Introduction to Optimization

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[1]The nice slides were created by Sven Leyffer, Jorge More, and Todd Munson.

Outline: Six Topics

- ◇ Introduction
- ◇ Unconstrained optimization
  - Limited-memory variable metric methods
- ◇ Systems of Nonlinear Equations
  - Sparsity and Newton's method
- ◇ Automatic Differentiation
  - Computing sparse Jacobians via graph coloring
- ◇ Constrained Optimization
  - All that you need to know about KKT conditions
- ◇ Solving optimization problems
  - Modeling languages: AMPL and GAMS
  - NEOS

Topic 1: The Optimization Viewpoint

- Modeling
- Algorithms
- Software
- Automatic differentiation tools
- Application-specific languages
- High-performance architectures

Classification of Constrained Optimization Problems

$$\min \{ f(x) : x_l \le x \le x_u,\ c_l \le c(x) \le c_u \}$$

- Number of variables n
- Number of constraints m
- Number of linear constraints
- Number of equality constraints n_e
- Number of degrees of freedom $n - n_e$
- Sparsity of $c'(x) = (\partial_i c_j(x))$
- Sparsity of $\nabla_x^2 \mathcal{L}(x, \lambda) = \nabla^2 f(x) + \sum_{k=1}^m \nabla^2 c_k(x) \lambda_k$

Classification of Constrained Optimization Software

- Formulation
- Interfaces: MATLAB, AMPL, GAMS
- Second-order information options:
  - Differences
  - Limited memory
  - Hessian-vector products
- Linear solvers
  - Direct solvers
  - Iterative solvers
  - Preconditioners
- Partially separable problem formulation
- Documentation
- License

Life-Cycles Saving Problem

Maximize the utility

$$\sum_{t=1}^{T} \beta^t u(c_t)$$

where S_t are the saving, c_t is consumption, w_t are wages, and

$$S_{t+1} = (1 + r)S_t + w_{t+1} - c_{t+1}, \qquad 0 \le t < T$$

with $r = 0.2$ interest rate, $\beta = 0.9$, $S_0 = S_T = 0$, and

$$u(c) = -\exp(-c)$$

Assume that $w_t = 1$ for $t < R$ and $w_t = 0$ for $t \ge R$.

Question. What are the characteristics of the life-cycle problem?

Topic 2: Unconstrained Optimization

Augustin Louis Cauchy (August 21, 1789 – May 23, 1857)
Additional information at **Mac Tutor**
`www-history.mcs.st-andrews.ac.uk`

Unconstrained Optimization: Background

Given a continuously differentiable $f : \mathbb{R}^n \mapsto \mathbb{R}$ and

$$\min \{ f(x) : x \in \mathbb{R}^n \}$$

generate a sequence of iterates $\{x_k\}$ such that the gradient test

$$\|\nabla f(x_k)\| \le \tau$$

is eventually satisfied

Theorem. If $f : \mathbb{R}^n \mapsto \mathbb{R}$ is continuously differentiable and bounded below, then there is a sequence $\{x_k\}$ such that

$$\lim_{k \to \infty} \|\nabla f(x_k)\| = 0.$$

Exercise. Prove this result.

Unconstrained Optimization

What can I use if the gradient $\nabla f(x)$ is not available?

- Geometry-based methods: Pattern search, Nelder-Mead, ...
- Model-based methods: Quadratic, radial-basis models, ...

What can I use if the gradient $\nabla f(x)$ is available?

- Conjugate gradient methods
- Limited-memory variable metric methods
- Variable metric methods

Computing the Gradient

Hand-coded gradients

- ◇ Generally efficient
- ◇ Error prone
- ◇ The cost is usually less than 5 function evaluations

Difference approximations

$$\partial_i f(x) \approx \frac{f((x + he_i) - f(x)}{h_i}$$

- ◇ Choice of h_i may be problematic in the presence of noise.
- ◇ Costs n function evaluations
- ◇ Accuracy is about the $\varepsilon_f^{1/2}$ where ε_f is the noise level of f

Cheap Gradient via Automatic Differentiation

Code generated by automatic differentiation tools

- Accurate to full precision
- For the reverse mode the cost is $\Omega_T \, T\{f(x)\}$.
- In theory, $\Omega_T \le 5$.
- For the reverse mode the memory is proportional to the number of intermediate variables.

