

DISCRETE OPTIMIZATION

3-4 IP MODELS

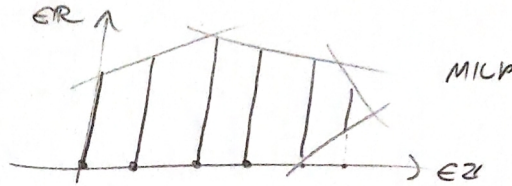
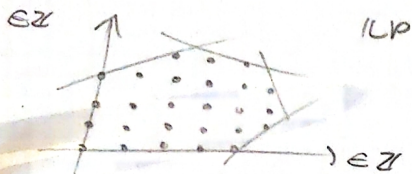
Def a mixed integer linear programming (MILP) problem is

$$\begin{aligned} \text{min } c^T x \\ \text{st } Ax \leq b \\ x \in \mathbb{Z}^{m_1} \times \mathbb{R}^{m_2} \end{aligned} \quad \left(\begin{array}{l} A \in \mathbb{Z}^{m \times (m_1 + m_2)} \\ c \in \mathbb{Z}^{m_1 + m_2} \\ b \in \mathbb{R}^m \end{array} \right)$$

$\underbrace{\mathbb{Z}^{m_1}}_{\text{integer part (m}_1 \text{ vars in } \mathbb{Z})}$ $\underbrace{\mathbb{R}^{m_2}}_{\text{mixed part (m}_2 \text{ vars in } \mathbb{R})}$

- $x_j \in \mathbb{Z} \forall j$ then we just call it ILP (integer linear prog)
- $x_j \in \mathbb{S} \{0, 1\} \forall j$ we talk of BILP (or 0/1 ILP, or linear bin prog)

BILPs are NP-hard, and (M)ILP are at least as difficult. We have $n = m_1 + m_2$ variables and m constraints. Feasible regions examples are



MODELING TECHNIQUES AND EXAMPLES

(1) A binary variable allows to model a choice between two alternatives.

EX Binary knapsack problem

variables $x_i = \begin{cases} 1 & \text{if object } i \text{ is chosen} \\ 0 & \text{otherwise} \end{cases}$

Model
$$\begin{aligned} \text{max } \sum p_i x_i \\ \text{st } \sum w_i x_i \leq b \quad (\text{capacity}) \\ x_i \in \mathbb{S} \{0, 1\} \forall i \end{aligned}$$

(2) Binary variables allow to model slow association between two entities. The decision var x_{ij} is to associate object/comp w to group/object j .

(3) Logical constraints (or linking-variables constraints) to impose that a decision x can be made only if slow y was made.

EX Unconstrained facility location (UFL)

variables x_{ij} : number of elements of client i served by plant j ;

$y_j = \begin{cases} 1 & \text{if plant } j \text{ is opened} \\ 0 & \text{otherwise} \end{cases}$

these because c_{ij} - we can have zero or more plants serving the client (i.e. demand)

Model
$$\text{min } \sum_i \sum_j c_{ij} x_{ij} + \sum_j f_j y_j$$

st
$$\sum_j x_{ij} = d_i \quad \forall i \quad (\text{natural clients demands})$$

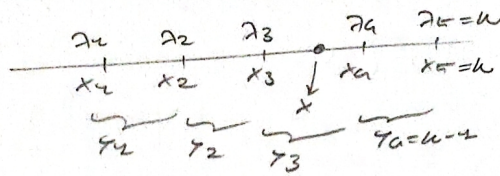
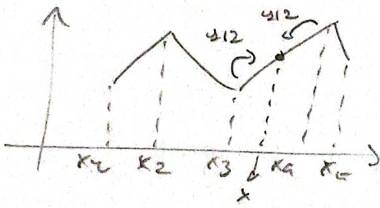
$$\sum_i x_{ij} \leq M \cdot y_j \quad \forall j \quad \text{OR} \quad x_{ij} \leq y_j \quad \forall i, j$$

(these constraints are to impose that)

$$y_j = 0 \Rightarrow x_{ij} = 0, \quad \exists x_{ij} > 0 \Rightarrow y_j = 1$$

$$0 \leq x_{ij} \leq d_i \\ y_j \in \mathbb{S} \{0, 1\} \forall j$$

(4) Piecewise linear cost functions: we have more nodes and a piecewise function there defined, and we want to choose the best all the x in that interval.



We can define $f(x) = \begin{cases} y_i & \text{if } x \text{ is inside interval } i, \text{ i.e. } (x_{i-1}, x_i) \\ 0 & \text{otherwise} \end{cases}$

min $f(x)$
 s.t. $x \in [x_1, x_5]$

(=) (can be re-computed)

min $\sum_{i=1}^k \lambda_i f(x_i)$

s.t. $\sum \lambda_i = 1$ (convex cover)
 $\sum \gamma_i = 1$ (one interval)

$\lambda_i \leq \gamma_{i-1} + \gamma_i \quad \forall i = 2, \dots, k-1$

$\lambda_1 \leq \gamma_1$

$\lambda_k \leq \gamma_{k-1}$

$\lambda_i \geq 0$

$\gamma_i \in \{0, 1\} \quad \forall i$

(5) Modeling with exponentially many constraints, eg an engine we use small components, engine variables but the we work on subsets of engines/vertices to add constraint

