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School of Mathematics



Massively Parallel Implementation of Interior Point Methods for Very Large Scale Optimization

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joint work with Andreas Grothey

Outline

- Optimality Conditions for LP
- Simplex Method vs Interior Point Method
- IPM Framework: LP, QP, NLP
- Features of Logarithmic Function
- From Sparse to Block-Sparse Problems
- Structured Very Large Optimization Problems
- Object-Oriented Parallel Solver
- Financial Planning Problems: Asset/Liability Models
- Conclusions

Primal-Dual Pair of Linear Programs

Primal Dual
min
$$c^T x$$
 max $b^T y$
s.t. $Ax = b$, s.t. $A^T y + s = c$,
 $x \ge 0$; $s \ge 0$.

Lagrangian

$$L(x,y) = c^T x - y^T (Ax - b).$$

Optimality Conditions

$$Ax = b,$$

$$A^{T}y + s = c,$$

$$XSe = 0, \quad (\text{ i.e., } x_{j} \cdot s_{j} = 0 \quad \forall j),$$

$$x \ge 0,$$

$$s \ge 0,$$

where $X = diag\{x_1, \dots, x_n\}, S = diag\{s_1, \dots, s_n\}$ and $e = (1, 1, \dots, 1) \in \mathbb{R}^n$.

Complementarity

Recall that the **Simplex Method** works with a partitioned formulation:

LP constraint matrix A = [B, N], B is nonsingular primal variables $x = (x_B, x_N),$ reduced costs $s = (s_B, s_N).$

The simplex method maintains the complementarity of primal and dual solutions:

$$x_j \cdot s_j = 0 \quad \forall j = 1, 2, \dots, n.$$

For **basic** variables, $s_B = 0$ and

$$(x_B)_j \cdot (s_B)_j = 0 \quad \forall j \in \mathcal{B}.$$

For **non-basic** variables, $x_N = 0$ hence

$$(x_N)_j \cdot (s_N)_j = 0 \quad \forall j \in \mathcal{N}.$$

What's wrong with the Simplex Method?

A **vertex** is defined by a set of n equations:

$$\begin{bmatrix} B & N \\ 0 & I_{n-m} \end{bmatrix} \begin{bmatrix} x_B \\ x_N \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}.$$

The linear program with m constraints and n variables $(n \ge m)$ has at most

$$N_V = \begin{pmatrix} n \\ m \end{pmatrix} = \frac{n!}{m!(n-m)!}$$

vertices and the simplex method can make a non-polynomial number of iterations to reach the optimality.

V. Klee and G. Minty's example LP: simplex method needs 2^n iterations. How good is the simplex algorithm, in: Inequalities-III, O. Shisha, ed., Academic Press, 1972, 159–175.

First Order Optimality Conditions



Theory: IPMs converge in $\mathcal{O}(\sqrt{n})$ or $\mathcal{O}(n)$ iterations **Practice:** IPMs converge in $\mathcal{O}(\log n)$ iterations ... but one iteration may be expensive!



The minimization of $-\sum_{j=1}^{n} \ln x_j$ is equivalent to the maximization of the product of distances from all hyperplanes defining the positive orthant: it prevents all x_j from approaching zero.

Use Logarithmic Barrier

Primal Problem

$$\begin{array}{ll} \min & c^T x\\ \text{s.t.} & Ax = b,\\ & x \ge 0; \end{array}$$

Dual Problem

$$\begin{array}{ll} \max & b^T y \\ \text{s.t.} & A^T y + s = c, \\ & s \ge 0. \end{array}$$

Primal Barrrier Problem

min
$$c^T x - \sum_{j=1}^n \ln x_j$$

s.t. $Ax = b$,

Dual Barrier Problem

max
$$b^T y + \sum_{j=1}^n \ln s_j$$

s.t. $A^T y + s = c$,

Primal Barrier Program:min
$$c^T x - \mu \sum_{j=1}^n \ln x_j$$
s.t. $Ax = b.$ Lagrangian: $L(x, y, \mu) = c^T x - y^T (Ax - b) - \mu \sum_{j=1}^n \ln x_j,$ Stationarity: $\nabla_x L(x, y, \mu) = c - A^T y - \mu X^{-1} e = 0$ Denote: $s = \mu X^{-1} e,$ i.e. $XSe = \mu e.$

