Algoritmi e Modelli di Ottimizzazione

Optimization Algorithms and Models

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A.A. 2015/2016

Course Introduction

Preliminary program:

- Introduction to non linear optimization
- Unconstrained optimization methods
- Constrained optimization algorithms
- Global Optimization
- Black box optimization
- Neural networks, machine learning, support vector machines
- Exact and heuristic methods for discrete optimization

General form

General form of an optimization problem:

$$\min_{x \in S} f(x)$$

with $S \subseteq \mathbb{R}^n$: feasible set, f: objective function, x decision variables.

Special cases

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

Unconstrained problem

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Unconstrained problem

$$\min_{x \geq 0} \sum_j c_j x_j$$
$$\sum_j a_{ij} x_j = b_i$$

Linear optimization problem

Special cases

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

Unconstrained problem

$$\min_{x \geq 0} \sum_j c_j x_j$$
$$\sum_j a_{ij} x_j = b_i$$

Linear optimization problem

$$\min_{x \geq 0} \sum_{ij} c_{ij} x_i x_j$$
$$\sum_j a_{ij} x_j = b_i$$

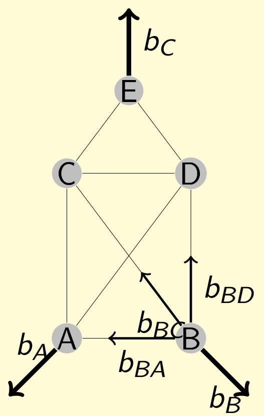
Quadratic optimization problem

Optimization application examples

Truss design

Problem: buid a structure (e.g., to hold a space telescope) which is as light–weight as possible, yet stiff enough to hold the telescope in place.

Example of a truss design:



Let $x_{ij} \in \mathbb{R}$ be the unknown tension between nodes i and j (it holds that $x_{ij} = -x_{ji}$). Negative tension: compression.

Force balance equations: for node A:

$$x_{AB} \begin{bmatrix} 1 \\ 0 \end{bmatrix} + x_{AC} \begin{bmatrix} 0 \\ 1 \end{bmatrix} + x_{AD} \begin{bmatrix} 0.6 \\ 0.8 \end{bmatrix} = -b_A$$

For node B:

$$x_{AB} \begin{bmatrix} -1 \\ 0 \end{bmatrix} + x_{BC} \begin{bmatrix} -0.6 \\ 0.8 \end{bmatrix} + x_{BD} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = -b_B$$

Truss design: balance constraints

Let p_i be the position – (x, y) coordinates – of joint i. Let

$$u_{ij} = \frac{p_j - p_i}{\|p_j - p_i\|}$$

and let b_i the required external forces. Let E be the set of pairs of nodes (joints) directly connected.
Then the equations become:

$$\sum_{j:(i,j)\in E} u_{ij} x_{ij} = -b_i \qquad \forall\, i$$

Assume now that the weight of a truss (i, j) is proportional to the absolute value of the tension $|x_{ij}|$. Then the optimization problem becomes

$$\min_x \sum_{(i,j)\in E} \ell_{ij} |x_{ij}|$$

$$\sum_{j:(i,j)\in E} u_{ij} x_{ij} = -b_i \qquad \forall\, i$$

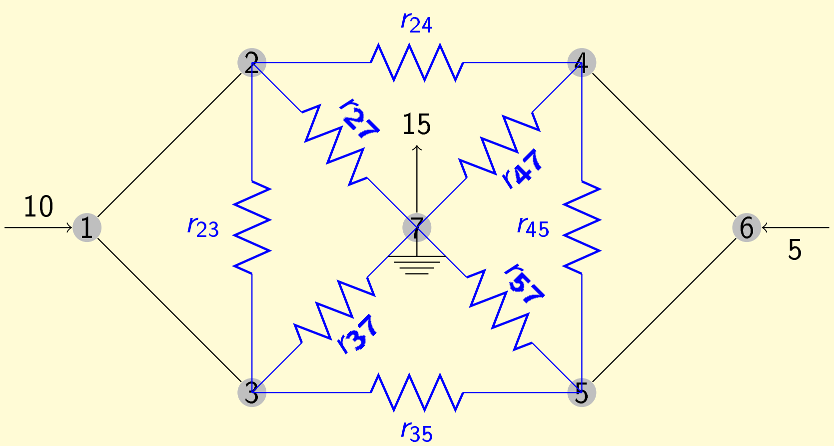
complete formulation

$$\min_x \ell_{AB}|x_{AB}| + \ell_{AC}|x_{AC}| + \cdots + \ell_{DE}|x_{DE}|$$

	AB	AC	AD	BC	BD	CD	CE	DE
A	1	0	.6					
A	0	1	.8					
B	−1			−.6	0			
B	0			.8	1			
C		0		.6		1	.6	
C		−1		−.8		0	.8	
D			−.6		0	−1		−.6
D			−.8		−1	0		.8
E							−.6	.6
							−.8	−.8

