(x_k)$
- Decrease constraint violation: $\|c_-(x_k + s)\| \leq \|c_-(x_k)\|$

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- Four possibilities
  1. step can decrease both $f(x)$ and $\|c_-(x)\|$ GOOD
  2. step can decrease $f(x)$ and increase $\|c_-(x)\|$???
  3. step can increase $f(x)$ and decrease $\|c_-(x)\|$???
  4. step can increase both $f(x)$ and $\|c_-(x)\|$ BAD

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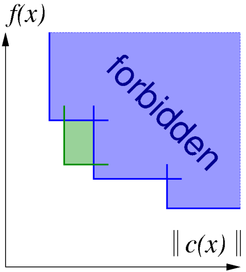
  4. step can increase both $f(x)$ and $\|c_-(x)\|$ BAD
- Filter uses concept from multi-objective optimization

(h_{k+1}, f_{k+1}) dominates (h_ℓ, f_ℓ) iff $h_{k+1} \leq h_\ell$ and $f_{k+1} \leq f_\ell$

Filter Framework

Filter $\mathcal{F}$: list of non-dominated pairs (h_ℓ, f_ℓ)

- new x_{k+1} is acceptable to filter $\mathcal{F}$ iff for all $\ell \in \mathcal{F}$
  1. $h_{k+1} \leq h_\ell$ or
  2. $f_{k+1} \leq f_\ell$



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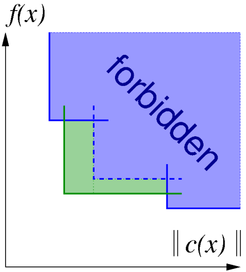
- remove redundant filter entries



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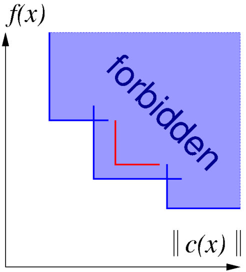
  1. $h_{k+1} \le h_\ell$ or
  2. $f_{k+1} \le f_\ell$
- remove redundant filter entries
- new x_{k+1} is rejected if for some $\ell \in \mathcal{F}$
  1. $h_{k+1} > h_\ell$ and
  2. $f_{k+1} > f_\ell$



Termination

- Feasible and complementary $\|\min(c(x_k), \lambda_k)\| \leq \tau_f$
- Optimal $\|\nabla_x \mathcal{L}(x_k, \lambda_k)\| \leq \tau_o$
- Other possible conditions
  - Slow progress
  - Iteration limit
  - Time limit
- Multipliers and reduced costs

Convergence Issues

- Quadratic convergence – best outcome
- Globally infeasible – linear constraints infeasible
- Locally infeasible – nonlinear constraints locally infeasible
- Unbounded objective – hard to detect
- Unbounded multipliers – constraint qualification not satisfied
- Linear convergence rate
  - Far from a solution – $\|\nabla f(x_k)\|$ is large
  - Hessian is incorrect – disrupts quadratic convergence
  - Hessian is rank deficient – $\|\nabla f(x_k)\|$ is small
  - Limits of finite precision arithmetic
- Domain violations such as $\frac{1}{x}$ when $x = 0$
  - Make implicit constraints explicit
- Nonglobal solutions
  - Apply a multistart heuristic
  - Use global optimization solver

Some Available Software

- filterSQP
  - trust-region SQP; robust QP solver
  - filter to promote global convergence
- SNOPT
  - line-search SQP; null-space CG option
  - ℓ_1 exact penalty function
- SLIQUE – part of KNITRO
  - SLP-EQP
  - trust-region with ℓ_1 penalty
  - use with `knitro_options = "algorithm=3";`

Interior-Point Method

- Reformulate optimization problem with slacks

$$
\begin{array}{ll}
\min\limits_{x} & f(x) \\
\text{subject to} & c(x) = 0 \\
& x \geq 0
\end{array}
$$

- Construct perturbed optimality conditions

$$
F_\tau(x, y, z) = \begin{bmatrix} \nabla f(x) - \nabla c(x)^T \lambda - \mu \\ c(x) \\ X\mu - \tau e \end{bmatrix}
$$

- Central path $\{x(\tau), \lambda(\tau), \mu(\tau) \mid \tau > 0\}$
- Apply Newton's method for sequence $\tau \searrow 0$

