DM587

Scientific Programming

Linear Programming

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

Outline

Outline

Closed Model

- Economic system consisting of a finite number of industries, $1, 2, \ldots, k$.
- Over some fixed period of time, each industry produces output of some good or service that is completely utilized in a predetermined manner by the k industries.
- Find suitable prices to be charged for these k outputs so that for each industry, total expenditures equal total income.
- Such a price structure represents an equilibrium position for the economy.

Closed Model

Three homeowners – a carpenter, an electrician, and a plumber – agree to make repairings in their three homes. They agree to work a total of 10 days each according to the following schedule:

	Work Performed by		
	Carpenter	**Electrician**	**Plumber**
Days of Work in Home of Carpenter	2	1	6
Days of Work in Home of Electrician	4	5	1
Days of Work in Home of Plumber	4	4	3

For tax purposes, they must report and pay each other a reasonable daily wage, even for the work each does on his or her own home.

Their normal daily wages are about \$100, but they agree to adjust their respective daily wages so that each homeowner will come out even—that is, so that the total amount paid out by each is the same as the total amount each receives. What should be the prices of their work?

Closed Model

- $$\begin{array}{rcrcrcr} 2p_1 & + & p_2 & + & 6p_3 & = & 10p_1 \\ 4p_1 & + & 5p_2 & + & p_3 & = & 10p_2 \\ 4p_1 & + & 4p_2 & + & 3p_3 & = & 10p_3 \end{array}$$
- $(I - A)\mathrm{p} = \mathrm{p}$. If $\det(I - A) \neq 0$ then non trivial solution. Moreover, it can be shown that for exchange matrices A that are stochastic matrices the solution p is such that its elements are non-negative and if A^m are positive for all m positive integer then all p entries are positive.

Open Model

- Consider a market with n industries producing n different commodities.
- The market is interdependent, meaning that each industry requires input from the other industries and possibly even its own commodity.
- In addition, there is an outside demand for each commodity that has to be satisfied.
- We wish to determine the amount of output of each industry which will satisfy all demands exactly; that is, both the demands of the other industries and the outside demand.

Open Model

- Let $n = 3$ and let a_{ij} indicate the amount of commodity i, $i = 1, 2, 3$ necessary to produce one unit of commodity j, $j = 1, 2, 3$.

- a_{ij} are given in monetary terms:
  a_{ij} cost of the commodity i necessary to produce one unit profit of commodity j.
  $\rightsquigarrow$ Hence, we will assume that $a_{ij} \geq 0$
  Example: to produce an amount of commodity j worth 100 dkk, one needs an amount of commodity i worth 30 dkk.

  For the sake of simplicity we scale all these values such that the profit of each commodity is 1 unity of currency.

  $\rightsquigarrow$ Hence, for each commodity j its production is not profitable unless

$$\sum_{i=1}^{3} a_{ij} < 1.$$

- d_i be the demand of commodity i expressed in units of currency.

For each commodity, the outside demand is covered by the production of the commodity after the subtraction of the amount of commodity that has to go in the other industries and the amount that has to go in the same industry.
Hence:

$$x_i - \sum_{j=1}^{n} a_{ij} x_j = d_i$$

For $n = 3$ we have:

$$\begin{aligned} x_1 - a_{11}x_1 - a_{12}x_2 - a_{13}x_3 &= d_1 \\ x_2 - a_{21}x_1 - a_{22}x_2 - a_{23}x_3 &= d_2 \\ x_3 - a_{31}x_1 - a_{32}x_2 - a_{33}x_3 &= d_3 \end{aligned}$$

In matrix terms:

$$I\mathrm{x} - A\mathrm{x} = \mathrm{d} \qquad \text{or} \qquad (I - A)\mathrm{x} = \mathrm{d}$$

which is a system of linear equations. To make sense the solution x must be non-negative. It can be shown that under the conditions expressd above the solution to the system is unique and non-negative.

Open Model

- Unique non-negative solution for x if and only if $(I - A)^{-1}$ exists and $(I - A)^{-1} \geq 0$.
- The matrix A such that $(I - A)^{-1}$ exists and $(I - A)^{-1} \geq 0$ is called productive.
- The matrix A is productive $\iff$ there exists $x \geq 0$ such that $x > Ax$
  $\iff \sum_{j=1}^{n} a_{ij} < 1$ (row sums)
  that is, there is some production plan such that each industry produces (monetarily) more than it consumes.
- A matrix is productive $\iff \sum_{i=1}^{m} a_{ij} < 1$ (column sums)
  that is, the jth industry is profitable if the total value of the outputs of all m industries needed to produce one unit of value of output of the industry j is less than one.

Decision Support Tools

- So far we considered a full economic system (country, region) and the decision making from the point of view of a Government planning
  IO Models and Linear Systems of Equations

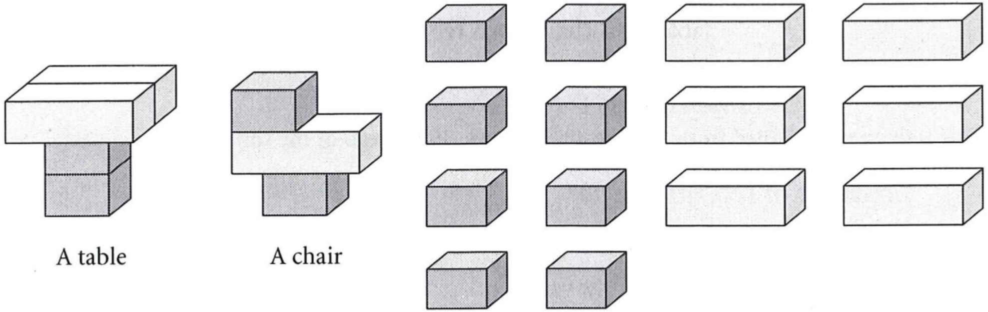
- Now, let's consider the Planning of Activities by a single Firm. Eg: Supply chain management, logistics, production scheduling
  Linear Programming

A firm can produce their items in many different ways. The planning problem is characterized by a large number of feasible ways of providing the same output.

Outline

Production Planning

Suppose a company produces only tables and chairs.
A table is made of 2 large Lego pieces and 2 small pieces, while a chair is made of 1 large and 2 small pieces.
The resources available are 8 small and 6 large pieces.



The profit for a table is 1600 dkk and for a chair 1000 dkk. What product mix maximizes the company's profile using the available resources?

Mathematical Model

	Tables	Chairs	Capacity
Small Pieces	2	2	8
Large Pieces	2	1	6
Profit	16	10	

Decision Variables

$x_1 \geq 0$ units of small pieces
$x_2 \geq 0$ units of large pieces

Object Function

$\max\ 16x_1 + 10x_2$ maximize profit

Constraints

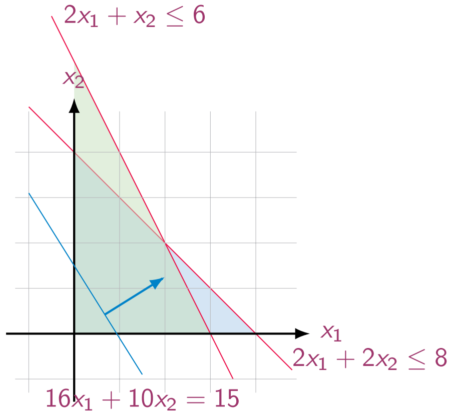
$$\begin{array}{rcrcll} 2x_1 & + & 2x_2 & \leq & 8 & \text{small pieces capacity} \\ 2x_1 & + & x_2 & \leq & 6 & \text{large pieces capacity} \end{array}$$

Mathematical Model

Materials A and B
Products 1 and 2

$$\begin{array}{rrcrcl} \max & 16x_1 & + & 10x_2 & & \\ & 2x_1 & + & 2x_2 & \leq & 8 \\ & 2x_1 & + & x_2 & \leq & 6 \\ & & & x_1 & \geq & 0 \\ & & & x_2 & \geq & 0 \end{array}$$

Graphical Representation:



Resource Allocation - General Model

Managing a production facility

$1, 2, \ldots, n$	products
$1, 2, \ldots, m$	materials
b_i	units of raw material at disposal
a_{ij}	units of raw material i to produce one unit of product j
σ_j	market price of unit of jth product
ρ_i	prevailing market value for material i
$c_j = \sigma_j - \sum_{i=1}^{n} \rho_i a_{ij}$	profit per unit of product j
x_j	amount of product j to produce

$$\begin{array}{rrcrcrcccrcl}
\max & c_1x_1 & + & c_2x_2 & + & c_3x_3 & + & \ldots & + & c_nx_n & = & z \\
\text{subject to} & a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + & \ldots & + & a_{1n}x_n & \leq & b_1 \\
 & a_{21}x_1 & + & a_{22}x_2 & + & a_{23}x_3 & + & \ldots & + & a_{2n}x_n & \leq & b_2 \\
 & \ldots & & & & & & & & & & \\
 & a_{m1}x_1 & + & a_{m2}x_2 & + & a_{m3}x_3 & + & \ldots & + & a_{mn}x_n & \leq & b_m \\
 & & & & & & & & & x_1, x_2, \ldots, x_n & \geq & 0
\end{array}$$

Notation

$$
\begin{array}{rrcrcrcccrcl}
\text{max} & c_1x_1 & + & c_2x_2 & + & c_3x_3 & + & \dots & + & c_nx_n & = & z \\
\text{s.t.} & a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + & \dots & + & a_{1n}x_n & \leq & b_1 \\
 & a_{21}x_1 & + & a_{22}x_2 & + & a_{23}x_3 & + & \dots & + & a_{2n}x_n & \leq & b_2 \\
 & \dots & & & & & & & & & & \\
 & a_{m1}x_1 & + & a_{m2}x_2 & + & a_{m3}x_3 & + & \dots & + & a_{mn}x_n & \leq & b_m \\
 & & & & & & & \multicolumn{3}{r}{x_1, x_2, \dots, x_n} & \geq & 0
\end{array}
$$

$$
\begin{array}{rrl}
\text{max} & \sum_{j=1}^{n} c_jx_j & \\
 & \sum_{j=1}^{n} a_{ij}x_j & \leq b_i, \quad i = 1, \dots, m \\
 & x_j & \geq 0, \quad j = 1, \dots, n
\end{array}
$$

In Matrix Form

$$
\begin{array}{rcccccccccl}
\max & c_1x_1 & + & c_2x_2 & + & c_3x_3 & + & \ldots & + & c_nx_n & = z \\
\text{s.t.} & a_{11}x_1 & + & a_{12}x_2 & + & a_{13}x_3 & + & \ldots & + & a_{1n}x_n & \leq b_1 \\
 & a_{21}x_1 & + & a_{22}x_2 & + & a_{23}x_3 & + & \ldots & + & a_{2n}x_n & \leq b_2 \\
 & \ldots & & & & & & & & & \\
 & a_{m1}x_1 & + & a_{m2}x_2 & + & a_{m3}x_3 & + & \ldots & + & a_{mn}x_n & \leq b_m \\
 & & & & & & & & & x_1, x_2, \ldots, x_n & \geq 0
\end{array}
$$

$$c^T = \begin{bmatrix} c_1 & c_2 & \ldots & c_n \end{bmatrix}$$

$$
\begin{array}{rcl}
\max \quad z & = & c^T x \\
Ax & \leq & b \\
x & \geq & 0
\end{array}
$$

$$A = \begin{bmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & & & \\ a_{31} & a_{32} & \ldots & a_{mn} \end{bmatrix}, x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

Vector and Matrices in Excel

$$\sum_{j=1}^{n} c_j = c_1 + c_2 + \ldots + c_n$$

$$\mathtt{SUM(B5:B14)}$$

Scalar product

$$\begin{aligned} \mathrm{u} \cdot \mathrm{v} &= u_1 v_1 + u_2 v_2 + \ldots + u_n v_n \\ &= \sum_{j=1}^{n} u_j v_j \end{aligned}$$

$$\mathtt{SUMPRODUCT(B5:B14,C5:C:14)}$$

Our Numerical Example

$$\begin{aligned} \max \ & \sum_{j=1}^{n} c_j x_j \\ & \sum_{j=1}^{n} a_{ij} x_j \leq b_i, \quad i = 1, \ldots, m \\ & x_j \geq 0, \quad j = 1, \ldots, n \end{aligned}$$

$$\begin{array}{rrcrcr} \max & 16x_1 & + & 10x_2 & & \\ & 2x_1 & + & 2x_2 & \leq & 8 \\ & 2x_1 & + & x_2 & \leq & 6 \\ & & & x_1, x_2 & \geq & 0 \end{array}$$

$$\begin{aligned} \max \ & c^T x \\ & Ax \leq b \\ & x \geq 0 \end{aligned}$$

$$\max \quad \begin{bmatrix} 16 & 10 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leq \begin{bmatrix} 8 \\ 6 \end{bmatrix}$$

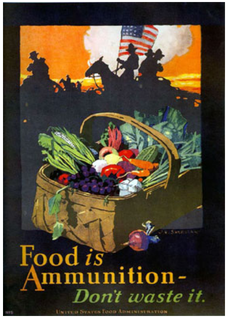
$$x \in \mathbb{R}^n, c \in \mathbb{R}^n, A \in \mathbb{R}^{m \times n}, b \in \mathbb{R}^m$$

$$x_1, x_2 \geq 0$$

Outline

The Diet Problem (Blending Problems)

- Select a set of foods that will satisfy a set of daily nutritional requirement at minimum cost.
- Motivated in the 1930s and 1940s by US army.
- Formulated as a linear programming problem by George Stigler
- First linear programming problem
- (programming intended as planning not computer code)



min cost/weight
subject to nutrition requirements:
eat enough but not too much of Vitamin A
eat enough but not too much of Sodium
eat enough but not too much of Calories
...

The Diet Problem

Suppose there are:

- 3 foods available, corn, milk, and bread,
- there are restrictions on the number of calories (between 2000 and 2250) and the amount of Vitamin A (between 5000 and 50,000)

Food	Corn	2% Milk	Wheat bread
Vitamin A	107	500	0
Calories	72	121	65
Cost per serving	\$0.18	\$0.23	\$0.05

The Mathematical Model

Parameters (given data)

F = set of foods
N = set of nutrients

a_{ij} = amount of nutrient j in food i, $\forall i \in F$, $\forall j \in N$
c_i = cost per serving of food $i, \forall i \in F$
F_{mini} = minimum number of required servings of food $i, \forall i \in F$
F_{maxi} = maximum allowable number of servings of food $i, \forall i \in F$
N_{minj} = minimum required level of nutrient $j, \forall j \in N$
N_{maxj} = maximum allowable level of nutrient $j, \forall j \in N$

Decision Variables

x_i = number of servings of food i to purchase/consume, $\forall i \in F$

The Mathematical Model

Objective Function: Minimize the total cost of the food

$$\text{Minimize} \sum_{i \in F} c_i x_i$$

Constraint Set 1: For each nutrient $j \in N$, at least meet the minimum required level

$$\sum_{i \in F} a_{ij} x_i \geq N_{minj}, \qquad \forall j \in N$$

Constraint Set 2: For each nutrient $j \in N$, do not exceed the maximum allowable level.

$$\sum_{i \in F} a_{ij} x_i \leq N_{maxj}, \qquad \forall j \in N$$

Constraint Set 3: For each food $i \in F$, select at least the minimum required number of servings

$$x_i \geq F_{mini}, \qquad \forall i \in F$$

Constraint Set 4: For each food $i \in F$, do not exceed the maximum allowable number of servings.

$$x_i \leq F_{maxi}, \qquad \forall i \in F$$

The Mathematical Model

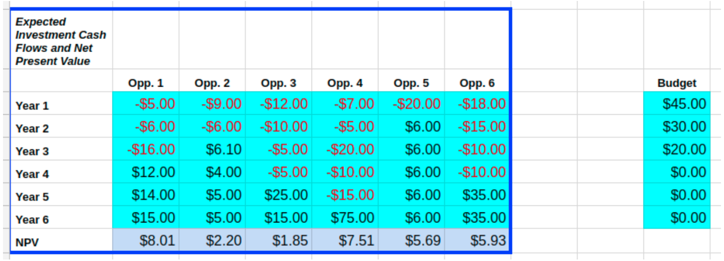
system of equalities and inequalities

$$
\begin{aligned}
\min \quad & \sum_{i \in F} c_i x_i \\
\sum_{i \in F} a_{ij} x_i \geq N_{minj}, & \qquad \forall j \in N \\
\sum_{i \in F} a_{ij} x_i \leq N_{maxj}, & \qquad \forall j \in N \\
x_i \geq F_{mini}, & \qquad \forall i \in F \\
x_i \leq F_{maxi}, & \qquad \forall i \in F
\end{aligned}
$$

Outline

Budget Allocation

- A company has six different opportunities to invest money.
- Each opportunity requires a certain investment over a period of 6 years or less.