$x = b$

Example: electrical networks



Formulation

FLow balance equations (Kirchof's law): let f_{ij} be the current flow on arc (i, j). Let E: arc set. Let b_i be the demand or supply of current of each node (positive if supply, negeative if demand, 0 if transit). Then

$$\sum_{j:(v,j)\in E} f_{vj} - \sum_{i:(i,v)\in E} f_{iv} = b_i$$

Moreover:

$$f_{ij} \geq 0 \qquad \forall\,(i, j)$$

And, from Ohm's law, if r_{ij} is the resistance of link (i, j) then

$$\min_f \sum_{(i,j)\in E} r_{ij} f_{ij}^2$$

(a quadratic optimization problem with linear constraints)

Portfolio selection – Markowitz model

Given:

- a finite set of possible investment options
- the expected return p_i in investing in each asset
- the variance–covariance matrix of all investments: assuming the return of investment i is a random variable R_i:

$$Q_{ij} = E\left((R_i - p_i)(R_j - p_j)\right)$$

- a target minimum expected desired return $\bar{p}$ or, alternatively, a maximum acceptable *risk* $\bar{r}$

Assuming an investement of $x_1, \ldots, x_n$ € in assets $1, 2, \ldots, n$, the expected return is

$$\sum_i p_i x_i$$

and the risk (standard deviation) is

$$\sqrt{x^T Q x} = \sqrt{\sum_i \sum_j Q_{ij} x_i x_j}$$

Portfolio: formulations

Min risk:

$$\begin{aligned} \min x^T Q x \\ \sum_i p_i x_i \geq \bar{p} \\ \sum_i x_i = 1 \\ x_i \geq 0 \end{aligned}$$

Alternative: max profit:

$$\begin{aligned} \max \sum_i p_i x_i \\ x^T Q x \leq \bar{r} \\ \sum_i x_i = 1 \\ x_i \geq 0 \end{aligned}$$

Lennard-Jones atomic clusters

Model pair potential due to two atoms located at $X_1, X_2 \in \mathbb{R}^3$:

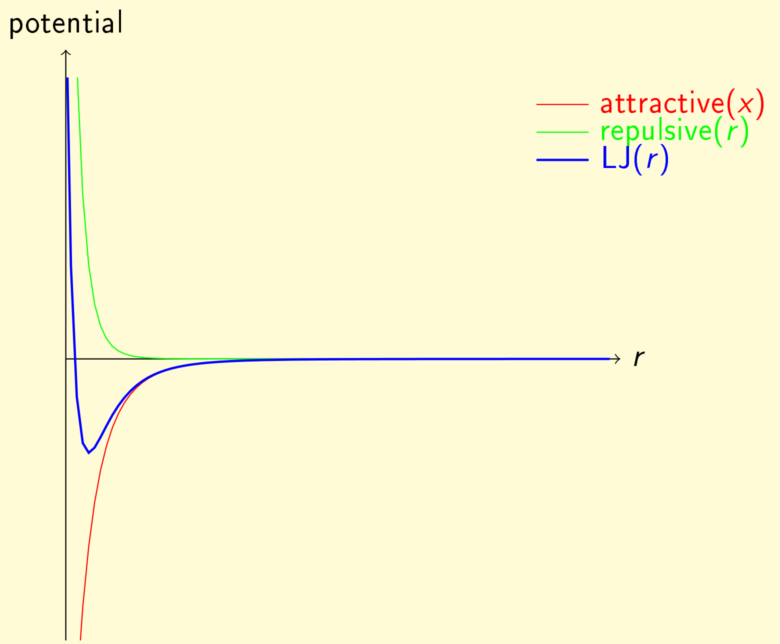
$$v(r) = \frac{1}{r^{12}} - \frac{2}{r^6}$$

where $r = \|X_1 - X_2\|$

Total energy of a cluster of N atoms located at $X_1, \ldots, X_N \in \mathbb{R}^3$ defined as:

$$\sum_{i=1,\ldots,N} \sum_{j<i} v(||X_i - X_j||)$$

Lennard–Jones pair potential



Global Unconstrained optimization model

Given N (number of atoms) find the coordinates of each so that the total potential is minimized:

$$\min_{X_1 \in \mathbb{R}^3, \ldots, X_N \in \mathbb{R}^3} \sum_{i=1}^{N} \sum_{j=i+1}^{N} v(\|X_i - X_j\|)$$