Exercise

Develop an order n code for computing the gradient of

$$f(x) = \prod_{k=1}^{n} x_k$$

Line Search Methods

A sequence of iterates $\{x_k\}$ is generated via

$$x_{k+1} = x_k + \alpha_k p_k,$$

where p_k is a descent direction at x_k, that is,

$$\nabla f(x_k)^T p_k < 0,$$

and α_k is determined by a line search along p_k.

Line searches

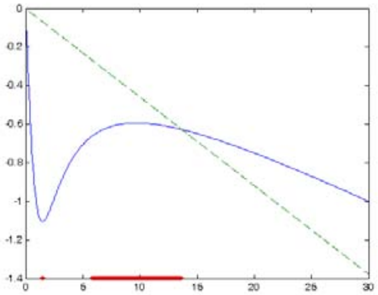
- Geometry-based: Armijo, ...
- Model-based: Quadratics, cubic models, ...

Powell-Wolfe Conditions on the Line Search

Given $0 \leq \mu < \eta \leq 1$, require that

$$f(x + \alpha p) \leq f(x) + \mu \, \alpha \nabla f(x_k)^T p_k \qquad \text{sufficent decrease}$$

$$|\nabla f(x + \alpha p)^T p| \leq \eta \, |\nabla f(x)^T p| \qquad \text{curvature condition}$$



Conjugate Gradient Algorithms

Given a starting vector x_0 generate iterates via

$$x_{k+1} = x_k + \alpha_k p_k$$
$$p_{k+1} = -\nabla f(x_k) + \beta_k p_k$$

where α_k is determined by a line search.

Three reasonable choices of β_k are ($g_k = \nabla f(x_k)$):

$$\beta_k^{FR} = \left(\frac{\|g_{k+1}\|}{\|g_k\|} \right)^2, \qquad \text{Fletcher-Reeves}$$

$$\beta_k^{PR} = \frac{\langle g_{k+1}, g_{k+1} - g_k \rangle}{\|g_k\|^2}, \qquad \text{Polak-Rivière}$$

$$\beta_k^{PR+} = \max\left\{ \beta_k^{PR}, 0 \right\}, \qquad \text{PR-plus}$$

Recommendations

But what algorithm should I use?

- If the gradient $\nabla f(x)$ is not available, then a model-based method is a reasonable choice. Methods based on quadratic interpolation are currently the best choice.
- If the gradient $\nabla f(x)$ is available, then a limited-memory variable metric method is likely to produce an approximate minimizer in the least number of gradient evaluations.
- If the Hessian is also available, then a state-of-the-art implementation of Newton's method is likely to produce the best results if the problem is large and sparse.

Topic 3: Newton's Method

Library of Congress

Sir Isaac Newton (January 4, 1643 – March 331, 1727)
Additional information at **Mac Tutor**
`www-history.mcs.st-andrews.ac.uk`

Motivation

Give a continuously differentiable $f : \mathbb{R}^n \mapsto \mathbb{R}^n$, solve

$$f(x) = \begin{pmatrix} f_1(x) \\ \vdots \\ f_n(x) \end{pmatrix} = 0$$

Linear models. The mapping defined by

$$L_k(s) = f(x_k) + f'(x_k)s$$

is a linear model of f near x_k, and thus it is sensible to choose s_k such that $L_k(s_k) = 0$ provided $x_k + s_k$ is near x_k.