Interior-Point Method

1. Compute a new iterate
   1.1 Solve linear system of equations

$$\left[\begin{array}{ccc} W_k & -\nabla c(x_k)^T & -I \\ \nabla c(x_k) & 0 & 0 \\ \mu_k & 0 & X_k \end{array}\right] \left(\begin{array}{c} s_x \\ s_\lambda \\ s_\mu \end{array}\right) = -F_\tau(x_k, \lambda_k, \mu_k)$$

   1.2 Accept or reject iterate
   1.3 Update parameters
2. Check convergence

Convergence Issues

- Quadratic convergence – best outcome
- Globally infeasible – linear constraints infeasible
- Locally infeasible – nonlinear constraints locally infeasible
- Dual infeasible – dual problem is locally infeasible
- Unbounded objective – hard to detect
- Unbounded multipliers – constraint qualification not satisfied
- Duality gap
- Domain violations such as $\frac{1}{x}$ when $x = 0$
  - Make implicit constraints explicit
- Nonglobal solutions
  - Apply a multistart heuristic
  - Use global optimization solver

Termination

- Feasible and complementary $\| \min(c(x_k), \lambda_k) \| \leq \tau_f$
- Optimal $\|\nabla_x \mathcal{L}(x_k, \lambda_k)\| \leq \tau_o$
- Other possible conditions
  - Slow progress
  - Iteration limit
  - Time limit
- Multipliers and reduced costs

Some Available Software

- IPOPT – open source in COIN-OR
  - line-search filter algorithm
- KNITRO
  - trust-region Newton to solve barrier problem
  - ℓ_1 penalty barrier function
  - Newton system: direct solves or null-space CG
- LOQO
  - line-search method
  - Newton system: modified Cholesky factorization

Part IV

Optimal Control

Optimal Technology

Optimize energy production schedule and transition between old and new reduced-carbon technology to meet carbon targets

- Maximize social welfare
- Constraints
  - Limit total greenhouse gas emissions
  - Low-carbon technology less costly as it becomes widespread
- Assumptions on emission rates, economic growth, and energy costs

Model Formulation

- Finite time: $t \in [0, T]$
- Instantaneous energy output: $q^o(t)$ and $q^n(t)$
- Cumulative energy output: $x^o(t)$ and $x^n(t)$

$$x^n(t) = \int_0^t q^n(\tau) d\tau$$

- Discounted greenhouse gases emissions

$$\int_0^T e^{-at} \left(b_o q^o(t) + b_n q^n(t) \right) dt \leq z_T$$

- Consumer surplus $S(Q(t), t)$ derived from utility
- Production costs
  - c_o per unit cost of old technology
  - $c_n(x^n(t))$ per unit cost of new technology (learning by doing)

Continuous-Time Model

$$\max_{\{q^o, q^n, x^n, z\}(t)} \quad \int_0^T e^{-rt} \left[S(q^o(t) + q^n(t), t) - c_o q^o(t) - c_n(x^n(t)) q^n(t) \right] dt$$

$$\text{subject to} \quad \dot{x}^n(t) = q^n(t) \quad x(0) = x_0 = 0$$

$$\dot{z}(t) = e^{-at} \left(b_o q^o(t) + b_n q^n(t) \right) \quad z(0) = z_0 = 0$$

$$z(T) \leq z_T$$

$$q^o(t) \geq 0, \quad q^n(t) \geq 0.$$

Optimal Technology Penetration

Discretization:

- $t \in [0, T]$ replaced by $N + 1$ equally spaced points $t_i = ih$
- $h := T/N$ time integration step-length
- approximate $q_i^n \simeq q^n(t_i)$ etc.

Replace differential equation

$$\dot{x}(t) = q^n(t)$$

by

$$x_{i+1} = x_i + hq_i^n$$

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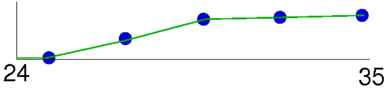
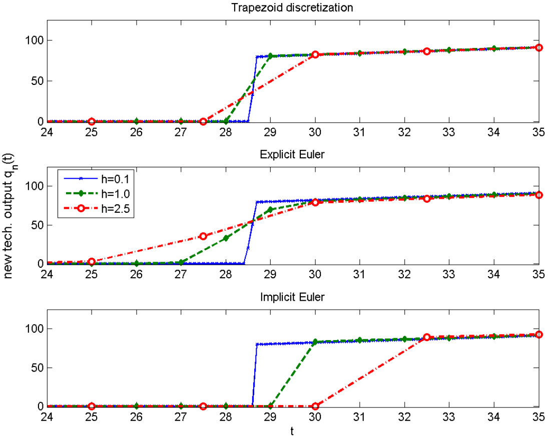