The First Order Optimality Conditions are:

$$Ax = b,$$

$$A^{T}y + s = c,$$

$$XSe = \mu e$$

$$(x, s) > 0.$$

Newton Method

The first order optimality conditions for the barrier problem form a large system of nonlinear equations E(x,y,z) = 0

$$F(x, y, s) = 0,$$

where $F : \mathcal{R}^{2n+m} \mapsto \mathcal{R}^{2n+m}$ is an application defined as follows:

$$F(x, y, s) = \begin{bmatrix} Ax - b \\ A^T y + s - c \\ XSe - \mu e \end{bmatrix}.$$

Actually, the first two terms of it are <u>linear</u>; only the last one, corresponding to the complementarity condition, is <u>nonlinear</u>.

For a given point (x, y, s) we find the Newton direction $(\Delta x, \Delta y, \Delta s)$ by solving the system of linear equations:

$$\begin{bmatrix} A & 0 & 0 \\ 0 & A^T & I \\ S & 0 & X \end{bmatrix} \cdot \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta s \end{bmatrix} = \begin{bmatrix} b - Ax \\ c - A^Ty - s \\ \mu e - XSe \end{bmatrix}$$

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IPM for QP
min
$$c^T x + \frac{1}{2} x^T \mathbf{Q} x \rightarrow \min c^T x + \frac{1}{2} x^T \mathbf{Q} x - \mu \sum_{j=1}^n \ln x_j$$

s.t. $Ax = b$, s.t. $Ax = b$,
 $x \ge 0$.

The first order conditions (for the barrier problem)

$$Ax = b,$$

$$A^{T}y + s - \mathbf{Q}x = c,$$

$$XSe = \mu e.$$

Newton direction

$$\begin{bmatrix} A & 0 & 0 \\ -\mathbf{Q} & A^T & I \\ S & 0 & X \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta s \end{bmatrix} = \begin{bmatrix} \xi_p \\ \xi_d \\ \xi_\mu \end{bmatrix} = \begin{bmatrix} b - Ax \\ c - A^Ty - s + \mathbf{Q}x \\ \mu e - XSe \end{bmatrix}$$

Augmented system

$$\begin{bmatrix} -\mathbf{Q} - \Theta^{-1} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} \xi_d - X^{-1}\xi_\mu \\ \xi_p \end{bmatrix}$$

IPM for NLP s.t. g(x) + z = 0 $z \ge 0.$ $\min f(x) - \mu \sum_{i=1}^{m} \ln z_i$ s.t. g(x) + z = 0m

Lagrangian: $L(x, y, z, \mu) = f(x) + y^T(g(x) + z) - \mu \sum_{i=1}^{m} \ln z_i.$

The first order conditions (for the barrier problem)

$$abla f(x) +
abla g(x)^T y = 0, \\
g(x) + z = 0, \\
YZe = \mu e.$$

Newton direction

$$\begin{bmatrix} Q(x,y) & A(x)^T & 0 \\ A(x) & 0 & I \\ 0 & Z & Y \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta z \end{bmatrix} = \begin{bmatrix} -\nabla f(x) - A(x)^T y \\ -g(x) - z \\ \mu e - Y Z e \end{bmatrix}$$

Augmented system

$$\begin{bmatrix} Q(x,y) & A(x)^T \\ A(x) & -ZY^{-1} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} -\nabla f(x) - A(x)^T y \\ -g(x) - \mu Y^{-1} e \end{bmatrix} \text{ where } \begin{array}{c} A(x) = \nabla g \\ Q(x,y) = \nabla_{xx}^2 L \end{array}$$

Optimality Conditions:

Newton Direction:

Ax = b		
$A^T y + s = c$	$\begin{bmatrix} A & 0 & 0 \\ 0 & AT & I \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta x \end{bmatrix} \begin{bmatrix} \zeta p \\ \zeta \end{bmatrix}$	
$XSe = \mu e$	$\begin{vmatrix} 0 & A & I \\ S & 0 & Y \end{vmatrix} \begin{vmatrix} \Delta y \\ \Delta c \end{vmatrix} = \begin{vmatrix} \zeta_d \\ \zeta \end{vmatrix}$	
$x, s \geq 0.$	$\begin{bmatrix} \mathcal{S} & 0 & \mathcal{A} \end{bmatrix} \begin{bmatrix} \Delta S \end{bmatrix} \begin{bmatrix} \zeta \mu \end{bmatrix}$	

Linear Algebra involves an (ill-conditioned) scaling matrix $\Theta = XS^{-1}$.

Augmented System vs Normal Equations

 $\begin{array}{ccc} \mathbf{LP} & \mathbf{QP} & \mathbf{NLP} \\ \begin{bmatrix} \Theta^{-1} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} f \\ d \end{bmatrix} & \begin{bmatrix} Q + \Theta^{-1} & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} f \\ d \end{bmatrix} & \begin{bmatrix} Q(x,y) & A(x)^T \\ A(x) & -ZY^{-1} \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \end{bmatrix} = \begin{bmatrix} f \\ d \end{bmatrix} \\ (A\Theta A^T) \Delta y = g & (A(Q + \Theta^{-1})^{-1}A^T) \Delta y = g & (AQ^{-1}A^T + ZY^{-1}) \Delta y = g \end{array}$

Direct Methods: Symmetric LDL^T Factorization

Indefinite	Quasidefinite	Positive Definite		
$H = \begin{bmatrix} Q & A^T \\ A & 0 \end{bmatrix}$	$H = \begin{bmatrix} Q & A^T \\ A & -R \end{bmatrix}$	$H = AQ^{-1}A^T$		
2×2 pivots needed	1×1 pivots (any sign)	1×1 pivots (positive)		
$\begin{bmatrix} 0 & a \\ a & 0 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & a \\ a & d \end{bmatrix}$	strongly factorizable	easy		

Vanderbei, *SIOPT* (1995): Symmetric QDFM's are strongly factorizable. For any quasidefinite matrix there exists a **Cholesky-like** factorization

$$\bar{H} = LDL^T,$$

where D is **diagonal** but **not positive definite**: D has n negative pivots and m positive pivots.

OOPS (Object Oriented Parallel Solver)

- Mantra: "Truly large scale problems are not only sparse but structured" (due to e.g. dynamics, uncertainty, spatial distribution etc.)
- Exploiting structure is key to building efficient IPMs for large problems:
 - Faster linear algebra
 - Reduced memory use
 - Possibility to exploit (massive) parallelism
 - We assume that structure is known! \Rightarrow no automatic detection.
- OOPS currently solves LP/QP problems.
- Simple sequential-QP scheme solves nonlinear ALM models

OOPS: (Block) Elimination Trees:

Elimination tree orders rows/columns for elimination with minimum fill-in:



Elimination Tree can be extended to Block Elimination Tree





 \Rightarrow Organisation of linear algebra, Parallelism

Minimum Degree Ordering



Minimum degree ordering:

choose a diagonal element corresponding to a row with the \underline{min} number of nonzeros. Permute rows and columns of H accordingly.

From Sparsity to Block-Sparsity:

Apply minimum degree ordering to (sparse) blocks:



choose a diagonal block-pivot corresponding to a block-row with the \underline{min} number of blocks.

Permute block-rows and block-columns of H accordingly.

OOPS: Object-oriented linear algebra implementation

- Every node in *block elimination tree* has own linear algebra implementation (depending on its type)
- Implementation is realisation of an abstract linear algebra interface.
- Different implementations for different structures are available.



 \Rightarrow Rebuild *block elimination tree* with matrix interface structures

Application: Asset and Liability Management Problem

- A set of assets $\mathcal{J} = \{1, ..., J\}$ is given (e.g. bonds, stock, real estate).
- At every stage t = 0, ..., T-1 we can buy or sell different assets.
- The return of asset j at stage t is *uncertain* (but distribution is known).