Expected Investment Cash Flows and Net Present Value							
	Opp. 1	**Opp. 2**	**Opp. 3**	**Opp. 4**	**Opp. 5**	**Opp. 6**	**Budget**
Year 1	-\$5.00	-\$9.00	-\$12.00	-\$7.00	-\$20.00	-\$18.00	\$45.00
Year 2	-\$6.00	-\$6.00	-\$10.00	-\$5.00	\$6.00	-\$15.00	\$30.00
Year 3	-\$16.00	\$6.10	-\$5.00	-\$20.00	\$6.00	-\$10.00	\$20.00
Year 4	\$12.00	\$4.00	-\$5.00	-\$10.00	\$6.00	-\$10.00	\$0.00
Year 5	\$14.00	\$5.00	\$25.00	-\$15.00	\$6.00	\$35.00	\$0.00
Year 6	\$15.00	\$5.00	\$15.00	\$75.00	\$6.00	\$35.00	\$0.00
NPV	\$8.01	\$2.20	\$1.85	\$7.51	\$5.69	\$5.93	

- The company has an investment budget that needs to be met for each year.
- It also has the wish of investing in those opportunities that maximize the combined Net Present Value (NPV) after the 6th year.

Digression: What is the Net Present Value?

- P: value of the original payment presently due
- the debtor wants to delay the payment for t years,
- let r be the market rate of return that the creditor would obtain from a similar investment asset
- the future value of P is $F = P(1+r)^t$

Viceversa, consider the task of finding:

- the present value P of \$100 that will be received in five years, or equivalently,
- which amount of money today will grow to \$100 in five years when subject to a constant discount rate.

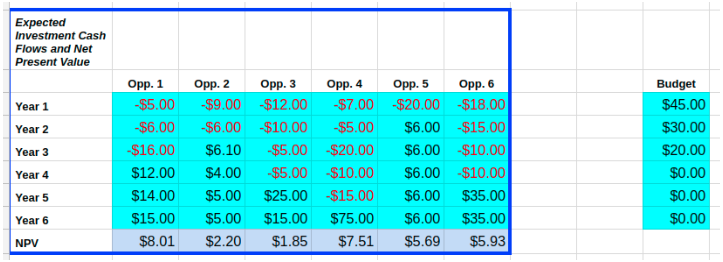
Assuming a 5% per year interest rate, it follows that

$$P = \frac{F}{(1+r)^t} = \frac{\$100}{(1+0.05)^5} = \$78.35.$$

Budget Allocation

Net Present Value calculation:
for each opportunity we calculate the NPV at time zero (the time of decision) as:

$$P_0 = \sum_{t=1}^{5} \frac{F_t}{(1+0.05)^5}$$



Expected Investment Cash Flows and Net Present Value									
	Opp. 1	**Opp. 2**	**Opp. 3**	**Opp. 4**	**Opp. 5**	**Opp. 6**			**Budget**
Year 1	-$5.00	-$9.00	-$12.00	-$7.00	-$20.00	-$18.00			$45.00
Year 2	-$6.00	-$6.00	-$10.00	-$5.00	$6.00	-$15.00			$30.00
Year 3	-$16.00	$6.10	-$5.00	-$20.00	$6.00	-$10.00			$20.00
Year 4	$12.00	$4.00	-$5.00	-$10.00	$6.00	-$10.00			$0.00
Year 5	$14.00	$5.00	$25.00	-$15.00	$6.00	$35.00			$0.00
Year 6	$15.00	$5.00	$15.00	$75.00	$6.00	$35.00			$0.00
NPV	$8.01	$2.20	$1.85	$7.51	$5.69	$5.93			

Budget Allocation - Mathematical Model

- Let B_t be the budget available for investments during the years $t = 1..5$.
- Let a_{tj} be the cash flow for opportunity j and c_j its NPV
- Task: choose a set of opportunities such that the budget is never exceeded and the expected return is maximized. Consider both the case of indivisible and divisible opportunities.

Variables $x_j = 1$ if opportunity j is selected and $x_j = 0$ otherwise, $j = 1..6$

Objective

$$\max \sum_{j=1}^{6} c_j x_j$$

Constraints

$$\textstyle\sum_{j=1}^{6} a_{tj} x_j + B_t \geq 0 \qquad \forall t = 1..5$$

DM587
Scientific Programming

Affine Scaling Method

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

Outline

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Interior Point Methods

Interior point methods in linear programming are classified as:

- affine scaling methods
- potential reduction methods, and
- central path methods (or central trajectory methods)

and for almost every approach one can consider

- a primal version,
- a dual version,
- a primal–dual version, or
- a self-dual version.

- affine scaling by Dikin
- logarithmic barrier algorithm by Fiacco and McCormick
- ellipsoid algorithm by Khachian
- projective method by Karmarkar $\equiv$ logarithmic barrier
- primal-dual logarithmic barrier
- primal–dual barrier algorithm, combined with Mehrotra's predictor–corrector method

Applied with success also to semidefinite programming and other important classes of optimization problems, such as convex quadratic programming.

Interior point algorithm with affine scaling

- Historically, one of the first interior-point methods to be invented
- No longer considered the method of choice for practical implementations

- Concept 1: Shoot through the interior of the feasible region toward an optimal solution.
- Concept 2: Move in a direction that improves the objective function value at the fastest possible rate.
- Concept 3: Transform the feasible region to place the current trial solution near its center, thereby enabling a large improvement when concept 2 is implemented.

Affine Scaling Method — Phase II

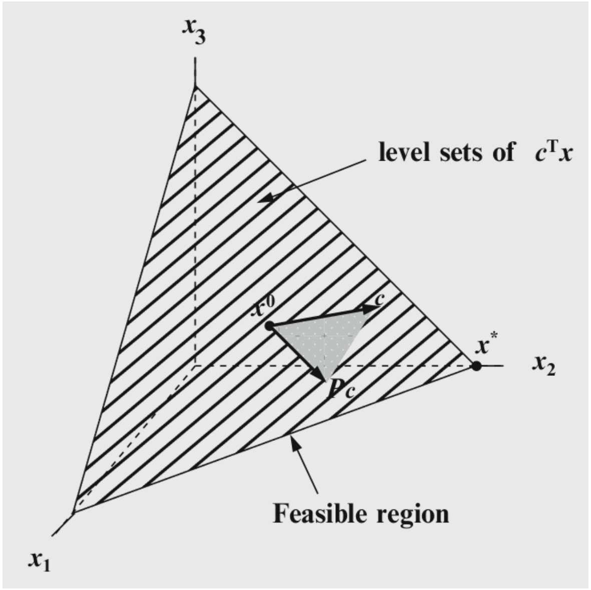
$$\begin{aligned} \text{maximize } & \boldsymbol{c}^T\boldsymbol{x} \\ \text{subject to } & A\boldsymbol{x} = \boldsymbol{b} \\ & \boldsymbol{x} \geq 0 \end{aligned}$$

Two-phase method:

- Phase I uses only the feasibility direction
- Phase II uses only the optimality direction

Phase II
We assume that we have a feasible initial starting point, $\boldsymbol{x}_0$ that lies in the strict interior of the feasible set. That is:

$$A\boldsymbol{x}_0 = \boldsymbol{b} \qquad \text{and} \qquad \boldsymbol{x}_0 > 0$$


x_3
level sets of c^Tx
x^0
c
x^*
x_2
P_c
Feasible region
x_1

Hence, the steepest ascent direction will almost surely cause a move to infeasible points. This is also clear algebraically. Indeed,

$$A(x^0 + \Delta x) = Ax^0 + A\Delta x = b + Ac \neq b$$

(unless Ac = 0 which is not likely).

To see how to find a better direction, let us first review in what sense the gradient is the steepest ascent direction. The *steepest ascent direction* is defined to be the direction that gives the greatest increase in the objective function subject to the constraint that the displacement vector has unit length. That is, the steepest ascent direction is the solution to the following optimization problem:

$$\begin{array}{ll} \text{maximize} & c^T(x^0 + \Delta x) \\ \text{subject to} & \|\Delta x\|^2 = 1. \end{array} \tag{21.2}$$

We can solve this problem using Lagrange multipliers. Indeed, if we let λ denote the Lagrange multiplier for the constraint, the problem becomes

$$\max_{\Delta x, \lambda} c^T(x^0 + \Delta x) - \lambda(\Delta x^T \Delta x - 1).$$

Differentiating with respect to Δx and setting the derivative to zero, we get

$$c - 2\lambda \Delta x = 0,$$

which implies that

$$\Delta x = \frac{1}{2\lambda} c \propto c.$$

Then differentiating the Lagrangian with respect to λ and setting that derivative to zero, we see that

$$\|\Delta x\|^2 - 1 = 0,$$

which implies that

$$\|\Delta x\| = \pm 1.$$

Hence, the steepest ascent direction points in the direction of either c or its negative. Since the negative is easily seen not to be an ascent direction at all, it follows that the steepest ascent direction points in the direction of c.

The problem with the steepest ascent direction is that it fails to preserve feasibility. That is, it fails to preserve the equality constraints $Ax = b$. To remedy this problem, let's add these constraints to (21.2) so that we get the following optimization problem:

$$\begin{array}{ll} \text{maximize} & c^T(x^0 + \Delta x) \\ \text{subject to} & \|\Delta x\|^2 = 1 \\ & A(x^0 + \Delta x) = b. \end{array}$$

Again, the method of Lagrange multipliers is the appropriate tool. As before, let λ denote the Lagrange multiplier for the norm constraint, and now introduce a vector y containing the Lagrange multipliers for the equality constraints. The resulting unconstrained optimization problem is

$$\max_{\Delta x, \lambda, y} \; c^T(x^0 + \Delta x) - \lambda(\Delta x^T \Delta x - 1) - y^T(A(x^0 + \Delta x) - b).$$

$$\max_{\Delta x, \lambda, y} \; c^T(x^0 + \Delta x) - \lambda(\Delta x^T \Delta x - 1) - y^T(A(x^0 + \Delta x) - b).$$

Differentiating this Lagrangian with respect to Δx, λ, and y and setting these derivatives to zero, we get

$$\begin{aligned} c - 2\lambda\Delta x - A^T y &= 0 \\ \|\Delta x\|^2 - 1 &= 0 \\ A(x^0 + \Delta x) - b &= 0. \end{aligned}$$

The second equation tells us that the length of Δx is one. Since we are interested in the direction of Δx and are not concerned about its length, we ignore this second equation. The first equation tells us that Δx is proportional to $c - A^T y$, and again, since we aren't concerned about lengths, we put $\lambda = 1/2$ so that the first equation reduces to

$$\Delta x = c - A^T y. \tag{21.3}$$

Since $Ax^0 = b$, the third equation says that

$$A\Delta x = 0.$$

Substituting (21.3) into this equation, we get

$$Ac - AA^T y = 0,$$

which, assuming that AA^T has full rank (as it should), can be solved for y to get

$$y = (AA^T)^{-1} Ac.$$

Now, substituting this expression into (21.3), we see that

$$\Delta x = c - A^T(AA^T)^{-1}Ac.$$

It is convenient to let P be the matrix defined by

$$P = I - A^T(AA^T)^{-1}A.$$

With this definition, Δx can be expressed succinctly as

$$\Delta x = Pc.$$

We claim that P is the matrix that maps any vector, such as c, to its orthogonal projection onto the null space of A. To justify this claim, we first need to define some of the terms we've used. The *null space* of A is defined as $\{d \in \mathbb{R}^n : Ad = 0\}$. We shall denote the null space of A by $N(A)$. A vector $\tilde{c}$ is the *orthogonal projection* of c onto $N(A)$ if it lies in the null space,

$$\tilde{c} \in N(A),$$

and if the difference between it and c is orthogonal to every other vector in $N(A)$. That is,

$$d^T(c - \tilde{c}) = 0, \qquad \text{for all } d \in N(A).$$

Hence, to show that Pc is the orthogonal projection of c onto the null space of A, we simply check these two conditions. Checking the first, we see that

$$APc = Ac - AA^T(AA^T)^{-1}Ac,$$

which clearly vanishes. To check the second condition, let d be an arbitrary vector in the null space, and compute

$$d^T(c - Pc) = d^T A^T (AA^T)^{-1} Ac,$$

which also vanishes, since $d^T A^T = (Ad)^T = 0$. The orthogonal projection Pc is shown in Figure 21.1.

Scaling

- If it is close to a "wall", the overall increase in one step will be small

- scale the variables in the problem so that the current feasible solution is far from the walls, compute the step direction as the projected gradient in the scaled problem, and then translate this direction back into the original system.

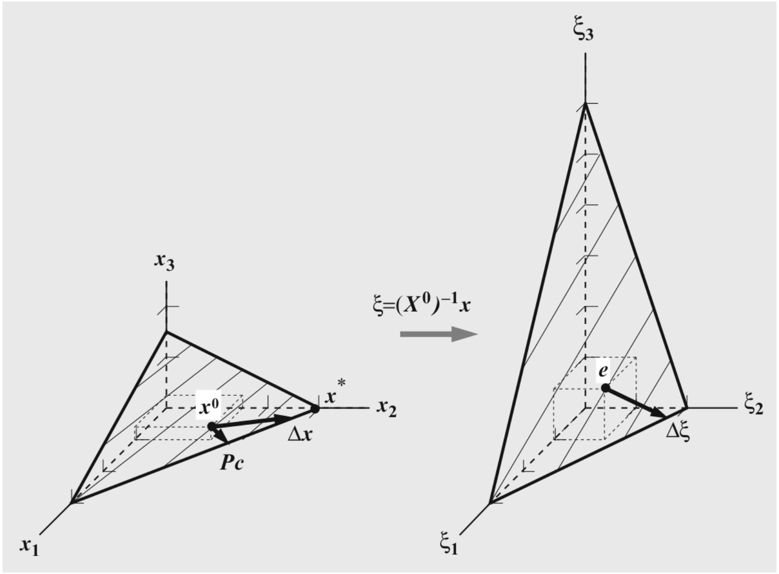
- scale each variable in such a manner that its initial value gets mapped to 1. That is, for each $j = 1, 2, \ldots, n$, we introduce new variables given by

$$\xi_j = \frac{x_j}{x_j^0} \qquad \Longrightarrow \qquad x_j = x_j^0 \xi_j$$

  In matrix notation:

$$\boldsymbol{x} = X^0 \boldsymbol{\xi}$$

  (X^0 diagonal matrix of diagonal $\boldsymbol{x}^0$)
  under this change of variables, the initial solution $\boldsymbol{x}_0$ gets mapped to the vector $\boldsymbol{e}$ of all ones, which is at least one unit away from each wall.


x_3
x^0
x^*
x_2
Δx
Pc
x_1
$\xi=(X^0)^{-1}x$
ξ_3
e
ξ_2
$\Delta\xi$
ξ_1

After substitution:

$$\begin{aligned} \text{maximize} \quad & \boldsymbol{c}^T X^0 \xi \\ \text{subject to} \quad & A X^0 \xi = \boldsymbol{b} \\ & \xi \geq 0 \end{aligned}$$

It is a linear programmming problem in standard form with constraint matrix AX^0 and vector of objective function coeffcients $(\boldsymbol{c}^T X^0)^T = X^0 \boldsymbol{c}$ (since X^0 is diagonal matrix).