EX Symmetric travelling salesman problem (ATSP)

variables $x_{ij} = \begin{cases} 1 & \text{if we select arc } (i,j) \\ 0 & \text{otherwise} \end{cases}$

Model min $\sum_{(i,j) \in A} c_{ij} x_{ij}$

s.t. $\sum_{(i,j) \in \delta^+(i)} x_{ij} = 1 \quad \forall i$ (one outgoing)

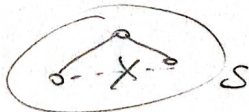
$\sum_{(i,j) \in \delta^-(i)} x_{ij} = 1 \quad \forall i$ (one incoming)

$\sum_{(i,j) \in \delta^+(i)} x_{ij} \geq 1 \quad \forall S \subset V, S \neq \emptyset$ (cutset requirements)

OR

$\sum_{(i,j) \in E(S)} x_{ij} \leq |S| - 1 \quad \forall S \subset V, 2 \leq |S| \leq n-1$

(sub-tour elimination)



$x_{ij} \in \{0, 1\} \quad \forall i, j$

$\delta^+(S) = \{(i,j) \in A : i \in S, j \notin S\}$
 $E(S) = \{(i,j) \in A : i, j \in S\}$



(6) With binary variables we can also impose disjunctive constraints. In this case let just one (binary) be valid.

$a_1 \cdot x_1 \leq b_1 \quad \text{or} \quad a_2 \cdot x_2 \leq b_2$ we solve them binary variables
 γ_1, γ_2 to decide which to activate

\Rightarrow transform from integer $a_1 \cdot x_1 - b_1 \leq M(1 - \gamma_1)$
 together with $\gamma_1 + \gamma_2 = 1$

≤ 0 if $\gamma_1 = 1$
 $\leq M$ if $\gamma_1 = 0$, and
 M is $\gg 0$ to make
 that constraint
 trivially always
 true

(7) Description of product variables.

- product of binary variables

$$z = y_1 \cdot y_2 \text{ with both } y_i \in \{0, 1\}$$

⇒ we introduce z and add the following constraint on it:

$$\begin{aligned} z &\leq y_1 \\ z &\leq y_2 \\ z &\geq y_1 + y_2 - 1 \end{aligned}$$

- product of binary and bounded continuous variable

$$z = y \cdot x \text{ with } y \in \{0, 1\} \text{ and } x \in [0, u]$$

⇒ we introduce z and the constraint:

$$\begin{aligned} z &\leq y \cdot u \\ z &\leq x \\ z &\geq 0 \\ z &\geq x - (1 - y)u \end{aligned}$$

$$\left. \begin{aligned} z &\leq y \cdot u \\ z &\leq x \\ z &\geq 0 \end{aligned} \right\} \begin{aligned} z &\leq g(y, x) \\ z &\geq x \end{aligned} \quad \begin{cases} y=0 \\ y=1 \end{cases}$$

3.2 STRONG FORMULATIONS

For MILP, the formulation of the problem is crucial. Often we will try to simplify them, hence consider to solve, to relax the integrality constraint.

Is now we talk about relaxations.

MILP

$$\begin{aligned} z_{MILP} &= \max c^T x \\ \text{s.t. } Ax &\leq b \\ x &\in \mathbb{Z}^{m_1} \times \mathbb{R}^{m_2} \end{aligned}$$

LP-relaxation

$$\begin{aligned} z_{LP} &= \max c^T x \\ \text{s.t. } Ax &\leq b \\ x &\in \mathbb{R}^{m_1+m_2} \end{aligned}$$

Prop. We know that the LP relaxation problem will end in either a better opt (i.e. for max problem, $z_{LP} \geq z_{MILP}$). If that set however is unbounded then no optimal sol for the MILP problem.

Def. A polyhedron $P = \{x \in \mathbb{R}^{m_1+m_2} : Ax \leq b, x \geq 0\} \subset \mathbb{R}^{m_1+m_2}$ is a convex hull for a mixed integer set $X \subseteq \mathbb{Z}^{m_1} \times \mathbb{R}^{m_2}$ if we know that $X = P \cap (\mathbb{Z}^{m_1} \times \mathbb{R}^{m_2})$.

Convex hulls are relaxed, continuous

Working with X a (possibly mixed) integer set, there could be different polyhedrons that lead to the same X , we different convex hulls. We look for stronger ones.

Def. Given X a mixed integer set $X \subseteq \mathbb{Z}^{m_1} \times \mathbb{R}^{m_2}$, and two polyhedrons P_1 and P_2 for X , we say that

$$P_1 \text{ is stronger than } P_2 \quad (\Leftrightarrow) \quad P_1 \subset P_2$$

$$(\Leftrightarrow) \quad P_1 \text{ is "smaller" (no more smaller to } X) \text{ than } P_2$$

To show that a convex hull P_1 is stronger than another one P_2 we need to show that:

- $P_1 \subset P_2$ (i.e. all the results of P_1 are also results of P_2)
- \exists a set $S \in P_2$ but $S \notin P_1$

Reverse that with convex hulls we are dealing with relaxed problems.