Output of new technology between $t = 24$ and $t = 35$

Solution with Varying h



Output for different discretization schemes and step-sizes

Optimal Technology Penetration

Add adjustment cost to model building of capacity:

Capital and Investment:

- $K^j(t)$ amount of capital in technology j at t.
- $I^j(t)$ investment to increase $K^j(t)$.
- initial capital level as $\bar{K}_0^j$:

Notation:

- $Q(t) = q^o(t) + q^n(t)$
- $C(t) = C^o(q^o(t), K^o(t)) + C^n(q^n(t), K^n(t))$
- $I(t) = I^o(t) + I^n(t)$
- $K(t) = K^o(t) + K^n(t)$

Optimal Technology Penetration

$$\underset{\{q^j, K^j, I^j, x, z\}(t)}{\text{maximize}} \quad \left\{ \int_0^T e^{-rt} \left[\tilde{S}(Q(t), t) - C(t) - K(t) \right] dt + e^{-rT} K(T) \right\}$$

$$\text{subject to} \quad \dot{x}(t) = q^n(t), \quad x(0) = x_0 = 0$$

$$\dot{K}^j(t) = -\delta K^j(t) + I^j(t), \quad K^j(0) = \bar{K}_0^j, \quad j \in \{o, n\}$$

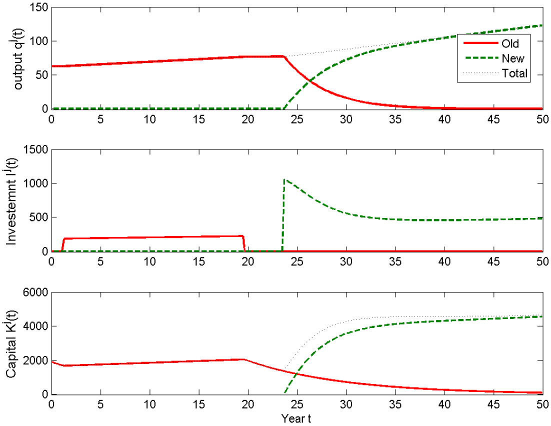
$$\dot{z}(t) = e^{-at}[b_o q^o(t) + b_n q^n(t)], \quad z(0) = z_0 = 0$$

$$z(T) \leq z_T$$

$$q^j(t) \geq 0, \ j \in \{o, n\}$$

$$I^j(t) \geq 0, \ j \in \{o, n\}$$

Optimal Technology Penetration



Optimal output, investment, and capital for 50% CO2 reduction.

Pitfalls of Discretizations [Hager, 2000]

Optimal Control Problem

$$\text{minimize } \frac{1}{2}\int_0^1 u^2(t) + 2y^2(t)dt$$

subject to

$$\begin{aligned} \dot{y}(t) &= \frac{1}{2}y(t) + u(t), \; t \in [0,1], \\ y(0) &= 1. \end{aligned}$$

$$\begin{aligned} \Rightarrow y^*(t) &= \frac{2e^{3t} + e^3}{e^{3t/2}(2+e^3)}, \\ u^*(t) &= \frac{2(e^{3t} - e^3)}{e^{3t/2}(2+e^3)}. \end{aligned}$$

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Discretize with 2nd order RK

$$\text{minimize } \frac{h}{2}\sum_{k=0}^{K-1} u^2_{k+1/2} + 2y^2_{k+1/2}$$

subject to $(k = 0, \ldots, K)$:

$$\begin{aligned} y_{k+1/2} &= y_k + \frac{h}{2}(\frac{1}{2}y_k + u_k), \\ y_{k+1} &= y_k + h(\frac{1}{2}y_{k+1/2} + u_{k+1/2}), \end{aligned}$$

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$$\text{minimize } \frac{h}{2}\sum_{k=0}^{K-1} u_{k+1/2}^2 + 2y_{k+1/2}^2$$

subject to $(k = 0, \ldots, K)$:

$$\begin{aligned} y_{k+1/2} &= y_k + \frac{h}{2}(\frac{1}{2}y_k + u_k), \\ y_{k+1} &= y_k + h(\frac{1}{2}y_{k+1/2} + u_{k+1/2}), \end{aligned}$$

Discrete solution $(k = 0, \ldots, K)$:

$$y_k = 1, \quad y_{k+1/2} = 0,$$

$$u_k = -\frac{4+h}{2h}, \quad u_{k+1/2} = 0,$$

DOES NOT CONVERGE!