We can determine the steepest ascent direction applying what seen in the previous slides:

$$\Delta \xi = \left(I - X^0 A^T (A {X^0}^2 A^T)^{-1} A X^0 \right) X^0 \boldsymbol{c}.$$

and

$$\xi^1 = \xi^0 + \Delta \xi = \boldsymbol{e} + \Delta \xi$$

Transforming the new point ξ^1 back into the original unscaled variables, we get a new point $\boldsymbol{x}^1$:

$$\boldsymbol{x}^1 = X^0 \xi^1 = X^0(\boldsymbol{e} + \Delta\xi) = \boldsymbol{x}^0 + X^0 \Delta\xi$$

The difference between $\boldsymbol{x}^1$ and $\boldsymbol{x}^0$ is the step direction in the original variables. Denoting this difference by $\Delta\boldsymbol{x}$, we see that:

$$\begin{aligned}\Delta\boldsymbol{x} &= \boldsymbol{x}_1 - \boldsymbol{x}_0 = \boldsymbol{x}^0 + X^0\Delta\xi - \boldsymbol{x}^0 = \\ &= X^0\left(I - X^0 A^T (A{X^0}^2 A^T)^{-1} A X^0\right) X^0 \boldsymbol{c} = \\ &= (E - EA^T(AEA^T)^{-1}AE)\boldsymbol{c}\end{aligned}$$

where $E = {X^0}^2$.
This expression for $\Delta\boldsymbol{x}$ is called affine-scaling step direction.

Recall that we worked with $\| \Delta\xi \| = 1$. We can then choose step lengths in such a manner as to ensure "strict" feasibility of each iteration.

Step Length

If all components of $\Delta\boldsymbol{\xi}$ are nonnegative, then we can increase the objective function without bound; stop the algorithm with an unbounded solution.

Otherwise, if the step were chosen so that the new point were to lie exactly on the boundary of the feasible region, then the multiplier for $\Delta\boldsymbol{\xi}$ in the transformed system would be equal to the inverse of the absolute value of the negative component of $\Delta\boldsymbol{\xi}$ with the largest absolute value. That is:

$$\boldsymbol{\xi}^1 = \boldsymbol{\xi}^0 + \theta\Delta\boldsymbol{\xi} = \boldsymbol{e} + \theta\Delta\boldsymbol{\xi}$$

$$\theta = \frac{1}{\max_j\{-\Delta\xi_j\}} = \frac{1}{\max_j\{-\Delta x_j/x_j^0\}}$$

With this definition of θ the smallest component of $\boldsymbol{\xi}^1$ goes to zero.

We then shorten the step by introducing a parameter $0 < \alpha < 1$ and setting the iterations of the affine-scaling algorithm defined by

$$\boldsymbol{x} \leftarrow \boldsymbol{x} + \alpha\theta\Delta\boldsymbol{x}$$

Convergence

Theorem (Convergence Results)

1. *If the problem and its dual are nondegenerate, then for every $\alpha < 1$, the sequence generated by the algorithm converges to the optimal solution.*
2. *For $\alpha \leq 2/3$, the sequence generated by the algorithm converges to an optimal solution (regardless of degeneracy).*
3. *There exists an example and an associated $\alpha < 1$ for which the algorithm converges to a nonoptimal solution.*

As for the speed of convergence, there is no example but it is believed that the Klee–Minty problem might arise here as well.

Affine-Scaling Algorithm

At iteration k:

1. Centering Let $D = X^k = \text{Diag}(\boldsymbol{x}^k)$. Rescale the problem to center the current interior feasible solution by letting $\tilde{A} = AD$, $\tilde{\boldsymbol{c}}^T = \boldsymbol{c}^T D$. Hence, $\boldsymbol{\xi}^k = D^{-1}\boldsymbol{x}^k = \boldsymbol{e}$, the vector consisting of all 1's. Note that $\tilde{A}\boldsymbol{\xi}^k = \boldsymbol{b}$.
2. Search Direction Computation For the rescaled problem, project the steepest ascent direction $\tilde{\boldsymbol{c}}^T$ onto the null space of the constraint matrix $\tilde{A}$, resulting in the search direction $\Delta\boldsymbol{\xi} = (I - \tilde{A}^T(\tilde{A}\tilde{A}^T)^{-1}\tilde{A})\tilde{c}$.
3. Step Length Add a positive multiple θ of the search direction $\Delta\boldsymbol{\xi}$ to the scaled interior feasible point, by computing $\boldsymbol{\xi}^{k+1} = \boldsymbol{e} + \theta\Delta\boldsymbol{\xi}$. If $\Delta\boldsymbol{\xi} \geq 0$, then $\boldsymbol{\xi}^{k+1}$, and hence $\boldsymbol{x}^{k+1}$, can increase without bound; stop the algorithm with an unbounded solution. Otherwise, because $\tilde{A}\Delta\boldsymbol{\xi} = 0$ and $\tilde{A}\boldsymbol{\xi}^{k+1} = \boldsymbol{b}$, then θ must be chosen to ensure that $\boldsymbol{\xi}^{k+1} > 0$, avoiding the border. For any constant α such that $0 < \alpha < 1$, the update $\boldsymbol{\xi}^{k+1} = \boldsymbol{e} + \left(\frac{\alpha}{\max_j\{-\Delta\xi_j\}}\right)\Delta\boldsymbol{\xi}$ suffices.
4. Optimality Test Unscale the problem, setting $x^{k+1} = D\boldsymbol{\xi}^{k+1}$. Test $\boldsymbol{x}^{k+1}$ for optimality by checking whether $\| \boldsymbol{x}^{k+1} - \boldsymbol{x}^k \|$ is small. If $\boldsymbol{x}^{k+1}$ is optimal, stop the algorithm. Otherwise, return to Step 1 with feasible interior point solution $\boldsymbol{x}^{k+1}$.

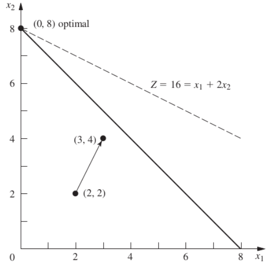
Outline

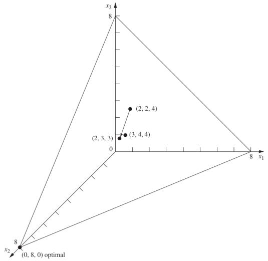
Example

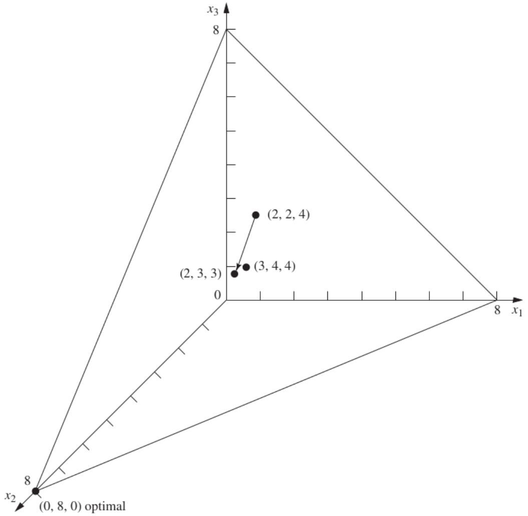
$$\max z = x_1 + 2x_2$$
$$x_1 + x_2 \leq 8$$
$$x_1 \geq 0, x_2 \geq 0$$

In equational standard form:

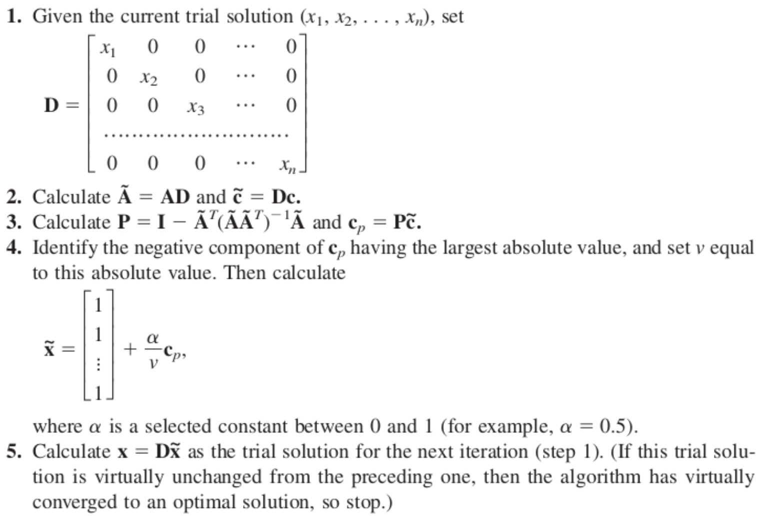
$$\max z = x_1 + 2x_2$$
$$x_1 + x_2 + x_3 = 8$$
$$x_1 \geq 0, x_2 \geq 0, x_3 \geq 0$$






x_3
8
(2, 2, 4)
(3, 4, 4)
(2, 3, 3)
0
8
x_1
8
x_2
(0, 8, 0) optimal

Affine-Scaling Method



1. Given the current trial solution $(x_1, x_2, \dots, x_n)$, set
$$\mathbf{D} = \begin{bmatrix} x_1 & 0 & 0 & \cdots & 0 \\ 0 & x_2 & 0 & \cdots & 0 \\ 0 & 0 & x_3 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & x_n \end{bmatrix}$$
2. Calculate $\tilde{\mathbf{A}} = \mathbf{AD}$ and $\tilde{\mathbf{c}} = \mathbf{Dc}$.
3. Calculate $\mathbf{P} = \mathbf{I} - \tilde{\mathbf{A}}^T(\tilde{\mathbf{A}}\tilde{\mathbf{A}}^T)^{-1}\tilde{\mathbf{A}}$ and $\mathbf{c}_p = \mathbf{P}\tilde{\mathbf{c}}$.
4. Identify the negative component of $\mathbf{c}_p$ having the largest absolute value, and set v equal to this absolute value. Then calculate
$$\tilde{\mathbf{x}} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} + \frac{\alpha}{v}\mathbf{c}_p,$$
where α is a selected constant between 0 and 1 (for example, $\alpha = 0.5$).
5. Calculate $\mathbf{x} = \mathbf{D}\tilde{\mathbf{x}}$ as the trial solution for the next iteration (step 1). (If this trial solution is virtually unchanged from the preceding one, then the algorithm has virtually converged to an optimal solution, so stop.)

Watch out the change of notation:

$$\Delta\xi \to \boldsymbol{c}_p$$

$$\xi \to \tilde{\boldsymbol{x}}$$

$$\theta = \frac{1}{v} = \frac{1}{\max_j\{-\Delta\xi_j\}} = \frac{1}{\max_j\{-\Delta x_j / x_j^k\}}$$

$$\mathbf{D} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix}.$$

The rescaled variables then are the components of

$$\tilde{\mathbf{x}} = \mathbf{D}^{-1}\mathbf{x} = \begin{bmatrix} \frac{1}{2} & 0 & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & \frac{1}{4} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \frac{x_1}{2} \\ \frac{x_2}{2} \\ \frac{x_3}{4} \end{bmatrix}.$$

In these new coordinates, **A** and **c** have become

$$\tilde{\mathbf{A}} = \mathbf{AD} = [1 \quad 1 \quad 1] \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix} = [2 \quad 2 \quad 4],$$

$$\tilde{\mathbf{c}} = \mathbf{Dc} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}.$$

Therefore, the projection matrix is

$$\mathbf{P} = \mathbf{I} - \tilde{\mathbf{A}}^T(\tilde{\mathbf{A}}\tilde{\mathbf{A}}^T)^{-1}\tilde{\mathbf{A}}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} \left([2 \quad 2 \quad 4] \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} \right)^{-1} [2 \quad 2 \quad 4]$$

$$\mathbf{P} = \mathbf{I} - \tilde{\mathbf{A}}^T(\tilde{\mathbf{A}}\tilde{\mathbf{A}}^T)^{-1}\tilde{\mathbf{A}}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} \left([2 \quad 2 \quad 4] \begin{bmatrix} 2 \\ 2 \\ 4 \end{bmatrix} \right)^{-1} [2 \quad 2 \quad 4]$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{24} \begin{bmatrix} 4 & 4 & 8 \\ 4 & 4 & 8 \\ 8 & 8 & 16 \end{bmatrix} = \begin{bmatrix} \frac{5}{6} & -\frac{1}{6} & -\frac{1}{3} \\ -\frac{1}{6} & \frac{5}{6} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{bmatrix},$$

so that the projected gradient is

$$\mathbf{c}_p = \mathbf{P}\tilde{\mathbf{c}} = \begin{bmatrix} \frac{5}{6} & -\frac{1}{6} & -\frac{1}{3} \\ -\frac{1}{6} & \frac{5}{6} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{1}{3} \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 3 \\ -2 \end{bmatrix}.$$

Define v as the *absolute value* of the *negative* component of $\mathbf{c}_p$ having the *largest* absolute value, so that $v = |-2| = 2$ in this case. Consequently, in the current coordinates, the algorithm now moves from the current trial solution $(\tilde{x}_1, \tilde{x}_2, \tilde{x}_3) = (1, 1, 1)$ to the next trial solution

$$\tilde{\mathbf{x}} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + \frac{\alpha}{v}\mathbf{c}_p = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + \frac{0.5}{2} \begin{bmatrix} 1 \\ 3 \\ -2 \end{bmatrix} = \begin{bmatrix} \frac{5}{4} \\ \frac{7}{4} \\ \frac{1}{2} \end{bmatrix},$$

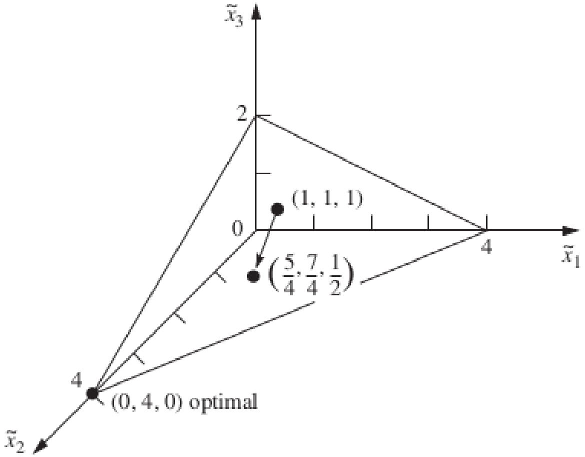
as shown in Fig. 8.5. (The definition of v has been chosen to make the smallest component of $\tilde{\mathbf{x}}$ equal to zero when $\alpha = 1$ in this equation for the next trial solution.) In the original coordinates, this solution is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \mathbf{D}\tilde{\mathbf{x}} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} \frac{5}{4} \\ \frac{7}{4} \\ \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{5}{2} \\ \frac{7}{2} \\ 2 \end{bmatrix}.$$

This completes the iteration, and this new solution will be used to start the next iteration.