Def. (Meyer). Let $X \subseteq \mathbb{Z}^{m_1} \times \mathbb{R}^{m_2}$ be the mixed integer feasible set of a MILP with rational coeffs. Then $\text{conv}(X)$ is a rational polyhedron, and all its extreme points belong to X .

Def. Is we use just a polyhedron $P \subseteq \mathbb{R}^{m_1+m_2}$ as the convex hull of X w/ $\text{conv}(X) = P$.

Best case we could solve the MILP problem by solving its relaxation of P , i.e. solving a simple (conv) LP.

All ideas will be to solve or show combinatorial, or reasoning about which constraints to add or how to model the problem.

EX Perfect matching problem (PM)
An n cycle with n even

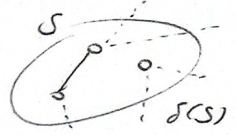
variables $x_e = \begin{cases} 1 & \text{if we select edge } e \\ 0 & \text{otherwise} \end{cases}$

Model $\min \sum_{e \in E} c_e x_e$

st $\sum_{e \in \delta(v)} x_e = 1 \quad \forall v \in V$ (one in one out - same edge)

$\left[\sum_{e \in \delta(S)} x_e \geq 1 \quad \forall S \subset V \text{ with } |S| \text{ odd} \right]$

this added constraint is needed to reach on ideal combinatorial



$x_e \in \{0, 1\} \quad \forall e \in E$

Or we can go to extended combinatorial, which is when we include additional variables, still to reach stronger combinatorial

EX Unrestricted lot sizing (ULS)

Determine the production plan for the next n time periods.

- original combinatorial:

$x_t =$ amount produced at time t

$y_t = 1$ if production occurs at time t

$z_t =$ amount in stock at the end of time t

- extended combinatorial:

$w_t =$ amount produced in time w to meet demand of future period t

(Even this we can derive x_t, y_t and z_t, w_t)

How do we compare the strength of extended combinatorial?

Def: Given a relaxation $P \subset \mathbb{R}^m \times \mathbb{R}^n$, the orthogonal projection onto the x -subspace \mathbb{R}^m is the relaxation

$$\pi_{\mathbb{R}^m}(P) = \{x \in \mathbb{R}^m : \exists w \in \mathbb{R}^n \text{ st } (x, w) \in P\}$$

variables of the extended combinatorial

We can obtain the projection using the Fourier-Motzkin method, which for simple systems is just the idea of

- isolating a variable x_i in the equations
- remove it out and add all the inequalities governing from lower and upper bounds of x_i , on the other variables.

Def: a compact combinatorial is a combinatorial with a number of variables/ constraints polynomial with the instance size.

However as usual we like strong and ideal combinatorial, which are often achieved introducing variables and/or constraints.

So often compact combinatorial are weak.

3.3 EASY ILP PROBLEMS (TU)

Convert a given ILP problem and its relaxation:

$$\begin{aligned} \min \quad & c^T x \\ \text{st} \quad & Ax = b \\ & x \in \mathbb{Z}^n \end{aligned} \quad (\text{ILP})$$

$$\begin{aligned} \min \quad & c^T x \\ \text{st} \quad & Ax = b \\ & x \geq 0 \end{aligned} \quad (\text{LP relax})$$

Assume that $A \in \mathbb{Z}^{m \times n}$, with $n \geq m$ (more variables than constraints) and also $b \in \mathbb{Z}^m$. We know that if the LP relaxation has an optimal set which is integer, then it is optimal also for the ILP.

- on LP has the optimal set on a vertex
- to each vertex components (at least) are basic feasible sol, i.e.

$$x = \begin{pmatrix} x_B \\ x_N \end{pmatrix} = \begin{pmatrix} B^{-1}b \\ 0 \end{pmatrix} \quad A = \left(\begin{array}{c|c} B & N \end{array} \right)$$

B is a basis of A , i.e. a $m \times m$ non-singular submatrix

$$\Rightarrow Ax = b \text{ becomes} \\ Bx_B + Nx_N = b \\ Bx_B = (b - Nx_N)$$

- w/ an optimal basis B has set of ± 1 , then the set $x = (x_B, x_N)$ will be integer and then optimal for ILP.

How do we guarantee that last condition? with this Def. A matrix $A \in \mathbb{Z}^{m \times n}$ is totally unimodular (TU) if every squared submatrix B of A has determinant $-1, 0, \text{ or } 1$.

Prop. We have the following properties:

- (P1) A is TU $\Leftrightarrow A^T$ is TU
- (P2) A is TU $\Leftrightarrow (A; I_m)$ is TU
- (P3) A' obtained permuting or changing the sign of some cols/rows of A is TU $\Leftrightarrow A$ is TU

Wd) this condition is useful?