Tips to Solve Continuous-Time Problems

- Use discretize-then-optimize with different schemes
- Refine discretization: $h = 1$ discretization is nonsense
- Check implied discretization of adjoints

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Alternative: Optimize-Then-Discretize

- Consistent adjoint/dual discretization
- Discretized gradients can be wrong!
- Harder for inequality constraints

Part V

Complementarity Constraints

Nash Games

- Non-cooperative game played by n individuals
  - Each player selects a strategy to optimize their objective
  - Strategies for the other players are fixed
- Equilibrium reached when no improvement is possible

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- Characterization of two player equilibrium (x^*, y^*)

$$
\begin{aligned}
x^* &\in \left\{ \begin{array}{ll} \displaystyle\operatorname*{arg\,min}_{x \geq 0} & f_1(x, y^*) \\ \text{subject to} & c_1(x) \leq 0 \end{array} \right. \\
y^* &\in \left\{ \begin{array}{ll} \displaystyle\operatorname*{arg\,min}_{y \geq 0} & f_2(x^*, y) \\ \text{subject to} & c_2(y) \leq 0 \end{array} \right.
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\end{aligned}
$$

- Many applications in economics
  - Bimatrix games
  - Cournot duopoly models
  - General equilibrium models
  - Arrow-Debreau models

Complementarity Formulation

- Assume each optimization problem is convex
  - $f_1(\cdot, y)$ is convex for each y
  - $f_2(x, \cdot)$ is convex for each x
  - $c_1(\cdot)$ and $c_2(\cdot)$ satisfy constraint qualification
- Then the first-order conditions are necessary and sufficient

$$\begin{array}{ll} \min\limits_{x \geq 0} & f_1(x, y^*) \\ \text{subject to} & c_1(x) \leq 0 \end{array} \quad \Leftrightarrow \quad \begin{array}{lcl} 0 \leq x & \perp & \nabla_x f_1(x, y^*) + \lambda_1^T \nabla_x c_1(x) \geq 0 \\ 0 \leq \lambda_1 & \perp & -c_1(x) \geq 0 \end{array}$$

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$$\begin{array}{ll} \min\limits_{y \geq 0} & f_2(x^*, y) \\ \text{subject to} & c_2(y) \leq 0 \end{array} \quad \Leftrightarrow \quad \begin{array}{lcl} 0 \leq y & \perp & \nabla_y f_2(x^*, y) + \lambda_2^T \nabla_y c_2(y) \geq 0 \\ 0 \leq \lambda_2 & \perp & -c_2(y) \geq 0 \end{array}$$

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- Assume each optimization problem is convex
  - $f_1(\cdot, y)$ is convex for each y
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- Then the first-order conditions are necessary and sufficient

$$
\begin{array}{lcl}
0 \leq x & \perp & \nabla_x f_1(x, y) + \lambda_1^T \nabla_x c_1(x) \geq 0 \\
0 \leq y & \perp & \nabla_y f_2(x, y) + \lambda_2^T \nabla_y c_2(y) \geq 0 \\
0 \leq \lambda_1 & \perp & -c_1(y) \geq 0 \\
0 \leq \lambda_2 & \perp & -c_2(y) \geq 0
\end{array}
$$

- Nonlinear complementarity problem
  - Square system – number of variables and constraints the same
  - Each solution is an equilibrium for the Nash game