These steps can be summarized as follows for any iteration.

Example


$\tilde{x}_3$
2
0
$(1, 1, 1)$
$\left(\frac{5}{4}, \frac{7}{4}, \frac{1}{2}\right)$
4
$\tilde{x}_1$
4
$(0, 4, 0)$ optimal
$\tilde{x}_2$

Iteration 2

Step 1:
Given the current trial solution $(x_1, x_2, x_3) = (\frac{5}{2}, \frac{7}{2}, 2)$, set

$$\mathbf{D} = \begin{bmatrix} \frac{5}{2} & 0 & 0 \\ 0 & \frac{7}{2} & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

(Note that the rescaled variables are

$$\begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \tilde{x}_3 \end{bmatrix} = \mathbf{D}^{-1}\mathbf{x} = \begin{bmatrix} \frac{2}{5} & 0 & 0 \\ 0 & \frac{2}{7} & 0 \\ 0 & 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} \frac{2}{5}x_1 \\ \frac{2}{7}x_2 \\ \frac{1}{2}x_3 \end{bmatrix},$$

so that the BF solutions in these new coordinates are

$$\tilde{\mathbf{x}} = \mathbf{D}^{-1}\begin{bmatrix} 8 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{16}{5} \\ 0 \\ 0 \end{bmatrix}, \qquad \tilde{\mathbf{x}} = \mathbf{D}^{-1}\begin{bmatrix} 0 \\ 8 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{16}{7} \\ 0 \end{bmatrix},$$

and

$$\tilde{\mathbf{x}} = \mathbf{D}^{-1}\begin{bmatrix} 0 \\ 0 \\ 8 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 4 \end{bmatrix},$$

as depicted in Fig. 8.6.)

Step 2:

$$\tilde{\mathbf{A}} = \mathbf{AD} = [\tfrac{5}{2}, \tfrac{7}{2}, 2] \quad \text{and} \quad \tilde{\mathbf{c}} = \mathbf{Dc} = \begin{bmatrix} \frac{5}{2} \\ 7 \\ 0 \end{bmatrix}.$$

Step 3:

$$\mathbf{P} = \begin{bmatrix} \frac{13}{18} & -\frac{7}{18} & -\frac{2}{9} \\ -\frac{7}{18} & \frac{41}{90} & -\frac{14}{45} \\ -\frac{2}{9} & -\frac{14}{45} & \frac{37}{45} \end{bmatrix} \quad \text{and} \quad \mathbf{c}_p = \begin{bmatrix} -\frac{11}{12} \\ \frac{133}{60} \\ -\frac{41}{15} \end{bmatrix}.$$

Step 4:
$\left|-\frac{41}{15}\right| > \left|-\frac{11}{12}\right|$, so $v = \frac{41}{15}$ and

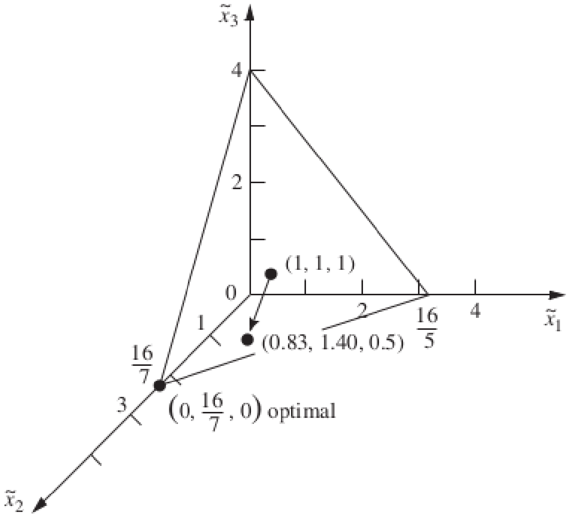
$$\tilde{\mathbf{x}} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} + \frac{0.5}{\frac{41}{15}} \begin{bmatrix} -\frac{11}{12} \\ \frac{133}{60} \\ -\frac{41}{15} \end{bmatrix} = \begin{bmatrix} \frac{273}{328} \\ \frac{461}{328} \\ \frac{1}{2} \end{bmatrix} \approx \begin{bmatrix} 0.83 \\ 1.40 \\ 0.50 \end{bmatrix}.$$

Step 5:

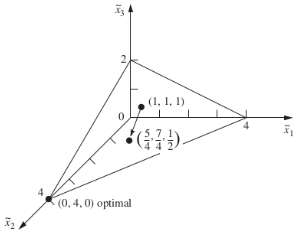
$$\mathbf{x} = \mathbf{D}\tilde{\mathbf{x}} = \begin{bmatrix} \frac{1365}{656} \\ \frac{3227}{656} \\ 1 \end{bmatrix} \approx \begin{bmatrix} 2.08 \\ 4.92 \\ 1.00 \end{bmatrix}$$

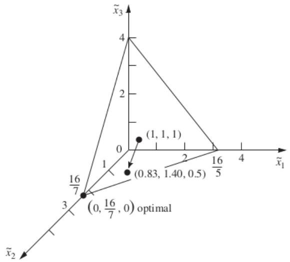
is the trial solution for iteration 3.

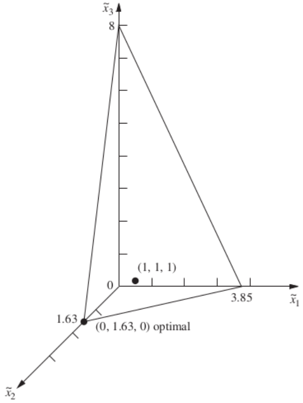
Example


$\tilde{x}_3$
4
2
(1, 1, 1)
0
1
2
4
$\frac{16}{5}$
$\tilde{x}_1$
(0.83, 1.40, 0.5)
$\frac{16}{7}$
3
$\left(0, \frac{16}{7}, 0\right)$ optimal
$\tilde{x}_2$

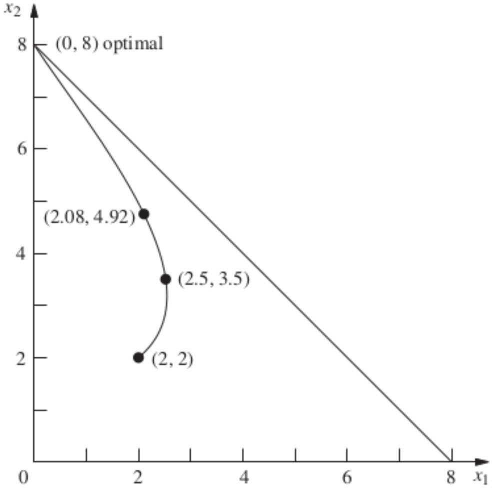
Example


$\tilde{x}_3$
2
0
(1, 1, 1)
$\left(\frac{5}{4}, \frac{7}{4}, \frac{1}{2}\right)$
4
$\tilde{x}_1$
4
(0, 4, 0) optimal
$\tilde{x}_2$


$\tilde{x}_3$
4
2
0
(1, 1, 1)
2
$\frac{16}{5}$
4
$\tilde{x}_1$
(0.83, 1.40, 0.5)
1
$\frac{16}{7}$
3
$\left(0, \frac{16}{7}, 0\right)$ optimal
$\tilde{x}_2$


$\tilde{x}_3$
8
(1, 1, 1)
0
3.85
$\tilde{x}_1$
1.63
(0, 1.63, 0) optimal
$\tilde{x}_2$

Example



Projection Calculations

Projection matrix:

$$P = (I - \tilde{A}^T(\tilde{A}\tilde{A}^T)^{-1}\tilde{A})$$

$$\Delta\boldsymbol{\xi} = P\tilde{\boldsymbol{c}} = \tilde{\boldsymbol{c}} - \tilde{A}^T(\tilde{A}\tilde{A}^T)^{-1}\tilde{A}\tilde{\boldsymbol{c}}$$

Solved by:

- $\tilde{A}\tilde{\boldsymbol{c}} = \boldsymbol{v}$
- $\boldsymbol{w} = (\tilde{A}\tilde{A}^T)^{-1}\boldsymbol{v}$ solved as $(\tilde{A}\tilde{A}^T)\boldsymbol{w} = \boldsymbol{v}$ by Cholesky decomposition
- $\tilde{\boldsymbol{c}} - \tilde{A}^T\boldsymbol{w}$

Phase I: Feasibility Direction

To derive a Phase I procedure for the affine-scaling algorithm, we consider a starting point $\boldsymbol{x}^0$ that has strictly positive components but does not necessarily satisfy the equality constraints $A\boldsymbol{x} = \boldsymbol{b}$. We then let

$$\rho = \boldsymbol{b} - A\boldsymbol{x}^0$$

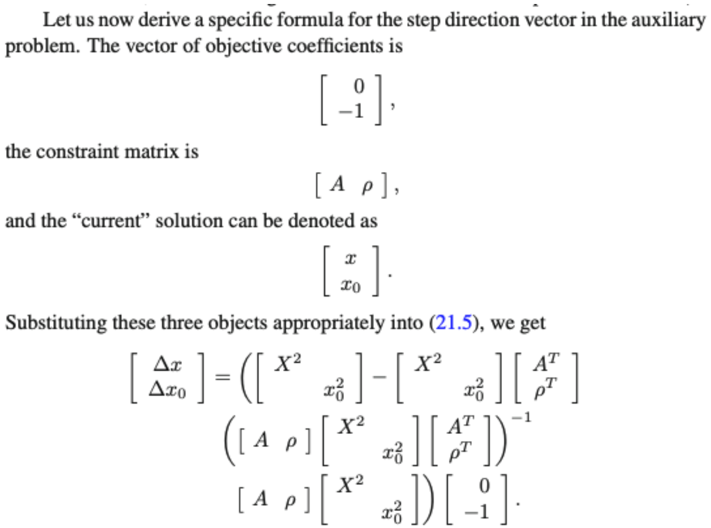
denote the vector of infeasibilities.

Auxiliary problem:

$$\begin{aligned} \max\ & -\boldsymbol{x}_0 \\ & A\boldsymbol{x} + \boldsymbol{x}_0\rho = \boldsymbol{b} \\ & \boldsymbol{x} \geq 0, \boldsymbol{x}_0 \geq 0 \end{aligned}$$

$\begin{bmatrix} \boldsymbol{x}^0 \\ 1 \end{bmatrix}$ is feasible solution

If $\boldsymbol{x}_0^* > 0$, then the original problem is infeasible.
If $\boldsymbol{x}_0^* = 0$, then the optimal solution to the auxiliary problem provides a feasible starting solution to the original problem (it may not be a strictly interior feasible solution)



Let us now derive a specific formula for the step direction vector in the auxiliary problem. The vector of objective coefficients is

$$\begin{bmatrix} 0 \\ -1 \end{bmatrix},$$

the constraint matrix is

$$\begin{bmatrix} A & \rho \end{bmatrix},$$

and the "current" solution can be denoted as

$$\begin{bmatrix} x \\ x_0 \end{bmatrix}.$$

Substituting these three objects appropriately into (21.5), we get

$$\begin{bmatrix} \Delta x \\ \Delta x_0 \end{bmatrix} = \left(\begin{bmatrix} X^2 & \\ & x_0^2 \end{bmatrix} - \begin{bmatrix} X^2 & \\ & x_0^2 \end{bmatrix} \begin{bmatrix} A^T \\ \rho^T \end{bmatrix} \right.$$
$$\left(\begin{bmatrix} A & \rho \end{bmatrix} \begin{bmatrix} X^2 & \\ & x_0^2 \end{bmatrix} \begin{bmatrix} A^T \\ \rho^T \end{bmatrix} \right)^{-1}$$
$$\left. \begin{bmatrix} A & \rho \end{bmatrix} \begin{bmatrix} X^2 & \\ & x_0^2 \end{bmatrix} \right) \begin{bmatrix} 0 \\ -1 \end{bmatrix}.$$

which yeilds $\Delta \boldsymbol{x} = X^2 A^T (A X^2 A^T)^{-1} \rho$.

DM587
Scientific Programming

Numerical Methods
LU Factorization

Marco Chiarandini

Department of Mathematics & Computer Science
University of Southern Denmark

[*Based on slides by Lieven Vandenberghe, UCLA*]

Outline

In solving large scale-linear systems, Gaussian elimination and Gauss-Jordan elimination are not suitable because of:

- computer roundoff errors
- memory usage
- speed

Computer methods are based on LU decomposition.

Outline

Complexity of matrix algorithms

- flop counts
- vector-vector operations
- matrix-vector product
- matrix-matrix product

Floating point numbers

$$x = m \cdot \beta^e \; ; \qquad l \leq e \leq u$$

with mantissa m, base β, and exponent e

$$m = \pm d_0.d_1 d_2 \cdots d_t \;\; , \quad 0 \leq d_i < \beta$$

	β	t	l	u
IEEE SP	2	23	-126	127
IEEE DP	2	52	-1022	1023
Cray	2	48	-16383	16384
HP calculator	10	12	-499	499
IBM mainframe	16	6	-64	63

Flop counts

floating-point operation (flop)

- one floating-point addition, subtraction, multiplication, or division
- other common definition: one multiplication followed by one addition

flop counts of matrix algorithm

- total number of flops is typically a polynomial of the problem dimensions
- usually simplified by ignoring lower-order terms

applications

- a simple, machine-independent measure of algorithm complexity
- not an accurate predictor of computation time on modern computers

Vector-vector operations

- inner product of two n-vectors

  $$\boldsymbol{x}^T\boldsymbol{y} = x_1y_1 + x_2y_2 + \ldots + x_ny_n$$

  n multiplications and $n-1$ additions $= 2n$ flops ($2n$ if $n \gg 1$)

- addition or subtraction of n-vectors: n flops

- scalar multiplication of n-vector : n flops

Matrix-vector product

matrix-vector product with $m \times n$-matrix A:

$$\boldsymbol{y} = A\boldsymbol{x}$$

m elements in y; each element requires an inner product of length n:

$$(2n-1)m \text{ flops}$$

approximately $2mn$ for large n special cases

- $m = n$, A diagonal: n flops
- $m = n$, A lower triangular: $n(n+1)$ flops
- A very sparse (lots of zero coefficients): $\#\mathit{flops} \ll 2mn$

Matrix-matrix product

product of $m \times n$-matrix A and $n \times p$-matrix B:

$$C = AB$$

mp elements in C; each element requires an inner product of length n:

$$mp(2n - 1) flops$$

approximately $2mnp$ for large n.

Approximate Cost for an $n \times n$ Matrix A with Large n	
Algorithm	**Cost in Flops**
Gauss–Jordan elimination (forward phase)	$\approx \frac{2}{3}n^3$
Gauss–Jordan elimination (backward phase)	$\approx n^2$
LU-decomposition of A	$\approx \frac{2}{3}n^3$
Forward substitution to solve $L\mathbf{y} = \mathbf{b}$	$\approx n^2$
Backward substitution to solve $U\mathbf{x} = \mathbf{y}$	$\approx n^2$
A^{-1} by reducing $[A \mid I]$ to $[I \mid A^{-1}]$	$\approx 2n^3$
Compute $A^{-1}\mathbf{b}$	$\approx 2n^3$

Outline

Overview

- factor-solve method
- LU factorization
- solving $Ax = b$ with A nonsingular
- the inverse of a nonsingular matrix
- LU factorization algorithm
- effect of rounding error
- sparse LU factorization

Definitions

Definition (Triangular Matrices)

An $n \times n$ matrix is said to be upper triangular if $a_{ij} = 0$ for $i > j$ and lower triangular if $a_{ij} = 0$ for $i < j$. Also A is said to be triangular if it is either upper triangular or lower triangular.