We have to make investment decisions: what to buy or sell, at which time stage Objectives:

 \Rightarrow

- maximize the final wealth
- minimize the associated risk

- \Rightarrow Stochastic Program:
 - Can formulate deterministic equivalent problem
 - standard QP, but huge

ALM: Structure of matrices A and Q:



ALM: Structure of Augmented System matrix:



ALM: Largest Problem Attempted

- Optimization of 21 assets (stock market indices) over 7 time stages.
- Using multistage stochastic programming Scenario tree geometry: $128-30-16-10-5-4 \Rightarrow 16$ million scenarios.
- Scenario Tree generated using geometric Brownian motion.
- \Rightarrow 1.01 billion variables, 353 million constraints

Issues for Massive Parallelism

- Sparsity of multilevel linear Algebra
- Memory Management



BlueGene (Edinburgh, Scotland)

- 2048 Processors
- 0.7GHz, 256Mb
- 4.7 TFlops
- **#64** in top500.org list

HPCx (Daresbury, England)

- 1600 IBM Power-4 Processors
- 1.7GHz, 800Mb
- 6.2 TFlops
- #45 in top500.org list



Sparsity of Linear Algebra I

- In ALM problems matrices up to \approx 500.000 1.000.000 variables can be treated as unstructured sparse matrices
- Problem has: -128 first level nodes with 10.000.000 variables each.
 - 3840 second level nodes with 350.000 variables each.
 - \Rightarrow need to decompose problem at second level (with 1280 processors \Rightarrow 3 blocks per processor)



Sparsity of Linear Algebra II



. . .

- $-63 + 128 \times 63 = 8127$ columns for Schur-complement
- Prohibitively expensive

- Need facility to exploit nested structure
 - Need to be careful that Schur-complement calculations stay sparse on second level

Memory Management

- Data for problem requires > 1GB of memory.
 ⇒ need to split information between processors
- To each node in block-elimination tree a set of processors is assigned
- Linear Algebra is implemented so that processors communicate when needed

Distribution of leading matrix blocks among processors implies

- Distribution of subordinate blocks
- Distribution of row/column vector contributions



Results (ALM: Mean-Variance QP formulation):

Problem	Stages	Blk	Assets	Scenarios	Constraints	Variables	iter	time	procs	machine
ALM8	7	128	6	12.831.873	64.159.366	153.982.477	42	3923	512	BlueGene
ALM9	7	64	14	6.415.937	96.239.056	269.469.355	39	4692	512	BlueGene
ALM10	7	128	13	12.831.873	179.646.223	500.443.048	45	6089	1024	BlueGene
ALM11	7	128	21	16.039.809	352.875.799	1.010.507.968	53	3020	1280	HPCx

The problem with

- 353 million of constraints
- 1 billion of variables

solved in 50 minutes using 1280 procs.

Object-Oriented Parallel Solver (OOPS): http://www.maths.ed.ac.uk/~gondzio/parallel/solver.html

References:

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- J. Gondzio and A. Grothey, *Reoptimization with the primal-dual interior point method*, SIAM J. on Optimization 13 (2003) pp 842-864.
- J. Gondzio and A. Grothey, *Parallel interior point solver for structured quadratic programs: application to financial planning problems*, Tech. Rep. MS-03-001, School of Maths, University of Edinburgh, April 2003 (to appear in **Annals of OR**).
- J. Gondzio and A. Grothey, *Solving nonlinear portfolio optimization problems with the primal-dual interior point method*, Tech. Rep. MS-04-001, School of Maths, University of Edinburgh, May 2004.
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Conclusions:

- Interior Point Methods are the key optimization technique.
- The theory of IPMs is well understood.
- IPMs demonstrate spectacular efficiency.
- Today IPMs can solve problems of dimension 10^9 .

IPMs are well-suited to exploit parallelism

Thank you for your attention!