Def. If $A \in \mathbb{Z}^{m \times n}$ is TU, b is integral ($\in \mathbb{Z}^m$) and

$$P(b) = \{x \in \mathbb{R}^n : Ax = b, x \geq 0\} \neq \emptyset \quad \text{relaxation of } Ax = b$$

$$\text{OR} \\ P(b) = \{x \in \mathbb{R}^n : Ax \leq b, x \geq 0\} \neq \emptyset \quad \text{relaxation of } Ax \leq b$$

\Rightarrow then all vertices of $P(b)$ are integer

\Rightarrow we to optimally solve the ILP it will be the same as LP relaxation

In practice, how do we check (often that we built the model for the machine) that a matrix is TU? We use the properties P1-P3 and the following

Prop (a sufficient condition for TUness)

- (1) $a_{ij} \in \{-1, 0, 1\} \forall i, j$
- (2) each col of A contains at most two non-zero coefficients
- (3) we can divide the rows into two groups I_1 and I_2 st for all cols j which have two non-zero coeffs we have that

$$\sum_{i \in I_1} a_{ij} = \sum_{i \in I_2} a_{ij}$$

eg for this A

$$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{array}{l} \\ I_1 \\ \\ I_2 \end{array}$$

\downarrow check $0=0$ \downarrow don't check \downarrow check $0=0$ \downarrow check $1=1$

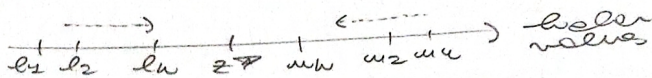
The TUness is useful when it gives us well-structured

But for some problems there are better, polynomial-time solvers, also that exploit the problem structure.

3.6 RELAXATIONS AND BOUNDS

In casual situations solving discrete optimization problems (like LPs) normally as set a reference of upper bounds and a reference of lower bounds.

$$z^D = \min_{x \in X} c(x)$$



- dual bounds:
- are LBs for a min pb
 - are obtained through a relaxation

- primal bounds:
- are UBs for a min pb
 - are obtained through heuristics (to get an feasible set X)

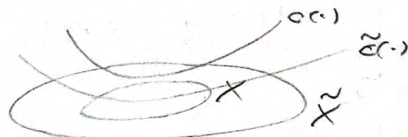
where the termination criterion will be $(uu - lu) \leq \epsilon$ (to have a desired accuracy on the obtained set).

RELAXATIONS

Def. Given the problem: we say that

(P) $z^D = \min \{ c(x) : x \in X \subseteq \mathbb{R}^n \}$

(RP) $\tilde{z} = \min \{ \tilde{c}(x) : x \in \tilde{X} \subseteq \mathbb{R}^n \}$



- RP is a relaxation of P \Leftrightarrow
- $X \subseteq \tilde{X}$ (bigger feasible region)
 - $\tilde{c}(x) \leq c(x) \forall x \in X$ (smaller obj function on X)

Prop. If RP is a relaxation of P then $\tilde{z} \leq z^D$ (we get a better optimal val)

Prop. Let \tilde{x}_{RP} be the optimal set of the RP.

- if $\tilde{x}_{RP} \in X$ (we could be P)
- and $\tilde{c}(\tilde{x}_{RP}) = c(\tilde{x}_{RP})$ (obj are equal) $\Rightarrow \tilde{x}_{RP}$ is also optimal for P

There are different possible relaxation methods:

- (1) the LP (Linear programming) relaxation: the only one we know till now. Just to remove the integrality constraint.
- (2) relaxation by elimination: simply remove one or more constraints. It's a very weak relaxation when.
- (3) surrogate relaxation (SR): replace a subset of constraints with their linear combination with multipliers $\lambda_i \geq 0$. Then look for the dual problem to get the best bound.
- (4) Lagrangian relaxation (LR): remove a "difficult" constraint and add a term in the obj function that penalizes its violation.

EX Multiple bin packing approach $x_{ij} = \begin{cases} 1 & \text{if we take object } j \text{ into bin } i \\ 0 & \text{otherwise} \end{cases}$

$$\begin{aligned} \max \quad & \sum_j w_j x_{ij} \\ \text{st} \quad & (1) \sum_j w_j x_{ij} \leq W_i \quad \forall \text{ bin } i \\ & (2) \sum_i x_{ij} \leq 1 \quad \forall \text{ item } j \\ & (3) x_{ij} \in \{0, 1\} \end{aligned}$$

- SR: $\max //$
 $\text{st} (2), (3)$
 $\sum_i \lambda_i \left(\sum_j w_j x_{ij} \right) \leq \sum_i \lambda_i (W_i)$

- LR: $\max //$ + $\sum_j \mu_j \left(1 - \sum_i x_{ij} \right)$
 $\text{st} (1)$
 (3)
 (no penalization if constraint violated)

(5) combinatorial relaxations: when we try to simplify the problem by relaxing or recalling when possible even structures to deal with (like spanning trees or cycles).

Pror. SR and LR demonstrate the relaxation b) elimination
Pror. SR demonstrates LR.
 But in practice LR is more used since it leads to fewer problems to solve.

HEURISTICS

(1) Greedy methods: build a feasible set piece-by-piece, selecting the option that leads to the best local result and without reconsidering past choices.

(2) Local search methods: We start with a current feasible set.

- start from initial \pm feasible
- at iteration k :
 - Find a best set x^* in $N(x^k)$, the neighborhood of x^k (set of nearby feasible sets)
 - if $C(x^*) < C(x^k)$, we improve, then continue with the search, otherwise return x^k

(3) Metaheuristics: try to escape from local optima. An example is Tabu search, where we allow moves to nearby sets even if they worsen the objective function, and we store the moves / directions taken to avoid come back.