Newton's Method

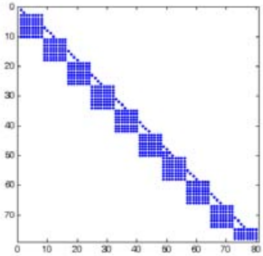
Given a starting point x_0, Newton's method generates iterates via

$$f'(x_k)s_k = -f(x_k), \qquad x_{k+1} = x_k + s_k.$$

Computational Issues

- How do we solve for s_k?
- How do we handle a (nearly) singular $f'(x_k)$?
- How do we enforce convergence if x_0 is not near a solution?
- How do we compute/approximate $f'(x_k)$?
- How accurately do we solve for s_k?
- Is the algorithm scale invariant?
- Is the algorithm mesh-invariant?

Sparsity



Assume that the Jacobian matrix is sparse, and let ρ_i be the number of non-zeroes in the i-th row of $f'(x)$.

- Sparse linear solvers can solve $f'(x)s = -f(x)$ in order ρ_A operations, where $\rho_A = \mathrm{avg}\{\rho_i^2\}$.
- Graph coloring techniques (see Topic 4) can compute or approximate the Jacobian matrix with ρ_M function evaluations where $\rho_M = \max\{\rho_i\}$

Topic 4: Automatic Differentiation

Gottfried Wilhelm Leibniz (July 1, 1646 – November 14, 1716)
Additional information at **Mac Tutor**
`www-history.mcs.st-andrews.ac.uk`

Computing Gradients and Sparse Jacobians

Theorem. Given $f : \mathbb{R}^n \mapsto \mathbb{R}^m$, automatic differentiation tools compute $f'(x)v$ at a cost comparable to $f(x)$

Tasks

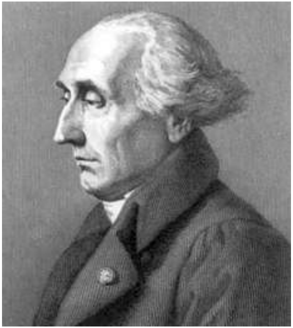
- Given $f : \mathbb{R}^n \mapsto \mathbb{R}^m$ with a sparse Jacobian, compute $f'(x)$ with $p \ll n$ evaluations of $f'(x)v$
- Given a partially separable $f : \mathbb{R}^n \mapsto \mathbb{R}$, compute $\nabla f(x)$ with $p \ll n$ evaluations of $\langle \nabla f(x), v \rangle$

Requirements:

$$T\{f'(x)\} \leq \Omega_T \, T\{f(x)\}, \qquad M\{\nabla f(x)\} \leq \Omega_M \, M\{f(x)\}$$

where $T\{\cdot\}$ is computing time and $M\{\cdot\}$ is memory.

Topic 5: Constrained Optimization



Joseph-Louis Lagrange (January 25, 1736 – April 10, 1813)
Additional information at **Mac Tutor**
`www-history.mcs.st-andrews.ac.uk`

Geometric Viewpoint of the KKT Conditions

For any closed set Ω, consider the abstract problem

$$\min\{f(x) : x \in \Omega\}$$

The tangent cone

$$T(x^*) = \left\{ v : v = \lim_{k\to\infty} \frac{x_k - x^*}{\alpha_k},\ x_k \in \Omega,\ \alpha_k \geq 0 \right\}$$

The normal cone

$$N(x^*) = \{ w : \langle w, v \rangle \leq 0,\ v \in T(x^*) \}$$

First order conditions

$$-\nabla f(x^*) \in N(x^*)$$

Computational Viewpoint of the KKT Conditions

In the case $\Omega = \{x \in \mathbb{R}^n : c(x) \geq 0\}$, define

$$C(x^*) = \left\{ w : w = \sum_{i=1}^{m} \lambda_i \left(-\nabla c_i(x^*)\right), \ \lambda_i \geq 0 \right\}$$

In general $C(x^*) \subset N(x^*)$, and under a **constraint qualification**

$$C(x^*) = N(x^*)$$

Hence, for some multipliers $\lambda_i \geq 0$,

$$\nabla f(x) = \sum_{i=1}^{m} \lambda_i \nabla c_i(x), \qquad \lambda_i \geq 0,$$

Constraint Qualifications

In the case where

$$\Omega = \{x \in \mathbb{R}^n : l \le c(x) \le u\}$$

the main two constraint qualifications are

Linear independence
The active constraint normals are positively linearly independent, that is, if

$$C_{\mathcal{A}} = (\nabla c_i(x) : c_i(x) \in \{l_i, u_i\})$$

then $C_{\mathcal{A}}$ has full rank.