Example:

$$\begin{bmatrix} 3 & 0 & 0 \\ 2 & 1 & 0 \\ 1 & 4 & 3 \end{bmatrix} \qquad \begin{bmatrix} 3 & 5 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 7 \end{bmatrix}$$

Definition (Diagonal Matrices)

An $n \times n$ matrix is diagonal if $a_{ij} = 0$ whenever $i \neq j$.

Example:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix}$$

Multiple right-hand sides

two equations with the same matrix but different right-hand sides

$$Ax = b, \qquad A\tilde{x} = \tilde{b}$$

- factor A once (f flops)
- solve with right-hand side b (s flops)
- solve with right-hand side $\tilde{b}$ (s flops)

cost: $f + 2s$ instead of $2(f + s)$ if we solve second equation from scratch

conclusion: if $f \gg s$, we can solve the two equations at the cost of one

LU factorization

LU factorization without pivoting

$$A = LU$$

- L unit lower triangular, U upper triangular
- does not always exist (even if A is nonsingular)

LU factorization (with row pivoting)

$$A = PLU$$

- P permutation matrix, L unit lower triangular, U upper triangular
- exists if and only if A is nonsingular (see later)

cost: $(2/3)n^3$ if A has order n

Solving linear equations by LU factorization

solve $Ax = b$ with A nonsingular of order n

factor-solve method using LU factorization

1. factor A as $A = PLU$ ($(2/3)n^3$ flops)
2. solve $(PLU)x = b$ in three steps
   - permutation: $z_1 = P^T b$ (0 flops)
   - forward substitution: solve $Lz_2 = z_1$ (n^2 flops)
   - back substitution: solve $Ux = z_2$ (n^2 flops)

total cost: $(2/3)n^3 + 2n^2$ flops, or roughly $(2/3)n^3$

this is the standard method for solving $Ax = b$

Multiple right-hand sides

two equations with the same matrix A (nonsingular and $n \times n$):

$$Ax = b, \qquad A\tilde{x} = \tilde{b}$$

- factor A once
- forward/back substitution to get x
- forward/back substitution to get $\tilde{x}$

cost: $(2/3)n^3 + 4n^2$ or roughly $(2/3)n^3$

exercise: propose an efficient method for solving

$$Ax = b, \qquad A^T\tilde{x} = \tilde{b}$$

Inverse of a nonsingular matrix

suppose A is nonsingular of order n, with LU factorization

$$A = PLU$$

- inverse from LU factorization

$$A^{-1} = (PLU)^{-1} = U^{-1}L^{-1}P^T$$

- gives interpretation of solve step: evaluate

$$x = A^{-1}b = U^{-1}L^{-1}P^T b$$

  in three steps

$$z_1 = P^T b, \qquad z_2 = L^{-1}z_1, \qquad x = U^{-1}z_2$$

Computing the inverse

solve $AX = I$ by solving n equations

$$AX_1 = e_1, \qquad AX_2 = e_2, \qquad \ldots, \qquad AX_n = e_n$$

X_i is the ith column of X; e_i is the ith unit vector of size n

- one LU factorization of A: $2n^3/3$ flops
- n solve steps: $2n^3$ flops

total: $(8/3)n^3$ flops

conclusion: do not solve $Ax = b$ by multiplying A^{-1} with b

LU factorization without pivoting

partition A, L, U as block matrices:

$$A = \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \qquad L = \begin{bmatrix} 1 & 0 \\ L_{21} & L_{22} \end{bmatrix}, \qquad U = \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

- a_{11} and u_{11} are scalars
- L_{22} unit lower-triangular, U_{22} upper triangular of order $n-1$

determine L and U from $A = LU$, *i.e.*,

$$\begin{aligned} \begin{bmatrix} a_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} u_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix} \\ &= \begin{bmatrix} u_{11} & U_{12} \\ u_{11}L_{21} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix} \end{aligned}$$

recursive algorithm:

- determine first row of U and first column of L

$$u_{11} = a_{11}, \qquad U_{12} = A_{12}, \qquad L_{21} = (1/a_{11})A_{21}$$

- factor the $(n-1) \times (n-1)$-matrix $A_{22} - L_{21}U_{12}$ as

$$A_{22} - L_{21}U_{12} = L_{22}U_{22}$$

  this is an LU factorization (without pivoting) of order $n-1$

cost: $(2/3)n^3$ flops (no proof)

Example

LU factorization (without pivoting) of

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix}$$

write as $A = LU$ with L unit lower triangular, U upper triangular

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- first row of U, first column of L:

$$\begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- second row of U, second column of L:

$$\begin{aligned} \begin{bmatrix} 9 & 4 \\ 7 & 9 \end{bmatrix} - \begin{bmatrix} 1/2 \\ 3/4 \end{bmatrix} \begin{bmatrix} 2 & 9 \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{22} & u_{23} \\ 0 & u_{33} \end{bmatrix} \\ \begin{bmatrix} 8 & -1/2 \\ 11/2 & 9/4 \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & -1/2 \\ 0 & u_{33} \end{bmatrix} \end{aligned}$$

- third row of U: $u_{33} = 9/4 + 11/32 = 83/32$

conclusion:

$$A = \begin{bmatrix} 8 & 2 & 9 \\ 4 & 9 & 4 \\ 6 & 7 & 9 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1/2 & 1 & 0 \\ 3/4 & 11/16 & 1 \end{bmatrix} \begin{bmatrix} 8 & 2 & 9 \\ 0 & 8 & -1/2 \\ 0 & 0 & 83/32 \end{bmatrix}$$

Not every nonsingular A can be factored as $A = LU$

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_{21} & 1 & 0 \\ l_{31} & l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- first row of U, first column of L:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 2 \\ 0 & 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & l_{32} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}$$

- second row of U, second column of L:

$$\begin{bmatrix} 0 & 2 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ l_{32} & 1 \end{bmatrix} \begin{bmatrix} u_{22} & u_{23} \\ 0 & u_{33} \end{bmatrix}$$

$u_{22} = 0$, $u_{23} = 2$, $l_{32} \cdot 0 = 1$?

LU factorization (with row pivoting)

if A is $n \times n$ and nonsingular, then it can be factored as

$$A = PLU$$

P is a permutation matrix, L is unit lower triangular, U is upper triangular

- not unique; there may be several possible choices for P, L, U
- interpretation: permute the rows of A and factor P^TA as $P^TA = LU$
- also known as *Gaussian elimination with partial pivoting* (GEPP)
- cost: $(2/3)n^3$ flops

we will skip the details of calculating P, L, U

Example

$$\begin{bmatrix} 0 & 5 & 5 \\ 2 & 9 & 0 \\ 6 & 8 & 8 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 1/3 & 1 & 0 \\ 0 & 15/19 & 1 \end{bmatrix} \begin{bmatrix} 6 & 8 & 8 \\ 0 & 19/3 & -8/3 \\ 0 & 0 & 135/19 \end{bmatrix}$$

the factorization is not unique; the same matrix can be factored as

$$\begin{bmatrix} 0 & 5 & 5 \\ 2 & 9 & 0 \\ 6 & 8 & 8 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 3 & -19/5 & 1 \end{bmatrix} \begin{bmatrix} 2 & 9 & 0 \\ 0 & 5 & 5 \\ 0 & 0 & 27 \end{bmatrix}$$

Effect of rounding error

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

exact solution:

$$x_1 = \frac{-1}{1 - 10^{-5}}, \qquad x_2 = \frac{1}{1 - 10^{-5}}$$

let us solve the equations using LU factorization, rounding intermediate results to 4 significant decimal digits

we will do this for the two possible permutation matrices:

$$P = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{or} \quad P = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

first choice of P: $P = I$ (no pivoting)

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} 10^{-5} & 1 \\ 0 & 1 - 10^5 \end{bmatrix}$$

L, U rounded to 4 decimal significant digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix}$$

forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^5 & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \Longrightarrow \qquad z_1 = 1, \quad z_2 = -10^5$$

back substitution

$$\begin{bmatrix} 10^{-5} & 1 \\ 0 & -10^5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^5 \end{bmatrix} \qquad \Longrightarrow \qquad x_1 = 0, \quad x_2 = 1$$

error in x_1 is 100%

second choice of P: interchange rows

$$\begin{bmatrix} 1 & 1 \\ 10^{-5} & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 - 10^{-5} \end{bmatrix}$$

L, U rounded to 4 decimal significant digits

$$L = \begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix}, \qquad U = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

forward substitution

$$\begin{bmatrix} 1 & 0 \\ 10^{-5} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \Longrightarrow \qquad z_1 = 0, \quad z_2 = 1$$

backward substitution

$$\begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \qquad \Longrightarrow \qquad x_1 = -1, \quad x_2 = 1$$

error in x_1, x_2 is about 10^{-5}

conclusion:

- for some choices of P, small rounding errors in the algorithm cause very large errors in the solution
- this is called **numerical instability**: for the first choice of P, the algorithm is unstable; for the second choice of P, it is stable
- from numerical analysis: there is a simple rule for selecting a good (stable) permutation (we'll skip the details, since we skipped the details of the factorization algorithm)
- in the example, the second permutation is better because it permutes the largest element (in absolute value) of the first column of A to the 1,1-position

Sparse linear equations

if A is sparse, it is usually factored as

$$A = P_1 L U P_2$$

P_1 and P_2 are permutation matrices

- interpretation: permute rows and columns of A and factor $\tilde{A} = P_1^T A P_2^T$

$$\tilde{A} = LU$$

- choice of P_1 and P_2 greatly affects the sparsity of L and U: many heuristic methods exist for selecting good permutations

- in practice: #flops $\ll (2/3)n^3$; exact value is a complicated function of n, number of nonzero elements, sparsity pattern

Conclusion

different levels of understanding how linear equation solvers work:

highest level: `x = A\b` costs $(2/3)n^3$; more efficient than `x = inv(A)*b`

intermediate level: factorization step $A = PLU$ followed by solve step

lowest level: details of factorization $A = PLU$

- for most applications, level 1 is sufficient
- in some situations ($e.g.$, multiple right-hand sides) level 2 is useful
- level 3 is important only for experts who write numerical libraries

Theorem

If A is a square matrix that can be reduced to a row echelon form U by Gaussian elimination without row interchanges, then A can be factored as $A = LU$, where L is a lower triangular matrix.

- If A is an invertible matrix that can be reduced to row echelon form without row interchanges, then A can be factored uniquely as

  $$A = LDU$$

  where L is a lower triangular matrix with 1's on the main diagonal, D is a diagonal matrix, and U is an upper triangular matrix with 1's on the main diagonal. This is called the LDU-decomposition (or LDU-factorization) of A.

- If desired, the diagonal matrix and the lower triangular matrix in the LU-decomposition can be multiplied to produce an LU-decomposition in which the 1's are on the main diagonal of U rather than L. (This is yet another example that LU decompositions are not unique)

Software

- In 1979 an important library of machine-independent linear algebra programs called LINPACK was developed at Argonne National Laboratories.
- Many of the programs in that library use the LU and other decomposition methods (SVD, Schur's decomposition, Cholesky decomposition, etc).
- Variations of the LINPACK routines in Fortran are used in many computer programs, including Scipy, MATLAB, Mathematica, and Maple.

Outline

Numerical Solutions

- A matrix A is said to be ill conditioned if relatively small changes in the entries of A can cause relatively large changes in the solutions of $A\boldsymbol{x} = \boldsymbol{b}$.
- A is said to be well conditioned if relatively small changes in the entries of A result in relatively small changes in the solutions of $A\boldsymbol{x} = \boldsymbol{b}$.
- reaching RREF as in Gauss-Jordan requires more computation and more numerical instability hence disadvantageous.
- Gauss elimination is a direct method: the amount of operations can be specified in advance. Indirect or Iterative methods work by iteratively improving approximate solutions until a desired accuracy is reached. Amount of operations depend on the accuracy required. (way to go if the matrix is sparse)

Gauss-Seidel Iterative Method
Example

$$\begin{array}{rcrcrcrcl}
x_1 & - & 0.25x_2 & - & 0.25x_3 & & & = & 50 \\
-0.25x_1 & + & x_2 & & & - & 0.25x_4 & = & 50 \\
-0.25x_1 & & & + & x_3 & - & 0.25x_4 & = & 25 \\
 & - & 0.25x_2 & - & 0.25x_3 & + & x_4 & = & 25
\end{array}$$

$$\begin{array}{rclcrcrcrcl}
x_1 & = & & & 0.25x_2 & + & 0.25x_3 & & & + & 50 \\
x_2 & = & 0.25x_1 & & & & & + & 0.25x_4 & + & 50 \\
x_3 & = & 0.25x_1 & & & & & + & 0.25x_4 & + & 25 \\
x_4 & = & & & 0.25x_2 & + & 0.25x_3 & & & + & 25
\end{array}$$

We start from an approximation, eg, $x_1^{(0)} = 100, x_2^{(0)} = 100, x_3^{(0)} = 100, x_4^{(0)} = 100$, and use the equatiuons above to find a perhaps better approximation:

$$\begin{array}{rclcrcrcrcrcr}
x_1^{(1)} & = & & & 0.25x_2^{(0)} & + & 0.25x_3^{(0)} & & & + & 50.00 & = & 100.00 \\
x_2^{(1)} & = & 0.25x_1^{(1)} & & & & & + & 0.25x_4^{(0)} & + & 50.00 & = & 100.00 \\
x_3^{(1)} & = & 0.25x_1^{(1)} & & & & & + & 0.25x_4^{(0)} & + & 25.00 & = & 75.00 \\
x_4^{(1)} & = & & & 0.25x_2^{(1)} & + & 0.25x_3^{(1)} & & & + & 25.00 & = & 68.75
\end{array}$$

$$\begin{aligned}
x_1^{(2)} &= & & 0.25x_2^{(1)} &+& 0.25x_3^{(1)} & & &+& 50.00 &=& 93.750\\
x_2^{(2)} &= 0.25x_1^{(2)} & & & & &+& 0.25x_4^{(1)} &+& 50.00 &=& 90.625\\
x_3^{(2)} &= 0.25x_1^{(2)} & & & & &+& 0.25x_4^{(1)} &+& 25.00 &=& 65.625\\
x_4^{(2)} &= & & 0.25x_2^{(2)} &+& 0.25x_3^{(2)} & & &+& 25.00 &=& 64.062
\end{aligned}$$

6. Cholesky factorization

- triangular matrices
- forward and backward substitution
- the Cholesky factorization
- solving $Ax = b$ with A positive definite
- inverse of a positive definite matrix
- permutation matrices
- sparse Cholesky factorization

Triangular matrix

a square matrix A is **lower triangular** if $a_{ij} = 0$ for $j > i$

$$A = \begin{bmatrix} a_{11} & 0 & \cdots & 0 & 0 \\ a_{21} & a_{22} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & 0 & 0 \\ a_{n-1,1} & a_{n-1,2} & \cdots & a_{n-1,n-1} & 0 \\ a_{n1} & a_{n2} & \cdots & a_{n,n-1} & a_{nn} \end{bmatrix}$$