Model Formulation

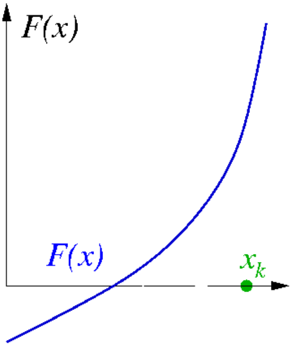
- Economy with n agents and m commodities
  - $e \in \Re^{n \times m}$ are the endowments
  - $\alpha \in \Re^{n \times m}$ and $\beta \in \Re^{n \times m}$ are the utility parameters
  - $p \in \Re^{m}$ are the commodity prices
- Agent i maximizes utility with budget constraint

$$\begin{array}{ll} \max\limits_{x_{i,*} \geq 0} & \sum\limits_{k=1}^{m} \dfrac{\alpha_{i,k}(1 + x_{i,k})^{1-\beta_{i,k}}}{1 - \beta_{i,k}} \\ \text{subject to} & \sum\limits_{k=1}^{m} p_k \left(x_{i,k} - e_{i,k}\right) \leq 0 \end{array}$$

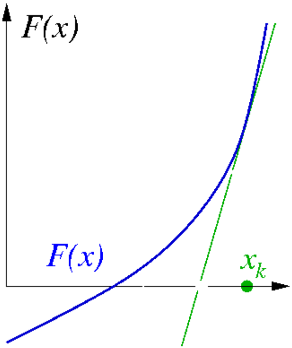
- Market k sets price for the commodity

$$0 \leq p_k \quad \perp \quad \sum_{i=1}^{n} (e_{i,k} - x_{i,k}) \geq 0$$

Newton Method for Nonlinear Equations



Newton Method for Nonlinear Equations



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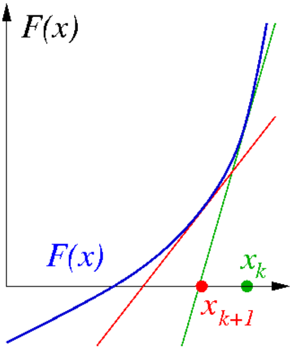

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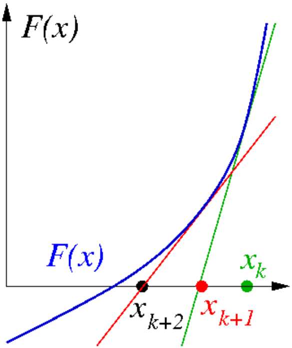

Methods for Complementarity Problems

- Sequential linearization methods (PATH)
    1. Solve the linear complementarity problem

$$0 \leq x \quad \perp \quad F(x_k) + \nabla F(x_k)(x - x_k) \geq 0$$

    2. Perform a line search along merit function
    3. Repeat until convergence

Methods for Complementarity Problems

- Sequential linearization methods (PATH)
  1. Solve the linear complementarity problem

$$0 \le x \quad \perp \quad F(x_k) + \nabla F(x_k)(x - x_k) \ge 0$$

  2. Perform a line search along merit function
  3. Repeat until convergence
- Semismooth reformulation methods (SEMI)
  - Solve linear system of equations to obtain direction
  - Globalize with a trust region or line search
  - Less robust in general
- Interior-point methods

Semismooth Reformulation

- Define Fischer-Burmeister function

$$\phi(a, b) := a + b - \sqrt{a^2 + b^2}$$

  - $\phi(a, b) = 0$ iff $a \geq 0$, $b \geq 0$, and $ab = 0$
- Define the system

$$[\Phi(x)]_i = \phi(x_i, F_i(x))$$

  - x^* solves complementarity problem iff $\Phi(x^*) = 0$
- Nonsmooth system of equations

Semismooth Algorithm

1. Calculate $H^k \in \partial_B \Phi(x^k)$ and solve the following system for d^k:

   $$H^k d^k = -\Phi(x^k)$$

   If this system either has no solution, or

   $$\nabla \Psi(x^k)^T d^k \leq -p_1 \|d^k\|^{p_2}$$

   is not satisfied, let $d^k = -\nabla \Psi(x^k)$.

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$$\nabla \Psi(x^k)^T d^k \leq -p_1 \|d^k\|^{p_2}$$

   is not satisfied, let $d^k = -\nabla \Psi(x^k)$.