Mangasarian-Fromovitz
The active constraint normals are positively linearly independent.

Lagrange Multipliers

For the general problem with 2-sided constraints

$$\min \{ f(x) : l \le c(x) \le u \}$$

the KKT conditions for a local minimizer are

$$\nabla f(x) = \sum_{i=1}^{m} \lambda_i \nabla c_i(x), \qquad l \le c(x) \le u,$$

where the multipliers satisfy complementarity conditions

- λ_i is unrestricted if $l_i = u_i$.
- $\lambda_i = 0$ if $c_i(x) \notin \{l_i, u_i\}$
- $\lambda_i \ge 0$ if $c_i(x) = l_i$
- $\lambda_i \le 0$ if $c_i(x) = u_i$

Lagrangians

The KKT conditions for the problem with constraints $l \le c(x) \le u$ can be written in terms of the Lagrangian

$$\mathcal{L}(x, \lambda) = f(x) - \sum_{i=1}^{m} \lambda_i c_i(x).$$

Examples.

The KKT conditions for the equality-constrained $c(x) = 0$ are

$$\nabla_x \mathcal{L}(x, \lambda) = 0, \qquad c(x) = 0.$$

The KKT conditions for the inequality-constrained $c(x) \ge 0$ are

$$\nabla_x \mathcal{L}(x, \lambda) = 0, \qquad c(x) \ge 0, \quad \lambda \ge 0, \quad \lambda \perp c(x)$$

where $\lambda \perp c(x)$ means that $\lambda_i c_i(x) = 0$.

Newton's Method: Equality-Constrained Problems

The KKT conditions for the equality-constrained problem $c(x) = 0$,

$$\nabla_x \mathcal{L}(x, \lambda) = \nabla f(x) - \sum_{i=1}^{m} \lambda_i \nabla c_i(x) = 0, \qquad c(x) = 0.$$

are a system of $n + m$ nonlinear equations.

Newton's method for this system can be written as

$$x_+ = x + s_x, \qquad \lambda_+ = \lambda + s_\lambda$$

where

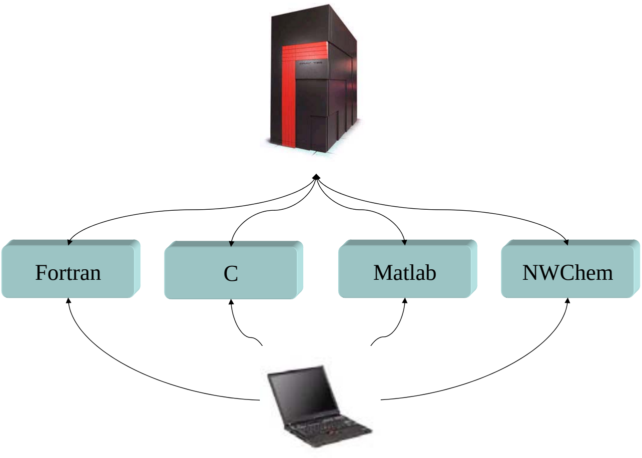
$$\begin{pmatrix} \nabla_x^2 \mathcal{L}(x, \lambda) & -\nabla c(x) \\ \nabla c(x)^T & 0 \end{pmatrix} \begin{pmatrix} s_x \\ s_\lambda \end{pmatrix} = - \begin{pmatrix} \nabla_x \mathcal{L}(x, \lambda) \\ c(x) \end{pmatrix}$$