- EX - Ex (1): in the binary knapsack problem we can order the items based on profit/weight ratio
- Ex (2): in STSP we can remove two random non-adjacent edges or add or and replace them to get another route
 - Ex (3): in JFL we can ex on) set of candidate objects to be added consist of $S \cup S'$ or $S' \cup S$ as nearby sets and then to move

3.6 CUTTING PLANE METHODS

We now that we solve for strong formulations. But cutting planes try to model one as complex, so the idea is to try to "remove" or restrict formulation b) solving it.

Def. $\Pi \cdot x \leq \pi_0$ is a valid inequality for $X \subseteq \mathbb{R}^n$ $\Leftrightarrow \Pi \cdot x \leq \pi_0 \quad \forall x \in X$
 \Leftrightarrow we use it as restriction b) all points of X

How do we use them? we cover

(1) add them a priori, but this will make the problem difficult to solve even for the LP relaxation or from a branch & bound approach, due to the huge # of constraints.

(2) generate them when needed, and this is the cutting plane's core idea.

Consider a convex LP form $\{STP: x \in X = P \cap Z^m\}$.

Def. A cutting plane is a candidate via $\Pi \cdot x \leq \pi_0$ or

- it is valid $\forall x \in X$, so $\Pi \cdot x \leq \pi_0 \quad \forall x \in X$
- it is not valid outside of X , so $\Pi \cdot x' > \pi_0 \quad \forall x' \in P \text{ (and } \notin X)$

actually, for us "cut" or "even $\notin X$ ", is that we cut it away

In this case there is no need to get for the whole formulation (redundant), but instead we just "trim" out regions of P bounding integer vertices, out as optimal sets.

Method: with solve $P' = P = \{x \in \mathbb{R}^n : Ax \leq b\}$, with initial LP relaxation relaxation problem. Then:

- (1) Solve the current LP relaxation with $\{s \leq x \leq t\}$.
 Let $\{s \leq x \leq t\}$ be the optimal set.
 (2) If $\{s \leq x \leq t\} \in \mathbb{Z}^n \Rightarrow$ end, with also optimal for LP
 Else:
 (2a) Solve the separation problem: given $\{s \leq x \leq t\}$, a cone, if of rows, and a row that separates $\{s \leq x \leq t\}$ from $\text{conv}(X)$ (or extended test there was none of them).
 If no found \Rightarrow that with the cutting plane and we update $P' = P \cap \{s \leq x \leq t\}$ and go back to (1)
 Else: stop, we can't further improve

We have different example/methods for generating cutting planes.
 - Chvatal-Gomory procedure: create rows via linear combinations of the constraints and rounding.

- Let $X = P \cap \mathbb{Z}^n = \{x \in \mathbb{R}^n : Ax \leq b\} \cap \mathbb{Z}^n$ is that
 $X = \{x \in \mathbb{Z}^n : \sum_{j=1}^n A_{ij} x_j \leq b_i\}$
 i -th col of A
- Choose the multiplier vector $u \in \mathbb{R}^m$ (not nec $\sum u_i = 1$) and consider $\sum_j (u^T A_{ij}) x_j \leq u^T b$
- Since $\lfloor u^T A_{ij} \rfloor \leq u^T A_{ij}$ and $x_j \geq 0$ we get that $\sum_j \lfloor u^T A_{ij} \rfloor x_j \leq u^T b$ is a row in P, X , and $\text{conv}(X)$.
- Then we can get to the integer version rounding both sides, and with a cutting plane we can valid cut and $\text{conv}(X)$ (but not nec in P).

$$\sum_{j=1}^n \lfloor u^T A_{ij} \rfloor x_j \leq \lfloor u^T b \rfloor$$

This method is very strong since we have that $\text{conv}(X)$ (Chvatal). Any row in $\text{conv}(X)$ can be obtained by applying this procedure a finite number of times.
 Also, given an fractional $\{s \leq x \leq t\}$, there exist a multiplier vector u at the CG procedure cuts within P .

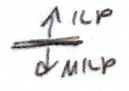
Def. Call conv Chvatal closure of P the set $P_1 = \{x \in \mathbb{R}^n : Ax \leq b, A^1 x \leq b^1\}$, where $A^1 x \leq b^1$ are all the inequalities generated by applying the vector $u \in \mathbb{R}^m$ in the CG procedure.

Def. We call Chvatal rank of $\text{conv}(X)$ the smallest integer k such that $P_k = \text{conv}(X)$.

- Gomory fractional/integers cutting planes: if $\{s \leq x \leq t\}$ is fractional, let $x^* \in \mathbb{R}^n$ be a fractional basic feasible solution. Then the integer part of the Gomory fractional cut, generated from a row t of the LP relaxation, is

$$x^* + \sum_{j \in N} \lfloor \bar{a}_{tj} \rfloor x_j \leq \lfloor \bar{b}_t \rfloor$$

\swarrow non basic variables \swarrow \bar{b} and \bar{a} come from
 $\bar{b} = B^{-1} b + B^{-1} N s$
 $\quad \quad \quad \bar{b} \quad \quad \quad \bar{a}$



- Mixed Integer Rounding (MIR) procedure, considering now MILP is $X = \{(x, y) \in \mathbb{Z} \times \mathbb{R}^+ : x - y \leq b\}$ with b not integer.
 $x - \frac{1}{1 - \{b\}} y \leq \lfloor b \rfloor$, where $\{b\} = b - \lfloor b \rfloor \geq 0$ is the fractional part of b