A is **upper triangular** if $a_{ij} = 0$ for $j < i$ (A^T is lower triangular)

a triangular matrix is **unit upper/lower triangular** if $a_{ii} = 1$ for all i

Forward substitution

solve $Ax = b$ when A is lower triangular with nonzero diagonal elements

$$\begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

algorithm:

$$\begin{aligned} x_1 &:= b_1/a_{11} \\ x_2 &:= (b_2 - a_{21}x_1)/a_{22} \\ x_3 &:= (b_3 - a_{31}x_1 - a_{32}x_2)/a_{33} \\ &\vdots \\ x_n &:= (b_n - a_{n1}x_1 - a_{n2}x_2 - \cdots - a_{n,n-1}x_{n-1})/a_{nn} \end{aligned}$$

cost: $1 + 3 + 5 + \cdots + (2n-1) = n^2$ flops

Back substitution

solve $Ax = b$ when A is upper triangular with nonzero diagonal elements

$$\begin{bmatrix} a_{11} & \cdots & a_{1,n-1} & a_{1n} \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & a_{n-1,n-1} & a_{n-1,n} \\ 0 & \cdots & 0 & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_{n-1} \\ b_n \end{bmatrix}$$

algorithm:

$$\begin{aligned} x_n &:= b_n/a_{nn} \\ x_{n-1} &:= (b_{n-1} - a_{n-1,n}x_n)/a_{n-1,n-1} \\ x_{n-2} &:= (b_{n-2} - a_{n-2,n-1}x_{n-1} - a_{n-2,n}x_n)/a_{n-2,n-2} \\ &\vdots \\ x_1 &:= (b_1 - a_{12}x_2 - a_{13}x_3 - \cdots - a_{1n}x_n)/a_{11} \end{aligned}$$

cost: n^2 flops

Inverse of a triangular matrix

triangular matrix A with nonzero diagonal elements is nonsingular

- $Ax = b$ is solvable via forward/back substitution; hence A has full range
- therefore A has a zero nullspace, is invertible, etc. (see p.4-8)

inverse

- can be computed by solving $AX = I$ column by column

$$A \begin{bmatrix} X_1 & X_2 & \cdots & X_n \end{bmatrix} = \begin{bmatrix} e_1 & e_2 & \cdots & e_n \end{bmatrix}$$

- inverse of lower triangular matrix is lower triangular
- inverse of upper triangular matrix is upper triangular

Cholesky factorization

every positive definite matrix A can be factored as

$$A = LL^T$$

where L is lower triangular with positive diagonal elements

cost: $(1/3)n^3$ flops if A is of order n

- L is called the *Cholesky factor* of A
- can be interpreted as 'square root' of a positive define matrix

Cholesky factorization algorithm

partition matrices in $A = LL^T$ as

$$\begin{aligned}\begin{bmatrix} a_{11} & A_{21}^T \\ A_{21} & A_{22} \end{bmatrix} &= \begin{bmatrix} l_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} l_{11} & L_{21}^T \\ 0 & L_{22}^T \end{bmatrix} \\ &= \begin{bmatrix} l_{11}^2 & l_{11}L_{21}^T \\ l_{11}L_{21} & L_{21}L_{21}^T + L_{22}L_{22}^T \end{bmatrix}\end{aligned}$$

algorithm

1. determine l_{11} and L_{21}:

$$l_{11} = \sqrt{a_{11}}, \qquad L_{21} = \frac{1}{l_{11}} A_{21}$$

2. compute L_{22} from

$$A_{22} - L_{21}L_{21}^T = L_{22}L_{22}^T$$

   this is a Cholesky factorization of order $n-1$

proof that the algorithm works for positive definite A of order n

- step 1: if A is positive definite then $a_{11} > 0$
- step 2: if A is positive definite, then

$$A_{22} - L_{21}L_{21}^T = A_{22} - \frac{1}{a_{11}}A_{21}A_{21}^T$$

  is positive definite (see page 4-23)

- hence the algorithm works for $n = m$ if it works for $n = m - 1$
- it obviously works for $n = 1$; therefore it works for all n

Example

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

- first column of L

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} 5 & 0 & 0 \\ 3 & l_{22} & 0 \\ -1 & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

- second column of L

$$\begin{bmatrix} 18 & 0 \\ 0 & 11 \end{bmatrix} - \begin{bmatrix} 3 \\ -1 \end{bmatrix} \begin{bmatrix} 3 & -1 \end{bmatrix} = \begin{bmatrix} l_{22} & 0 \\ l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{22} & l_{32} \\ 0 & l_{33} \end{bmatrix}$$

$$\begin{bmatrix} 9 & 3 \\ 3 & 10 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ 1 & l_{33} \end{bmatrix} \begin{bmatrix} 3 & 1 \\ 0 & l_{33} \end{bmatrix}$$

- third column of L: $10 - 1 = l_{33}^2$, $i.e.$, $l_{33} = 3$

conclusion:

$$\begin{bmatrix} 25 & 15 & -5 \\ 15 & 18 & 0 \\ -5 & 0 & 11 \end{bmatrix} = \begin{bmatrix} 5 & 0 & 0 \\ 3 & 3 & 0 \\ -1 & 1 & 3 \end{bmatrix} \begin{bmatrix} 5 & 3 & -1 \\ 0 & 3 & 1 \\ 0 & 0 & 3 \end{bmatrix}$$

Solving equations with positive definite A

$$Ax = b \qquad (A \text{ positive definite of order } n)$$

algorithm

- factor A as $A = LL^T$
- solve $LL^T x = b$
  - forward substitution $Lz = b$
  - back substitution $L^T x = z$

cost: $(1/3)n^3$ flops

- factorization: $(1/3)n^3$
- forward and backward substitution: $2n^2$

Inverse of a positive definite matrix

suppose A is positive definite with Cholesky factorization $A = LL^T$

- L is invertible (its diagonal elements are nonzero)
- $X = L^{-T}L^{-1}$ is a right inverse of A:

$$AX = LL^TL^{-T}L^{-1} = LL^{-1} = I$$

- $X = L^{-T}L^{-1}$ is a left inverse of A:

$$XA = L^{-T}L^{-1}LL^T = L^{-T}L^T = I$$

- hence, A is invertible and

$$A^{-1} = L^{-T}L^{-1}$$

Summary

if A is positive definite of order n

- A can be factored as LL^T
- the cost of the factorization is $(1/3)n^3$ flops
- $Ax = b$ can be solved in $(1/3)n^3$ flops
- A is invertible with inverse: $A^{-1} = L^{-T}L^{-1}$

Sparse positive definite matrices

- a matrix is *sparse* if most of its elements are zero
- a matrix is *dense* if it is not sparse

Cholesky factorization of dense matrices

- $(1/3)n^3$ flops
- on a current PC: a few seconds or less, for n up to a few 1000

Cholesky factorization of sparse matrices

- if A is very sparse, then L is often (but not always) sparse
- if L is sparse, the cost of the factorization is much less than $(1/3)n^3$
- exact cost depends on n, #nonzero elements, sparsity pattern
- very large sets of equations ($n \sim 10^6$) are solved by exploiting sparsity

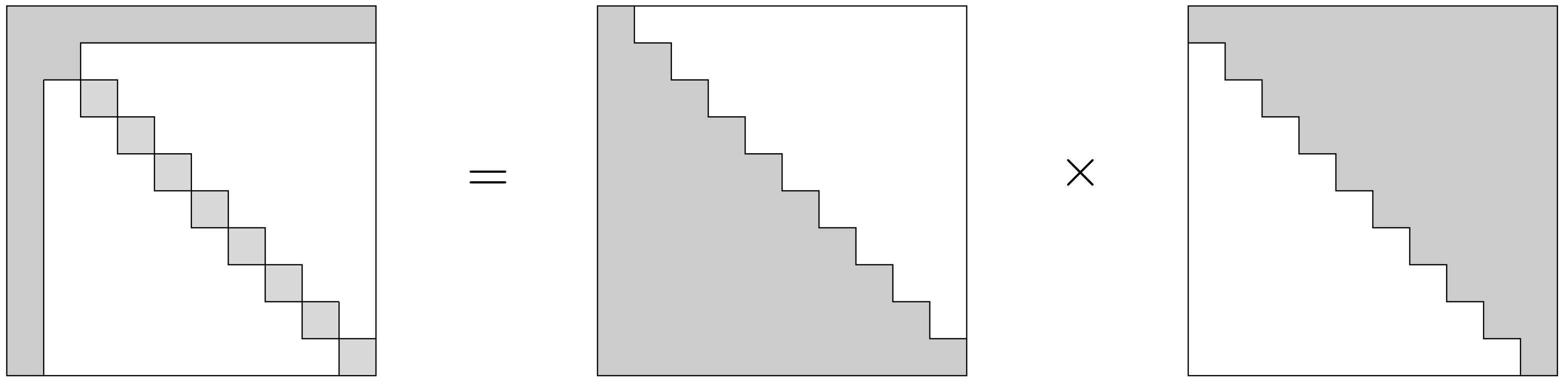
Effect of ordering

sparse equation (a is an $(n-1)$-vector with $\|a\| < 1$)

$$\begin{bmatrix} 1 & a^T \\ a & I \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} b \\ c \end{bmatrix}$$

factorization

$$\begin{bmatrix} 1 & a^T \\ a & I \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ a & L_{22} \end{bmatrix} \begin{bmatrix} 1 & a^T \\ 0 & L_{22}^T \end{bmatrix} \quad \text{where } I - aa^T = L_{22}L_{22}^T$$



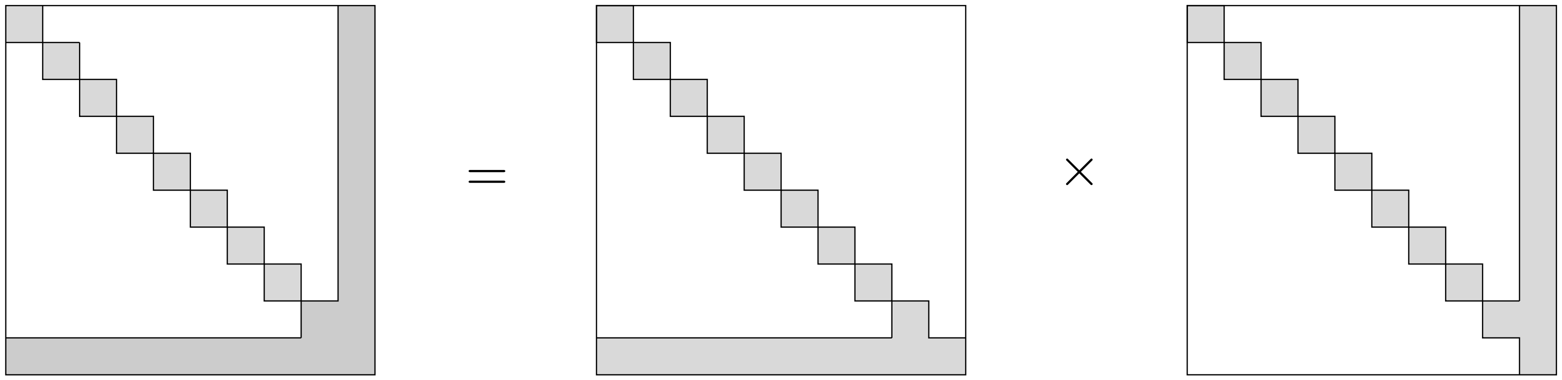
factorization with 100% fill-in

reordered equation

$$\begin{bmatrix} I & a \\ a^T & 1 \end{bmatrix} \begin{bmatrix} v \\ u \end{bmatrix} = \begin{bmatrix} c \\ b \end{bmatrix}$$

factorization

$$\begin{bmatrix} I & a \\ a^T & 1 \end{bmatrix} = \begin{bmatrix} I & 0 \\ a^T & \sqrt{1 - a^T a} \end{bmatrix} \begin{bmatrix} I & a \\ 0 & \sqrt{1 - a^T a} \end{bmatrix}$$



factorization with zero fill-in

Permutation matrices

a *permutation matrix* is the identity matrix with its rows reordered, $e.g.$,

$$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

- the vector Ax is a permutation of x

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_2 \\ x_3 \\ x_1 \end{bmatrix}$$

- $A^T x$ is the inverse permutation applied to x

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} x_3 \\ x_1 \\ x_2 \end{bmatrix}$$

- $A^T A = AA^T = I$, so A is invertible and $A^{-1} = A^T$

Solving $Ax = b$ when A is a permutation matrix

the solution of $Ax = b$ is $x = A^T b$

example

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 10.0 \\ -2.1 \end{bmatrix}$$

solution is $x = (-2.1, 1.5, 10.0)$

cost: zero flops

Sparse Cholesky factorization

if A is sparse and positive definite, it is usually factored as

$$A = PLL^T P^T$$

P a permutation matrix; L lower triangular with positive diagonal elements

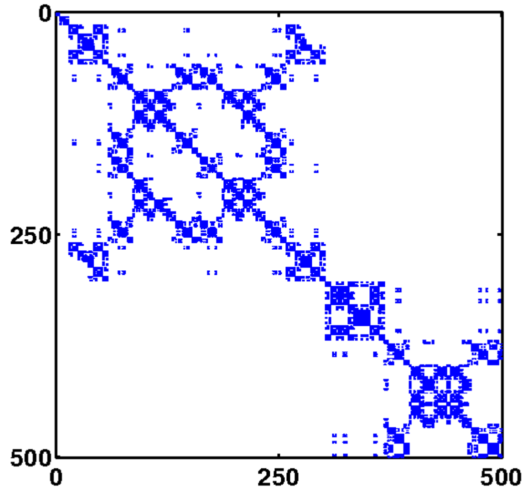
interpretation: we permute the rows and columns of A and factor

$$P^T AP = LL^T$$

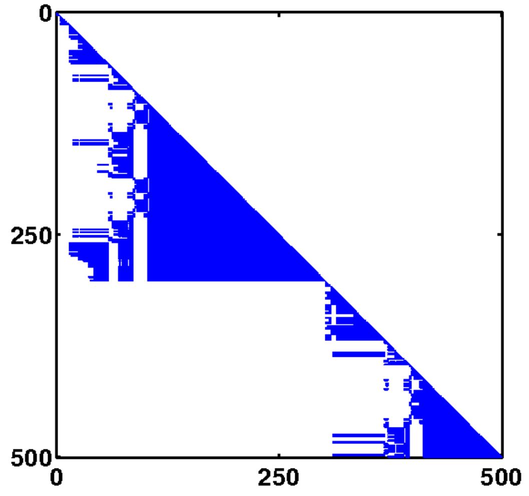
- choice of P greatly affects the sparsity L
- many heuristic methods (that we don't cover) exist for selecting good permutation matrices P

Example

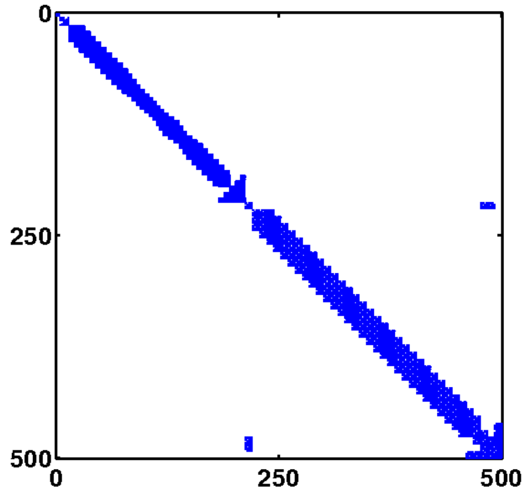
sparsity pattern of A



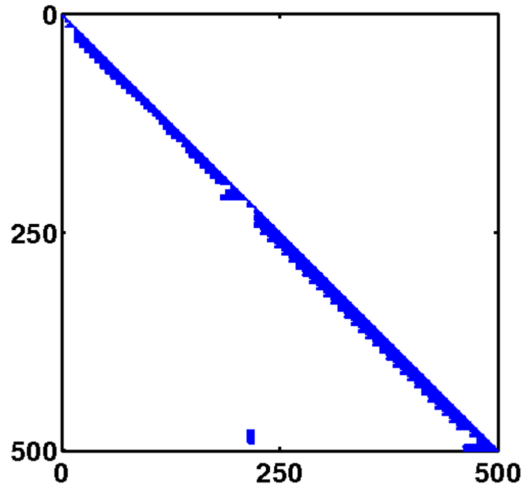
Cholesky factor of A



pattern of P^TAP



Cholesky factor of P^TAP



Solving sparse positive definite equations

solve $Ax = b$ via factorization $A = PLL^TP^T$

algorithm

1. $\tilde{b} := P^T b$
2. solve $Lz = \tilde{b}$ by forward substitution
3. solve $L^T y = z$ by back substitution
4. $x := Py$

interpretation: we solve

$$(P^T A P)\, y = \tilde{b}$$

using the Cholesky factorization of P^TAP

Interior-point methods
Path-following method

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Linear Programming

Consider the primal form in linear programming:

$$\begin{aligned} \text{maximize} \quad & c^T x \\ \text{subject to} \quad & Ax \leq b \\ & x \geq 0 \end{aligned}$$