Interior-Point Framework The logarithmic barrier

 $-\ln x_j$

added to the objective in the optimization problem prevents variable x_j from approaching zero and "replaces" the inequality

 $x_j \ge 0.$

Derive the **first order optimality conditions** for the primal barrier problem:

$$Ax = b,$$

$$A^Ty + s = c,$$

$$XSe = \mu e,$$

and apply **Newton method** to solve this system of nonlinear equations.

Actually, we fix the barrier parameter μ and make only **one** (damped) Newton step towards the solution of FOC. We do not solve the current FOC exactly. Instead, we immediately reduce the barrier parameter μ (to ensure progress towards optimality) and repeat the process.

Central Trajectory

Parameter μ controls the distance to optimality.

$$c^{T}\!x-b^{T}\!y=c^{T}\!x-x^{T}\!A^{T}\!y=x^{T}\!(c-A^{T}\!y)=x^{T}\!s=n\mu.$$

Analytic center (μ -center): a (unique) point

 $(x(\mu),y(\mu),s(\mu)), \quad x(\mu)>0, \ s(\mu)>0$

that satisfies the **first order optimality conditions**.

The path

 $\{(x(\mu), y(\mu), s(\mu)): \mu > 0\}$

is called the **primal-dual central trajectory**.

Follow the Central Path

$$\begin{aligned} Ax &= b, \\ A^T y + s &= c, \\ XSe &\approx \mu e, \quad \text{i.e.} \quad \|XSe - \mu e\| \leq \theta \mu, \end{aligned}$$

where $\theta \in (0, 1)$ and the barrier μ satisfies $x^T s = n\mu$.



Progress to optimality

Reduce the barrier: $\mu^{k+1} = \sigma \mu^k$, where $\sigma = 1 - \beta / \sqrt{n}$ for some $\beta \in (0, 1)$. Compute Newton direction:

$$\begin{bmatrix} A & 0 & 0 \\ 0 & A^T & I \\ S & 0 & X \end{bmatrix} \cdot \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta s \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \sigma \mu e - XSe \end{bmatrix},$$

and make step.

At the new iterate $(x^{k+1}, y^{k+1}, s^{k+1}) = (x^k, y^k, s^k) + (\Delta x^k, \Delta y^k, \Delta s^k)$ duality gap is reduced $1 - \beta/\sqrt{n}$ times.

Note that since at one iteration duality gap is reduced $1 - \beta/\sqrt{n}$ times, after \sqrt{n} iterations the reduction becomes:

$$(1 - \beta / \sqrt{n})^{\sqrt{n}} \approx e^{-\beta}.$$

After $C \cdot \sqrt{n}$ iterations, the reduction is $e^{-C\beta}$. For sufficiently large constant C the duality gap becomes arbitrarily small. Hence this algorithm has complexity $\mathcal{O}(\sqrt{n})$.

$\mathcal{O}(\sqrt{n})$ Complexity Result Theorem

Given $\epsilon > 0$, suppose that a feasible starting point $(x^0, y^0, s^0) \in N_2(0.1)$ satisfies

$$(x^0)^T s^0 = n\mu^0$$
, where $\mu^0 \le 1/\epsilon^{\kappa}$,

for some positive constant κ .

Then there exists an index K with $K = \mathcal{O}(\sqrt{n} \ln(1/\epsilon))$ such that

$$\mu^k \le \epsilon, \quad \forall k \ge K.$$

Interior Point Methods

• Fiacco & McCormick (1968)

handling inequality constraints - logarithmic barrier; minimization with inequality constraints replaced by a sequence of unconstrained minimizations

• Lagrange (1788)

handling equality constraints - multipliers; minimization with equality constraints replaced by unconstrained minimization

• Newton (1687)

solving unconstrained minimization problems;

Marsten, Subramanian, Saltzman, Lustig and Shanno:

"Interior point methods for linear programming: Just call Newton, Lagrange, and Fiacco and McCormick!", *Interfaces* 20 (1990) No 4, pp. 105–116.



From Sparsity to Block-Sparsity:



Object-Oriented Parallel Solver \Rightarrow problems of size $10^6, 10^7, 10^8, 10^9, ...$

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- G. & Grothey, AOR (to appear).