- Same) mixed integer (GMI) unrelaxed, still on MILPs, as now we deal with $(x \in P, \sum \mu_i x_i)$ an optimal linear feasible set of the LP relaxation. We set $\mu_i = 0$ or 1 on A and b then unrelaxed) for a constraint a at $x \in P \notin Z$:

$$x_a + \sum_{j \in N_1} (\bar{b}_{tj}) + \frac{(\sum \bar{b}_{tj} - \sum \bar{b}_{tj})^+}{4 - \sum \bar{b}_{tj}} x_j \leq \bar{b}_{tj} + \sum_{j \in N_2} \frac{(\bar{b}_{tj})^-}{4 - \sum \bar{b}_{tj}} x_j$$

non-linear integer vars
non-linear continuous vars

3.7 STRONG VIO FOR STRUCTURED ILPs

Studying the problem structure we can derive strong vns.

Def. For any $P = \{x \in \mathbb{R}^n : Ax \leq b\}$, a row $\pi \cdot x \leq \pi_0$ dominates another row $\mu \cdot x \leq \mu_0$ (valid both for P) if

$$\exists \mu > 0 : \mu \mu_0 \leq \pi_0 \text{ and } \mu \mu_0 \geq \pi_0 \text{ (with } (\frac{\pi}{\pi_0}) \neq \mu(\frac{\mu}{\mu_0}) \text{)}$$

which also means the feasible region of the first row is smaller than the one of the dominated second one.

Def. A row $\pi \cdot x \leq \pi_0$ is redundant in the description of P if exist other rows for P that their linear combination in non-neg. dominates that one. i.e.

$$\exists h \geq 2 \text{ rows } \pi_i \cdot x \leq \pi_i \text{ valid for } P, \text{ and } \exists \mu_i > 0 \text{ s.t. } \sum_{i=1}^h \mu_i \pi_i \cdot x \leq \sum_{i=1}^h \mu_i \pi_i$$

this new row dominates it

FACES AND FACETS

The sides then will be the lower bound rows which are "recessed" to describe the polyhedron $P = \{x \in \mathbb{R}^n : Ax \leq b\}$.

Def. (1) k points $x_1, \dots, x_k \in \mathbb{R}^n$ are affinely independent \Leftrightarrow the $k-1$ vectors $\{x_i - x_1\}$ can form an $(k-1)$ -plane \perp to $x_1 - x_2$ to $x_1 - x_k$

(2) $\dim(P) = (\max \# \text{ of aff. indep. pts. of } P) - 1$

(3) P is full dimensional $\Leftrightarrow \dim(P) = n$, i.e. no ineqs are active at any point $x \in P$

Def. $\dim(P) = n \Rightarrow P$ admits a unique minimal description $P = \{x \in \mathbb{R}^n : a_i \cdot x \leq b_i \text{ } i=1, \dots, m\}$ where we each ineq. is active and necessary (their deletion will lead to a different P)

and these necessary ineqs will be the facets ones.

Def. Let $F = \{x \in P : \pi \cdot x = \pi_0\}$ for any row $\pi \in P$. Then F is a face of P , and we say that the row represents/defines F . If moreover F is a face and $\dim(F) = \dim(P) - 1$, then we call it a facet.

Def. If P is full dimensional, $\dim(P) = n$

- a row is necessary to describe $P \Leftrightarrow$ it defines a facet of P
- $\Leftrightarrow \exists m$ aff. indep. points $\in P$ not w/ing it at equalty (w/ test $\dim(F) = n-1 = \dim(P)-1$)

Often the P we would be interested in ending in facets will be convex. If there is another method to show that a row defines a facet.

Let $X \subset \mathbb{Z}^n$ and $\Pi = \{ \pi_1, \dots, \pi_m \}$ be a set of m linear inequalities. Assume $\text{conv}(X)$ is bounded and $\dim(\text{conv}(X)) = n$. We check that the set is a facet if we can't:

(1) the definition (or the planar case) involves n points $x_1, \dots, x_n \in X$ not satisfying the set of inequalities and showing that they are affinely independent

(2) using our witness approach: select $t(n)$ points $x_1, \dots, x_t \in X$ not satisfying the set of inequalities. Suppose that all belong to the same extended facet $\psi^T x = \psi_0$

(2) without the extended facets $(\psi_1, \dots, \psi_m, \psi_0)$ solving the system

$$\sum_{j=1}^m \psi_j x_j = \psi^T x = \psi_0 \quad \forall k = 1, \dots, t$$

(3) if the set is not a facet $(\psi_0) = \gamma(\Pi)$ for $\gamma \neq 0$, then the set is not a facet

BINARY UNAPSACK CASE

We have $X = \{ x \in \{0,1\}^n : \sum_{j=1}^m a_j x_j \leq b_j \}$, for $N = \{1, \dots, m\}$.

Def. We call a subset $C \subseteq N$ a cover for X if $\sum_{j \in C} a_j \geq b$. A cover is minimal if $\forall j \in C, C \setminus \{j\}$ is not a cover.

Covers are useful since provide lower bounds:

Prop. If $C \subseteq N$ is a cover for X , then the following is a valid inequality:

$$\sum_{j \in C} x_j \leq |C| - 1$$

cover inequality

since covers we have to remove at least 1 when C is not a cover maybe possible set

But we have more:

Prop.