And the corresponding dual problem:

$$\begin{aligned} \text{minimize} \quad & b^T y \\ \text{subject to} \quad & A^T y \leq c \\ & y \geq 0 \end{aligned}$$

Linear Programming

Both problems can be converted into equality form:

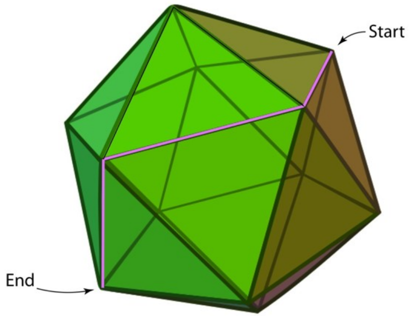
$$\begin{aligned} \text{maximize} \quad & c^T x \\ \text{subject to} \quad & Ax + w = b \\ & x, w \geq 0 \end{aligned}$$

And:

$$\begin{aligned} \text{minimize} \quad & b^T y \\ \text{subject to} \quad & A^T y + z = c \\ & y, z \geq 0 \end{aligned}$$

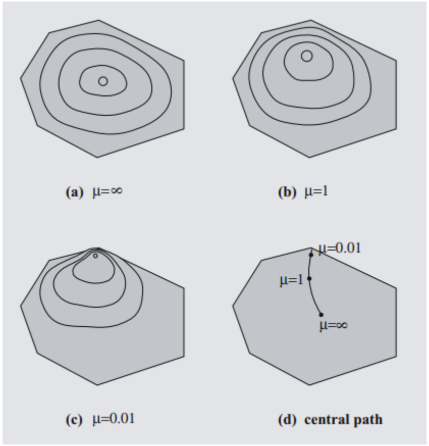
Simplex algorithm

Simplex Method finds the optimal solution by traversing along the edges from one vertex to another.



Interior Point method

The Interior Point method starts inside the polytope and iteratively converges to the optimal solution



Non-standard notation

Non-standard notation ahead! Given a lower-case letter denoting a vector quantity, we also have an upper-case letter denoting a diagonal matrix whose entries corresponds to elements the vector quantity.

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \implies X = \begin{bmatrix} x_1 & & & \\ & x_2 & & \\ & & \ddots & \\ & & & x_n \end{bmatrix}$$

Barrier function

- How do we avoid converging outside the feasibility region?
- Barrier problem:

$$BP(\mu): \begin{array}{rl} \text{maximize} & c^T x + \mu \sum_j \log x_j + \mu \sum_i \log w_i \\ \text{subject to} & Ax + w = b \end{array}$$

- Nonlinear objective function: logarithmic barrier function
- Family of problems indexed by parameter $\mu > 0$

Lagrange Multipliers and Barrier Problem

We Lagrange relax to the barrier function, we get the following problem:

$$L(x, w, y) = c^T x + \mu \sum_j \log x_j + \mu \sum_i \log w_i + y^T (b - Ax - w)$$

We get the first-order optimality conditions when we take the derivatives and set them to zero.

$$\begin{aligned}
\frac{\partial L}{\partial x_j} &= c_j + \mu \frac{1}{x_j} - \sum_i y_i a_{ij} && = 0, \quad j = 1, 2, ..., n. \\
\frac{\partial L}{\partial w_i} &= \mu \frac{1}{w_j} - y_1 && = 0, \quad i = 1, 2, ..., m. \\
\frac{\partial L}{\partial y_i} &= b_i - \sum_j a_{ij} x_j - w_i && = 0, \quad i = 1, 2, ..., m.
\end{aligned}$$

Lagrange Multipliers and Barrier Problem

This can be written in matrix form:

$$\begin{aligned} A^T y - \mu X^{-1} e &= c \\ y &= \mu W^{-1} e \\ Ax + w &= b \end{aligned}$$

Note: X and W are the diagonal matrices containing diagonal entries.

Lagrange Multipliers and Barrier Problem

When we introduce an extra vector $z = \mu X^{-1} e$, we can rewrite our first-order optimality conditions like this:

$$\begin{aligned} Ax + w &= b \\ A^T y - z &= c \\ z &= \mu X^{-1} e \\ y &= \mu W^{-1} e \end{aligned}$$

Important! e is the vector of all ones.

Lagrange Multipliers and Barrier Problem

When we multiply X and W on respectively the third and fourth equation, we get the following equations:

$$\begin{aligned} Ax + w &= b \\ A^T y - z &= c \\ XZe &= \mu e \\ YWe &= \mu e \end{aligned}$$

Lagrange Multipliers and Barrier Problem

When we multiply X and W on respectively the third and fourth equation, we get the following equations:

$$\begin{aligned} Ax + w &= b \\ A^T y - z &= c \\ XZe &= \mu e \\ YWe &= \mu e \end{aligned}$$

Componentwise, the third and fourth equation can be written like this:

$$\begin{aligned} x_j z_j &= \mu \qquad & j &= 1, 2, ..., n \\ y_i w_i &= \mu \qquad & i &= 1, 2, ..., m \end{aligned}$$

Lagrange Multipliers and Barrier Problem

When we multiply X and W on respectively the third and fourth equation, we get the following equations:

$$\begin{aligned} Ax + w &= b \\ A^T y - z &= c \\ XZe &= \mu e \\ YWe &= \mu e \end{aligned}$$

Componentwise, the third and fourth equation can be written like this:

$$\begin{aligned} x_j z_j &= \mu & \qquad j &= 1, 2, ..., n \\ y_i w_i &= \mu & \qquad i &= 1, 2, ..., m \end{aligned}$$

μ-complementarity conditions: $2n + 2m$ equations in $2n + 2m$ unknowns.

Does a solution exist and if so, is it unique?

Lagrange Multipliers and Barrier Problem

Theorem 1

There exists a solution to the barrier problem if and only if both the primal and the dual feasible regions have nonempty interior.

Corollary 2

If a primal feasible set (or, for that matter, its dual) has a nonempty interior and is bounded, then for each $\mu > 0$ there exists a unique solution

$$(x_\mu, w_\mu, y_\mu, z_\mu)$$

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Path-Following Method

1. Estimate appropriate value for μ.
2. Compute step directions $(\Delta x, \Delta w, \Delta y, \Delta z)$ pointing at the point $(x_\mu, w_\mu, y_\mu, z_\mu)$ on the central path.
3. Compute a new step length parameter θ such that the new point:

$$\begin{aligned} \tilde{x} &= x + \theta \Delta x, & \tilde{y} &= y + \theta \Delta y \\ \tilde{w} &= w + \theta \Delta w, & \tilde{z} &= z + \theta \Delta z \end{aligned}$$

4. Replace (x, w, y, z) with the new solution $(\tilde{x}, \tilde{y}, \tilde{w}, \tilde{z})$

Path-Following Method
1. Estimating μ

- We must find an appropriate value for μ.
- Too high, we might converge to the analytic center of the feasible set.
- Too low, we will converge to the edge of the feasible set that might be suboptimal.

$$\mu = \delta \frac{z^T x + y^T w}{n + m}$$

Path-Following Method
2. Compute step directions $(\Delta x, \Delta w, \Delta y, \Delta z)$

Recall the given equations defining the point $(x_\mu, w_\mu, y_\mu, z_\mu)$ on the central path:

$$\begin{aligned} Ax + w &= b \\ A^T y - z &= c \\ XZe &= \mu e \\ YWe &= \mu e \end{aligned}$$

Path-Following Method
2. Compute step directions $(\Delta x, \Delta w, \Delta y, \Delta z)$

Given a new point $(x_\mu + \Delta x, w_\mu + \Delta w, y_\mu + \Delta y, z_\mu + \Delta z)$, we get the following equations:

$$\begin{aligned} A(x + \Delta x) + (w + \Delta w) &= b \\ A^T(y + \Delta y) - (z + \Delta z) &= c \\ (X + \Delta X)(Z + \Delta Z)e &= \mu e \\ (Y + \Delta Y)(W + \Delta W)e &= \mu e \end{aligned}$$

Path-Following Method
2. Compute step directions $(\Delta x, \Delta w, \Delta y, \Delta z)$

We rewrite the equations so the unknowns are on the left and the data on the right:

$$\begin{aligned}
A\Delta x + \Delta w &= b - Ax - w \\
A^T\Delta y - \Delta z &= c - A^Ty + z \\
Z\Delta x + X\Delta z + \Delta X \Delta Z e &= \mu e - XZe \\
W\Delta y + Y\Delta w + \Delta Y \Delta W e &= \mu e - YWe
\end{aligned}$$

Path-Following Method
2. Compute step directions $(\Delta x, \Delta w, \Delta y, \Delta z)$

Then we transform the equations into a linear system by dropping the nonlinear terms:

$$\begin{aligned}
A\Delta x + \Delta w &= b - Ax - w \\
A^T\Delta y - \Delta z &= c - A^T y + z \\
Z\Delta x + X\Delta z &= \mu e - XZe \\
W\Delta y + Y\Delta w &= \mu e - YWe
\end{aligned}$$

Path-Following Method
3. Compute a new step length parameter θ

- Whenever we find the step direction, we need to determine the **step length** θ.
- Recall that we want to replace (x, w, y, z) with the new solution $(\tilde{x}, \tilde{y}, \tilde{w}, \tilde{z})$ by:

$$\begin{aligned} \tilde{x} &= x + \theta\Delta x, & \tilde{y} &= y + \theta\Delta y \\ \tilde{w} &= w + \theta\Delta w, & \tilde{z} &= z + \theta\Delta z \end{aligned}$$

The solution to this system of linear equation corresponds to the aplication of the Newton method on the primal-dual equations and μ-complementary equations.

Path-Following Method

3. Compute a new step length parameter θ

- We need to guarantee that:

$$x_j + \theta\Delta x > 0, \quad j = 1, 2, \ldots, n.$$

Path-Following Method
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- We need to guarantee that:

$$x_j + \theta \Delta x > 0, \quad j = 1, 2, \ldots, n.$$

- Similarly for w, y and z.

Path-Following Method
3. Compute a new step length parameter θ

- We need to guarantee that:

$$x_j + \theta \Delta x > 0, \quad j = 1, 2, \ldots, n.$$

- Similarly for w, y and z.

$$\frac{1}{\theta} = \max_{ij} \left\{ -\frac{\Delta x_j}{x_j}, -\frac{\Delta w_i}{w_i}, -\frac{\Delta y_i}{y_i}, -\frac{\Delta z_j}{z_j} \right\}$$

Path-Following Method

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- Similarly for w, y and z.

$$\frac{1}{\theta} = \max_{ij} \left\{ -\frac{\Delta x_j}{x_j}, -\frac{\Delta w_i}{w_i}, -\frac{\Delta y_i}{y_i}, -\frac{\Delta z_j}{z_j} \right\}$$

- We introduce a parameter r that is close to but strictly less than one.

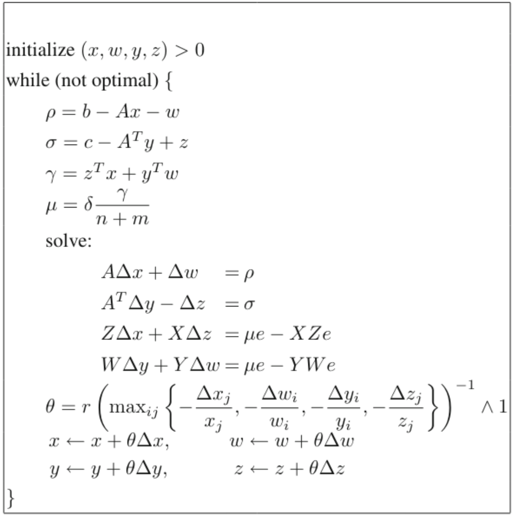
$$\theta = r \left(\max_{ij} \left\{ -\frac{\Delta x_j}{x_j}, -\frac{\Delta w_i}{w_i}, -\frac{\Delta y_i}{y_i}, -\frac{\Delta z_j}{z_j} \right\} \right)^{-1} \wedge 1$$

Path-Following Method
4. Replace (x, w, y, z) with $(\tilde{x}, \tilde{y}, \tilde{w}, \tilde{z})$

Now we can replace (x, w, y, z) with $(\tilde{x}, \tilde{y}, \tilde{w}, \tilde{z})$:

$$\begin{aligned} \tilde{x} &= x + \theta \Delta x, & \tilde{y} &= y + \theta \Delta y \\ \tilde{w} &= w + \theta \Delta w, & \tilde{z} &= z + \theta \Delta z \end{aligned}$$

Path-Following Method
Pseudo-code of the path-following method



```
initialize $(x, w, y, z) > 0$
while (not optimal) {
    $\rho = b - Ax - w$
    $\sigma = c - A^T y + z$
    $\gamma = z^T x + y^T w$
    $\mu = \delta \frac{\gamma}{n+m}$
    solve:
        $A\Delta x + \Delta w = \rho$
        $A^T \Delta y - \Delta z = \sigma$
        $Z\Delta x + X\Delta z = \mu e - XZe$
        $W\Delta y + Y\Delta w = \mu e - YWe$
    $\theta = r \left( \max_{ij} \left\{ -\frac{\Delta x_j}{x_j}, -\frac{\Delta w_i}{w_i}, -\frac{\Delta y_i}{y_i}, -\frac{\Delta z_j}{z_j} \right\} \right)^{-1} \wedge 1$
    $x \leftarrow x + \theta \Delta x,$        $w \leftarrow w + \theta \Delta w$
    $y \leftarrow y + \theta \Delta y,$        $z \leftarrow z + \theta \Delta z$
}
```

Optimality

- We have converged to a solution, but how do we know if it is optimal?

Optimality

- We have converged to a solution, but how do we know if it is optimal?
- Recall from the duality theory that we need to meet the following criteria for the solution to be optimal:
  Primal feasibility:
  $$\|\rho\|_1 = \|b - Ax - w\|_1$$
  Dual feasibility:
  $$\|\sigma\|_1 = \|c - A^T y + z\|_1$$
  Complementarity:
  $$\gamma = z^T x + y^T w$$

Optimality

- When do we stop?
- Let $\epsilon > 0$ be a small tolerance and $M < \infty$ be a large finite tolerance
- $\|x\|_\infty > M$ then the primal problem is unbounded.
- $\|y\|_\infty > M$ then the dual problem is unbounded.
- If $\|\rho\|_1 < \epsilon$, $\|\sigma\|_1 < \epsilon$, and $\gamma < \epsilon$ then we found our optimal solution!