Topic 6: Solving Optimization Problems

Environments

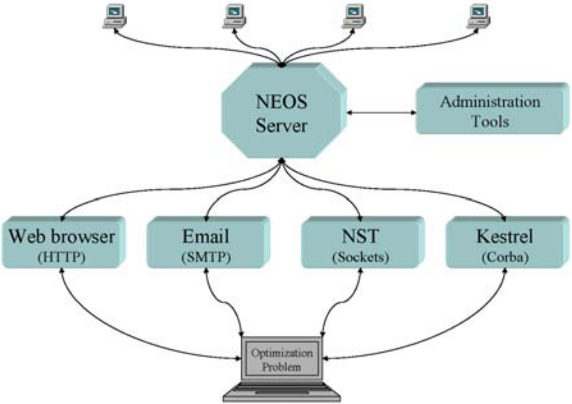
- Modeling Languages: AMPL, GAMS
- NEOS

The Classical Model



The NEOS Model

A collaborative research project that represents the efforts of the optimization community by providing access to 50+ solvers from both academic and commercial researchers.



NEOS: Under the Hood

- Modeling languages for optimization: AMPL, GAMS
- Automatic differentiation tools: ADIFOR, ADOL-C, ADIC
- Python
- Optimization solvers (50+)
  - Benchmark, GAMS/AMPL (Multi-Solvers)
  - MINLP, FortMP, GLPK, Xpress-MP, ...
  - CONOPT, FILTER, IPOPT, KNITRO, LANCELOT, LOQO, MINOS, MOSEK, PATHNLP, PENNON, SNOPT
  - BPMPD, FortMP, MOSEK, OOQP, Xpress-MP, ...
  - CSDP, DSDP, PENSDPP, SDPA, SeDuMi, ...
  - BLMVM, L-BFGS-B, TRON, ...
  - MILES, PATH
  - Concorde

Life-Cycles Saving Problem

Maximize the utility

$$\sum_{t=1}^{T} \beta^t u(c_t)$$

where S_t are the saving, c_t is consumption, w_t are wages, and

$$S_{t+1} = (1+r)S_t + w_{t+1} - c_{t+1}, \qquad 0 \leq t < T$$

with $r = 0.2$ interest rate, $\beta = 0.9$, $S_0 = S_T = 0$, and

$$u(c) = -\exp(-c)$$

Assume that $w_t = 1$ for $t < R$ and $w_t = 0$ for $t \geq R$.

Life-Cycles Saving Problem: Model

```
param T integer;                # Number of periods
param R integer;                # Retirement
param beta;                     # Discount rate
param r;                        # Interest rate
param S0;                       # Initial savings
param ST;                       # Final savings
param w{1..T};                  # Wages

var S{0..T};                    # Savings
var c{0..T};                    # Consumption

maximize utility: sum{t in 1..T} beta^t*(-exp(-c[t]));
subject to budget {t in 0..T-1}: S[t+1] = (1+r)*S[t] + w[t+1] - c[t+1];
subject to savings {t in 0..T}: S[t] >= 0.0;
subject to consumption {t in 1..T}: c[t] >= 0.0;

subject to bc1: S[0] = S0;
subject to bc2: S[T] = ST;
subject to bc3: c[0] = 0.0;
```

Life-Cycles Saving Problem: Data

```
param T    := 100;
param R    := 60;
param beta := 0.9;
param r    := 0.2;
param S0   := 0.0;
param ST   := 0.0;

# Wages

let {i in 1..R} w[i] := 1.0;
let {i in R..T} w[i] := 0.0;

let {i in 1..R} w[i] := (i/R);
let {i in R..T} w[i] :=  (i - T)/(R - T);
```

Life-Cycles Saving Problem: Commands

```
option show_stats 1;

option solver "filter";
option solver "ipopt";
option solver "knitro";
option solver "loqo";

model;
include life.mod;

data;
include life.dat;

solve;

printf {t in 0..T}: "%21.15e  %21.15e\n", c[t], S[t] > cops.dat;
```