C is a minimal cover for X

$$\Leftrightarrow \text{that } \bar{x} \text{ is a facet of } P_0 = \text{conv}(X) \cap \{ x \in \mathbb{R}^n : x_j = 0 \ \forall j \notin C \}$$

we if we just look for \bar{x} only in C we see where items out of C

(4) Separation problem. If we get (eg by LP relaxation) a fractional set \bar{x} , how can we find a cut to cut it (ie violated C)?

The idea was to rewrite the row from $\sum_{j \in C} x_j \leq |C| - 1$ to $\sum_{j \in C} (1 - x_j) \geq 1$, and we add w/ \tilde{c} a row \tilde{c} that makes that cut. So the idea was to

- solve $\beta = \min \sum_{j \in N} (1 - x_j^*) z_j$

(not nec to opt)

st $\sum_{j \in N} a_j z_j \geq b$ (we still set a cover for X)
 $z_j \in \{0,1\}^m$

- look at the objective function value: if $\beta \geq 1$ then \bar{x} satisfies all cover inequalities and there is no cut to cut it.

if $\beta < 1$ (with set \bar{x}) then we can add the classical cut with $\tilde{c} = \{j : z_j^* = 1\}$ and it cuts \bar{x} .

(2) Strengthening cover inequalities. We have list of a single cover inequality

Prop. If C is a cover for X , the extended cover inequality

$$\sum_{j \in E(C)} x_j \leq |C| - 1$$

where $E(C) = C \cup \{j \in N : a_j \geq a \ \forall j \in C\}$ is still valid for X .

The lifting procedure w/ the intermediate cut structure
 & cover inequality. It is useful since
 Prop. If C is a minimal cover and $a_j \leq b \forall j \in N$, then the lifting
 procedure will yield a facet-defining inequality for
 $conv(X)$.

How does it work?

- (1) we have $X = \{x \in \{0,1\}^n : \sum_{j \in N} a_j x_j \leq b\}$
- (2) set e (variable) minimal cover $C \subseteq N$ and the corresponding cut
- (3) set an order $e \in \{1, \dots, n\}$
- (4) consider $x_i \in N \setminus C$ and find the largest a_i st

$$a_i x_i + \sum_{j \in C} x_j \leq |C| - 1$$

by studying the relevant case of when $x_i = 1$:

$$a_i \leq |C| - 1 - \sum_{j \in C} x_j \leq |C| - 1 - \max_{\substack{\text{st } \sum_{j \in C} x_j \leq b - a_i \\ \text{or } \sum_{j \in C} x_j \leq b - a_i}} \sum_{j \in C} x_j$$

or we set $x_i = 1$ w/ we
 adjust the knapsack w/ the
 lvs weight

(5) Now consider the cut w/ variables under $\sum_{j \in C} x_j + a_i x_i \leq |C| - 1$
 and repeat from step (3) with the next variable

STSP CASE (AND ATSP)

EX Symmetric TSP problem. The ATSP but now
 we have an undirected (edges) graph.
Variable $x_e = 1$ if we close edge e
Model $\sum_{e \in E} c_e x_e$
 st $\sum_{e \in \delta(v)} x_e = 2 \quad \forall v \in V$ (1)
 $\sum_{e \in E(S)} x_e \leq |S| - 1 \quad \forall S \subseteq V: S \neq \emptyset$ (2)
 $x_e \in \{0,1\} \quad \forall e \in E$ (3)

Prop. $\forall S \subseteq V: 2 \leq |S| \leq n/2$ (and $n \geq 4$) we have that constraint (2)
 defines a facet of $conv(X)$.

To the rest use the ideas. Well, move the whole w/ to move
 to the ATSP (which had constraint of $\delta(v)$ violated in (1), and
 violate it w/ LP relaxation without considering constraint (2) of
 here, but move it to add structural cutting planes.

And we can find such cutting plane (to remove a set $S \subseteq V$)
 by solving a reformulation of instances of the min cut problem.

EQUIVALENCE BETWEEN SEPARATION AND OPTIMIZATION

Let $P \subseteq \mathbb{R}^n$ be a (bounded) polyhedral set.

Opt problem: $\min_{x \in P} c^T x \rightarrow$ find $\pm \delta \in P$ minimizing $c^T \delta$ st $\delta \in P$
 or otherwise that P is empty

Sep problem: $\min_{x \in P} c^T x \rightarrow$ find a cut that separates $\pm \delta \in P$
 or otherwise that $\pm \delta \in P$

Def. The sep problem can be solved in polynomial time in n and $\ln(V)$ \Leftrightarrow the opt problem can be solved in polynomial time in n and $\ln(V)$

So one of a problem (opt) seems hard to solve (as it may have an exp number of constraints), actually can be sep (reformulated) w/ all corresponding sep problem (of the cutting plane approach) is easy to solve.

3.8 BRANCH AND CUT

Idea: embed strong valid inequalities (on the problem solution) to meet up the classical branch and bound framework.
 Idea of other solving the LP relaxation we don't cut or branch yet, we don't directly branch (not the fractional variables) but we add cuts to the formulation.