2. Compute smallest nonnegative integer i^k such that

$$\Psi(x^k + \beta^{i^k} d^k) \leq \Psi(x^k) + \sigma \beta^{i^k} \nabla \Psi(x^k) d^k$$

3. Set $x^{k+1} = x^k + \beta^{i^k} d^k$, $k = k + 1$, and go to 1.

Convergence Issues

- Quadratic convergence – best outcome
- Linear convergence
  - Far from a solution – $r(x_k)$ is large
  - Jacobian is incorrect – disrupts quadratic convergence
  - Jacobian is rank deficient – $\|\nabla r(x_k)\|$ is small
  - Converge to local minimizer – guarantees rank deficiency
  - Limits of finite precision arithmetic
    1. $r(x_k)$ converges quadratically to small number
    2. $r(x_k)$ hovers around that number with no progress
- Domain violations such as $\frac{1}{x}$ when $x = 0$

Some Available Software

- PATH – sequential linearization method
- MILES – sequential linearization method
- SEMI – semismooth linesearch method
- TAO – Toolkit for Advanced Optimization
  - SSLS – full-space semismooth linesearch methods
  - ASLS – active-set semismooth linesearch methods
  - RSCS – reduced-space method

Definition

- Leader-follower game
  - Dominant player (leader) selects a strategy y^*
  - Then followers respond by playing a Nash game

$$x_i^* \in \begin{cases} \underset{x_i \geq 0}{\arg\min} & f_i(x, y) \\ \text{subject to} & c_i(x_i) \leq 0 \end{cases}$$

- Leader solves optimization problem with equilibrium constraints

$$\begin{array}{ll} \underset{y \geq 0, x, \lambda}{\min} & g(x, y) \\ \text{subject to} & h(y) \leq 0 \\ & 0 \leq x_i \quad \perp \quad \nabla_{x_i} f_i(x, y) + \lambda_i^T \nabla_{x_i} c_i(x_i) \geq 0 \\ & 0 \leq \lambda_i \quad \perp \quad -c_i(x_i) \geq 0 \end{array}$$

- Many applications in economics
  - Optimal taxation
  - Tolling problems

Model Formulation

- Economy with n agents and m commodities
  - $e \in \Re^{n \times m}$ are the endowments
  - $\alpha \in \Re^{n \times m}$ and $\beta \in \Re^{n \times m}$ are the utility parameters
  - $p \in \Re^{m}$ are the commodity prices
- Agent i maximizes utility with budget constraint

$$\begin{array}{ll} \max\limits_{x_{i,*} \geq 0} & \sum\limits_{k=1}^{m} \dfrac{\alpha_{i,k}(1 + x_{i,k})^{1-\beta_{i,k}}}{1 - \beta_{i,k}} \\ \text{subject to} & \sum\limits_{k=1}^{m} p_k \left(x_{i,k} - e_{i,k} \right) \leq 0 \end{array}$$

- Market k sets price for the commodity

$$0 \leq p_k \quad \perp \quad \sum_{i=1}^{n} (e_{i,k} - x_{i,k}) \geq 0$$

Nonlinear Programming Formulation

$$
\begin{array}{ll}
\min\limits_{x,y,\lambda,s,t\geq 0} & g(x,y) \\
\text{subject to} & h(y) \leq 0 \\
& s_i = \nabla_{x_i} f_i(x,y) + \lambda_i^T \nabla_{x_i} c_i(x_i) \\
& t_i = -c_i(x_i) \\
& \sum\limits_i \left(s_i^T x_i + \lambda_i t_i \right) \leq 0
\end{array}
$$

- Constraint qualification fails
  - Lagrange multiplier set unbounded
  - Constraint gradients linearly dependent
  - Central path does not exist
- Able to prove convergence results for some methods
- Reformulation very successful and versatile in practice

Penalization Approach

$$\begin{array}{ll}
\displaystyle\min_{x,y,\lambda,s,t\geq 0} & g(x,y) + \pi \sum_i \left(s_i^T x_i + \lambda_i t_i\right) \\
\text{subject to} & h(y) \leq 0 \\
 & s_i = \nabla_{x_i} f_i(x,y) + \lambda_i^T \nabla_{x_i} c_i(x_i) \\
 & t_i = -c_i(x_i)
\end{array}$$

- Optimization problem satisfies constraint qualification
- Need to increase π

Relaxation Approach

$$
\begin{array}{ll}
\min\limits_{x,y,\lambda,s,t \geq 0} & g(x,y) \\
\text{subject to} & h(y) \leq 0 \\
& s_i = \nabla_{x_i} f_i(x,y) + \lambda_i^T \nabla_{x_i} c_i(x_i) \\
& t_i = -c_i(x_i) \\
& \sum\limits_i \left(s_i^T x_i + \lambda_i t_i \right) \leq \tau
\end{array}
$$