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Implementation example

Consider the following LP problem:

Primal problem:

$$\begin{aligned} \max \quad & 5x_1 + 4x_2 + 3x_3 \\ \text{s.t.} \quad & 2x_1 + 3x_2 + x_3 \leq 5 \\ & 4x_1 + x_2 + 2x_3 \leq 11 \\ & 3x_1 + 4x_2 + 2x_3 \leq 8 \\ & x_1, x_2, x_3 \geq 0 \end{aligned}$$

Dual problem:

$$\begin{aligned} \max \quad & 5y_1 + 11y_2 + 8y_3 \\ \text{s.t.} \quad & 2y_1 + 4y_2 + 3_y3 \leq 5 \\ & 3y_1 + y_2 + 4y_3 \leq 4 \\ & y_1 + 2y_2 + 2y_3 \leq 3 \\ & y_1, y_2, y_3 \geq 0 \end{aligned}$$

Implementation example

Both are converted into equality form:

Primal problem:

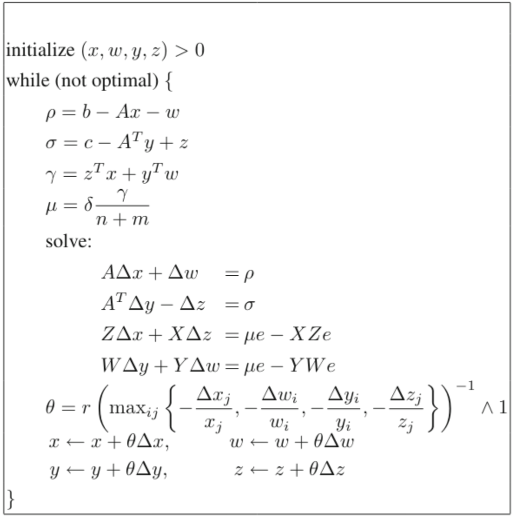
$$\begin{aligned} \max \quad & 5x_1 + 4x_2 + 3x_3 \\ \text{s.t.} \quad & 2x_1 + 3x_2 + x_3 + w_1 = 5 \\ & 4x_1 + x_2 + 2x_3 + w_2 = 11 \\ & 3x_1 + 4x_2 + 2x_3 + w_3 = 8 \\ & x_1, x_2, x_3, w_1, w_2, w_3 \geq 0 \end{aligned}$$

Dual problem:

$$\begin{aligned} \max \quad & 5y_1 + 11y_2 + 8y_3 \\ \text{s.t.} \quad & 2y_1 + 4y_2 + 3_{y_3} + z_1 \leq 5 \\ & 3y_1 + y_2 + 4y_3 + z_2 \leq 4 \\ & y_1 + 2y_2 + 2y_3 + z_3 \leq 3 \\ & y_1, y_2, y_3, z_1, z_2, z_3 \geq 0 \end{aligned}$$

Implementation example

Recall that we are following the pseudo-code:



```
initialize $(x, w, y, z) > 0$
while (not optimal) {
    $\rho = b - Ax - w$
    $\sigma = c - A^T y + z$
    $\gamma = z^T x + y^T w$
    $\mu = \delta \frac{\gamma}{n + m}$
    solve:
        $A\Delta x + \Delta w = \rho$
        $A^T \Delta y - \Delta z = \sigma$
        $Z\Delta x + X\Delta z = \mu e - XZe$
        $W\Delta y + Y\Delta w = \mu e - YWe$
    $\theta = r \left( \max_{ij} \left\{ -\frac{\Delta x_j}{x_j}, -\frac{\Delta w_i}{w_i}, -\frac{\Delta y_i}{y_i}, -\frac{\Delta z_j}{z_j} \right\} \right)^{-1} \wedge 1$
    $x \leftarrow x + \theta \Delta x,$        $w \leftarrow w + \theta \Delta w$
    $y \leftarrow y + \theta \Delta y,$        $z \leftarrow z + \theta \Delta z$
}
```

Implementation example

Initialize $(x, w, y, z) > 0$ with arbitrary values:

$$x = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}, w = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}, y = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}, z = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}$$

Implementation example

Initialize $(x, w, y, z) > 0$ with arbitrary values:

$$x = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}, w = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}, y = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}, z = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix}$$

Then initialize b, c, A and A^T

$$b = \begin{bmatrix} 5 \\ 11 \\ 8 \end{bmatrix}, c = \begin{bmatrix} 5 \\ 4 \\ 3 \end{bmatrix}, A = \begin{bmatrix} 2, 3, 1 \\ 4, 1, 2 \\ 3, 4, 2 \end{bmatrix}, A^T = \begin{bmatrix} 2, 4, 3 \\ 3, 1, 4 \\ 1, 2, 2 \end{bmatrix}$$

Implementation example

$$\rho = b - Ax - w = \begin{bmatrix} 5 \\ 11 \\ 8 \end{bmatrix} - \begin{bmatrix} 2,3,1 \\ 4,1,2 \\ 3,4,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} - \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.3 \\ 10.2 \\ 7 \end{bmatrix}$$

Implementation example

$$\rho = b - Ax - w = \begin{bmatrix} 5 \\ 11 \\ 8 \end{bmatrix} - \begin{bmatrix} 2,3,1 \\ 4,1,2 \\ 3,4,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} - \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.3 \\ 10.2 \\ 7 \end{bmatrix}$$

$$\sigma = c - A^T y + z = \begin{bmatrix} 5 \\ 4 \\ 3 \end{bmatrix} - \begin{bmatrix} 2,4,3 \\ 3,1,4 \\ 1,2,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.2 \\ 3.3 \\ 2.6 \end{bmatrix}$$

Implementation example

$$\rho = b - Ax - w = \begin{bmatrix} 5 \\ 11 \\ 8 \end{bmatrix} - \begin{bmatrix} 2,3,1 \\ 4,1,2 \\ 3,4,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} - \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.3 \\ 10.2 \\ 7 \end{bmatrix}$$

$$\sigma = c - A^T y + z = \begin{bmatrix} 5 \\ 4 \\ 3 \end{bmatrix} - \begin{bmatrix} 2,4,3 \\ 3,1,4 \\ 1,2,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.2 \\ 3.3 \\ 2.6 \end{bmatrix}$$

$$\gamma = z^T x + y^T w = \begin{bmatrix} 0.1, 0.1, 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + \begin{bmatrix} 0.1, 0.1, 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = 0.06$$

Implementation example

$$\rho = b - Ax - w = \begin{bmatrix} 5 \\ 11 \\ 8 \end{bmatrix} - \begin{bmatrix} 2,3,1 \\ 4,1,2 \\ 3,4,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} - \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.3 \\ 10.2 \\ 7 \end{bmatrix}$$

$$\sigma = c - A^T y + z = \begin{bmatrix} 5 \\ 4 \\ 3 \end{bmatrix} - \begin{bmatrix} 2,4,3 \\ 3,1,4 \\ 1,2,2 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = \begin{bmatrix} 4.2 \\ 3.3 \\ 2.6 \end{bmatrix}$$

$$\gamma = z^T x + y^T w = \begin{bmatrix} 0.1, 0.1, 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + \begin{bmatrix} 0.1, 0.1, 0.1 \end{bmatrix} \cdot \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} = 0.06$$

$$\mu = \delta \frac{\gamma}{n+m} = 0.1 \frac{0.06}{3+3} = 0.001$$

Where $\delta = 0.1$, $n = 3$ and $m = 3$.

Implementation example

Crucial part, we create our linear system of equations.

$$A\Delta x + \Delta w = \rho \tag{1}$$
$$A^T\Delta y - \Delta z = \sigma \tag{2}$$
$$Z\Delta x + X\Delta z = \mu e - XZe \tag{3}$$
$$W\Delta y + Y\Delta w = \mu e - YWe \tag{4}$$

We define right-hand side first:

$$rhs1 = \begin{bmatrix} 4.3 \\ 10.2 \\ 7 \end{bmatrix}, rhs2 = \begin{bmatrix} 4.2 \\ 3.3 \\ 2.6 \end{bmatrix}, rhs3 = \begin{bmatrix} -0.009 \\ -0.009 \\ -0.009 \end{bmatrix} rhs4 = \begin{bmatrix} -0.009 \\ -0.009 \\ -0.009 \end{bmatrix}$$

Recall that $X = \begin{bmatrix} 0.1, 0, 0 \\ 0, 0.1, 0 \\ 0, 0, 0.1 \end{bmatrix}$. Similarly for W, Y, and Z.

Implementation example

Left-hand side, we define M1, M2, M3 and M4 that corresponds to the right-hand side.

$$M1 = \begin{bmatrix} 2, 3, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0 \\ 4, 1, 2, 0, 1, 0, 0, 0, 0, 0, 0, 0 \\ 3, 4, 2, 0, 0, 1, 0, 0, 0, 0, 0, 0 \end{bmatrix}$$

$$M2 = \begin{bmatrix} 0, 0, 0, 0, 0, 0, 2, 4, 3, -1, -0, -0 \\ 0, 0, 0, 0, 0, 0, 3, 1, 4, -0, -1, -0 \\ 0, 0, 0, 0, 0, 0, 1, 2, 2, -0, -0, -1 \end{bmatrix}$$

$$M3 = \begin{bmatrix} 0.1, 0, 0, 0, 0, 0, 0, 0, 0, 0.1, 0, 0 \\ 0, 0.1, 0, 0, 0, 0, 0, 0, 0, 0, 0.1, 0 \\ 0, 0, 0.1, 0, 0, 0, 0, 0, 0, 0, 0, 0.1 \end{bmatrix}$$

$$M4 = \begin{bmatrix} 0, 0, 0, 0.1, 0, 0, 0.1, 0, 0, 0, 0, 0 \\ 0, 0, 0, 0, 0.1, 0, 0, 0.1, 0, 0, 0, 0 \\ 0, 0, 0, 0, 0, 0.1, 0, 0, 0.1, 0, 0, 0 \end{bmatrix}$$

Implementation example

Using Python (3.10) and numpy (1.26.4), we solve the system using `np.linalg.solve(M, rhs)` to retrieve the delta values:

$$\Delta x = \begin{bmatrix} 2.011 \\ -0.153 \\ 1.147 \end{bmatrix}, \Delta w = \begin{bmatrix} -0.411 \\ 0.015 \\ -0.716 \end{bmatrix}, \Delta y = \begin{bmatrix} 0.321 \\ -0.105 \\ 0.626 \end{bmatrix}, \Delta z = \begin{bmatrix} -2.101 \\ 0.063 \\ -1.237 \end{bmatrix}$$

Then we retrieve θ:

$$\begin{aligned} \theta = r\left(\max_{ij}\left\{-\frac{\Delta x_j}{x_j}, -\frac{\Delta w_i}{w_i}, -\frac{\Delta y_i}{y_i}, -\frac{\Delta z_j}{z_j}\right\}\right)^{-1} \wedge 1 \\ = 0.043 \end{aligned}$$

Implementation example

New solution:

$$x = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + 0.011 \cdot \begin{bmatrix} 2.011 \\ -0.153 \\ 1.147 \end{bmatrix} = \begin{bmatrix} 0.186 \\ 0.093 \\ 0.149 \end{bmatrix}$$

$$w = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + 0.011 \cdot \begin{bmatrix} -0.411 \\ 0.015 \\ -0.716 \end{bmatrix} = \begin{bmatrix} 0.082 \\ 0.100 \\ 0.069 \end{bmatrix}$$

$$y = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + 0.011 \cdot \begin{bmatrix} 0.321 \\ -0.105 \\ 0.626 \end{bmatrix} = \begin{bmatrix} 0.114 \\ 0.095 \\ 0.127 \end{bmatrix}$$

$$z = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \end{bmatrix} + 0.011 \cdot \begin{bmatrix} -2.101 \\ 0.063 \\ -1.237 \end{bmatrix} = \begin{bmatrix} 0.01 \\ 0.103 \\ 0.047 \end{bmatrix}$$

Implementation example

Is this the optimal solution?
Primal feasibility:

$$\|\rho\|_1 = 20.58$$

Dual feasibility:

$$\|\sigma\|_1 = 9.67$$

Complementarity:

$$\gamma = 0.068$$

As $\|\rho\|_1 \geq \epsilon$, $\|\sigma\|_1 \geq \epsilon$ and $\gamma \geq \epsilon$, we have not found an optimal solution yet. Therefore, we continue on our second iteration with the new x, w, y and z values.

Table of Contents

The KKT System

Given a system of equations:

$$A\Delta x + \Delta w = \rho \tag{5}$$

$$A^T \Delta y - \Delta z = \sigma \tag{6}$$

$$Z\Delta x + X\Delta z = \mu e - XZe \tag{7}$$

$$W\Delta y + Y\Delta w = \mu e - YWe \tag{8}$$

The KKT System

Given a system of equations:

$$A\Delta x + \Delta w = \rho \tag{5}$$
$$A^T\Delta y - \Delta z = \sigma \tag{6}$$
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In the previous example, it might be possible to solve a linear system of equations in a small problem. But what if the problem is larger? We transform the system into a **symmetric** linear system in matrix form:

$$\left[\begin{array}{cc|cc} -XZ^{-1} & & -I & \\ & & A & I \\ \hline -I & A^T & & \\ & I & & YW^{-1} \end{array}\right] \left[\begin{array}{cc} \Delta z & \Delta y \\ \hline \Delta x & \Delta w \end{array}\right] = \left[\begin{array}{cc} -\mu Z^{-1}e + x & \rho \\ \hline \sigma & \mu W^{-1}e - y \end{array}\right]$$

This is the Karush-Kuhn-Tucker system (KKT system)

The Reduced KKT System

The KKT system can be reduced further. We solve for Δz and Δw in equations **??** and **??**.

$$\begin{aligned} \Delta z &= X^{-1}(\mu e - XZ\epsilon - Z\Delta x) \\ \Delta w &= Y^{-1}(\mu e - YW\epsilon - W\Delta y) \end{aligned}$$

Then we substitute Δz and Δw into equations **??** and **??**.

$$\begin{aligned} A\Delta x - Y^{-1}W\Delta y &= \rho - \mu Y^{-1}e + w \\ A^T\Delta y - X^{-1}Z\Delta x &= \sigma + \mu X^{-1}e - z \end{aligned}$$

This gives us the following reduced KKT System.

The Reduced KKT System

$$\begin{bmatrix} -Y^{-1}W & A \\ A^T & X^{-1}Z \end{bmatrix} \begin{bmatrix} \Delta y \\ \Delta x \end{bmatrix} = \begin{bmatrix} b - Ax - \mu Y^{-1}e \\ c - A^T y + \mu X^{-1}e \end{bmatrix}$$

The Reduced KKT System is still symmetric. However, we can keep reducing the system into normal equations.

Normal Equations

Given the reduced KKT System:

$$A\Delta x - Y^{-1}W\Delta y = \rho - \mu Y^{-1}e + w \tag{9}$$
$$A^T\Delta y - X^{-1}Z\Delta x = \sigma + \mu X^{-1}e - z \tag{10}$$

We solve for Δy in equation **??** and eliminate it from **??** OR
We solve for Δx in equation **??** and eliminate it from **??**. We choose the latter.

$$\Delta x = -XZ^{-1}(c - A^T y + \mu X^{-1}e - A^T\Delta y)$$

Then we eliminate Δx:

$$\begin{aligned}-(Y^{-1}W + AXZ^{-1}A^T)\Delta y = b - Ax - \mu Y^{-1}e \\ - AXZ^{-1}(c - A^T y + \mu X^{-1}e)\end{aligned}$$

Normal Equations

- This gives us a system of normal equations in primal form.
- Similarly, if we choose the former option, we get a system of normal equations in dual form.
- Problem: If A has a dense column, then we end up with a dense matrix which is difficult to solve in primal form.
- Same problem if A has a dense row, which is also difficult to solve in dual form.
- Should we then use the reduced KKT matrix? Possible if the matrices are positive definite!