- Need to decrease τ

Limitations

- Multipliers may not exist
- Solvers can have a hard time computing solutions
  - Try different algorithms
  - Compute feasible starting point
- Stationary points may have descent directions
  - Checking for descent is an exponential problem
  - Strong stationary points found in certain cases
- Many stationary points – global optimization

Limitations

- Multipliers may not exist
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- Stationary points may have descent directions
  - Checking for descent is an exponential problem
  - Strong stationary points found in certain cases
- Many stationary points – global optimization
- Formulation of follower problem
  - Multiple solutions to Nash game
  - Nonconvex objective or constraints
  - Existence of multipliers

Part VI

Mixed Integer and Global Optimization

Global Optimization

I need to find the GLOBAL minimum!

- use any NLP solver (often work well!)
- use the multi-start trick from previous slides
- global optimization based on branch-and-reduce: `BARON`
  - constructs global underestimators
  - refines region by branching
  - tightens bounds by solving LPs
  - solve problems with 100s of variables
- "voodoo" solvers: genetic algorithm & simulated annealing
  no convergence theory ... usually worse than deterministic

Derivative-Free Optimization

My model does not have derivatives!

- Change your model ... good models have derivatives!
- pattern-search methods for min $f(x)$
  - evaluate $f(x)$ at stencil $x_k + \Delta M$
  - move to new best point
  - extend to NLP; some convergence theory h
  - matlab: `NOMADm.m`; parallel `APPSPACK`
- solvers based on building interpolating quadratic models
  - DFO project on `www.coin-or.org`
  - Mike Powell's `NEWUOA` quadratic model
- "voodoo" solvers: genetic algorithm & simulated annealing
  no convergence theory ... usually worse than deterministic

Optimization with Integer Variables

Mixed-Integer Nonlinear Program (MINLP)

- modeling discrete choices $\Rightarrow$ $0-1$ variables
- modeling integer decisions $\Rightarrow$ integer variables
  e.g. number of different stocks in portfolio (8-10)
  not number of beers sold at Goose Island (millions)

MINLP solvers:

- branch (separate $z_i = 0$ and $z_i = 1$) and cut
- solve millions of NLP relaxations: `MINLPBB`, `SBB`
- outer approximation: iterate MILP and NLP solvers
  `BONMIN (COIN-OR)` & `FilMINT` on NEOS

Portfolio Management

- N: Universe of asset to purchase
- x_i: Amount of asset i to hold
- B: Budget

$$\text{minimize} \;\; u(x) \quad \text{subject to} \; \sum_{i \in N} x_i = B, \quad x \geq 0$$

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$$\text{minimize } u(x) \quad \text{subject to } \sum_{i \in N} x_i = B, \quad x \geq 0$$

- Markowitz: $u(x) \stackrel{\text{def}}{=} -\alpha^T x + \lambda x^T Q x$
  - α: maximize expected returns
  - Q: variance-covariance matrix of expected returns
  - λ: minimize risk; aversion parameter

More Realistic Models

- $b \in \mathbb{R}^{|N|}$ of “benchmark” holdings
- Benchmark Tracking: $u(x) \stackrel{\text{def}}{=} (x - b)^T Q(x - b)$
  - Constraint on $\mathbb{E}$[Return]: $\alpha^T x \geq r$

More Realistic Models

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  - Constraint on $\mathbb{E}$[Return]: $\alpha^T x \geq r$
- Limit Names: $|i \in N \ : \ x_i > 0| \leq K$
  - Use binary indicator variables to model the implication $x_i > 0 \Rightarrow y_i = 1$
  - Implication modeled with variable upper bounds:

$$x_i \leq By_i \qquad \forall i \in N$$

  - $\sum_{i \in N} y_i \leq K$

Optimization Conclusions

Optimization is General Modeling Paradigm

- linear, nonlinear, equations, inequalities
- integer variables, equilibrium, control

AMPL (GAMS) Modeling and Programming Languages

- express optimization problems
- use automatic differentiation
- easy access to state-of-the-art solvers

Optimization Software

- open-source: COIN-OR, IPOPT, SOPLEX, & ASTROS (soon)
- current solver limitations on laptop:
  - 1,000,000 variables/constraints for LPs
  - 100,000 variables/constraints for NLPs/NCPs
  - 100 variables/constraints for global optimization
  - 500,000,000 variable LP on BlueGene/P