Advantages:

- (1) strengthening the formulation we get tighter dual bounds
- (2) slow convergence of pure cutting plane methods is mitigated by the branching step

3.9 COLUMN GENERATION METHOD

used on ILP problems with an exponential # of variables.
 The idea is:

- to enumerate all possible feasible sets
- represent the (additional) columns as a set machine / covering / partitioning type of formulation
- only create new variables when needed

It's also used in the cutting plane method, where we start on a set of constraints, which are not considered all explicitly but instead included/generated on the fly.

EX Cutting stock problem

2 common models, rolls of width w , but big small rolls of width w_0 instead are needed. So we cut the large one according to patterns.

- Kantorovich model:

$$z_{ILP} = \min \sum_{w \in K} y_w$$

$$\text{at } \sum_{w \in K} x_{iw} \geq b_i \quad \forall i \in I \quad (\text{demand constraint})$$

$$\sum_{i \in I} w_i x_{iw} \leq W \cdot y_w \quad \forall w \in K \quad (\text{width & vor limit})$$

$$x_{iw} = (\# \text{ of times a } w\text{-th small roll is cut in the } i\text{-th large roll}) \in \mathbb{Z}^+$$

$$y_w = (\# \text{ of } w\text{-th large rolls}) \in \{0, 1, 2, \dots\}$$

- Gilmore and Gomory model

$$z_{ILP} = \min \sum_{j \in J} x_j$$

$$\text{at } \sum_{j \in J} a_{ij} x_j \geq b_i \quad \forall i \in I \quad (\text{demand constraint})$$

$$x_j = (\# \text{ large rolls cut according to pattern } j) \in \mathbb{Z}^+$$

$$j \in J = (\text{index set of the patterns})$$

The matrix A is $m \times n$, where n will grow exponentially, not to m (ie with the number of small rolls w_1, \dots, w_m).

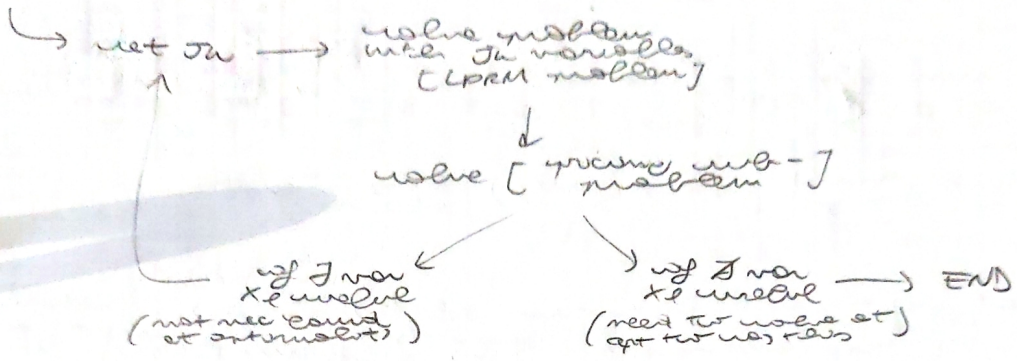
$$A = \left(\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} \right) \Bigg\}_m \quad A \text{ will be a wide matrix}$$

- But:
- at a given iteration not more than m of the n variables (the x_j) will have non zero values
 - remaining optimal LP gets will lead to (undesirable) results see

Column generation method:

- (1) consider the LP relaxation of the ILP, assuming $w=0$ and $J \subseteq I$ as the initial subset of variables.
- (2) solve w.r.t. the LP restricted master (LRM) problem on the variables selected in J .
- (3a) consider w.r.t. dual.
- (3b) solve the pricing subproblem for LRM with J to reach for an improving non-basic variable x_e .
- (4) if \exists such x_e , update $J = J \cup \{x_e\}$ and go to (2) otherwise we can't enter anymore, and LRM optimal is also optimal for the original LP relaxation of the ILP.

LP relaxation of ILP



EX Cutting stock problem ($I = \{1, \dots, m\}$) (I is the set of the small rolls)

$$\begin{aligned} \min \sum_{j \in J} x_j \\ \text{s.t. } \sum_{j \in J} a_{ij} x_j &\geq b_i \quad \forall i \in I \\ x_j &\geq 0 \quad \forall j \in J \end{aligned} \quad \left. \begin{array}{l} \text{LRM} \\ \text{dual} \end{array} \right\}$$

$$\begin{aligned} \max \sum_{i \in I} y_i b_i \\ \text{s.t. } \sum_{i \in I} a_{ij} y_i &\leq 1 \quad \forall j \in J \\ y_i &\geq 0 \quad \forall i \in I \end{aligned} \quad \left. \begin{array}{l} \text{LRM} \\ \text{dual} \end{array} \right\}$$

For the pricing subproblem we ask if there is an edge pattern (ie variable) which is feasible and useful to add to J :

(Before writing w.r.t. solve the above one optimize) \bar{c} and \bar{w} . Then:

$$\begin{aligned} \min \bar{c} = 1 - \sum_{i \in I} y_i^* d_i \\ \text{s.t. } \sum_{i \in I} w_i d_i &= W \quad (\text{pattern } w) \\ d_i &\in \mathbb{Z}^+ \end{aligned} \quad \left. \begin{array}{l} \text{pricing} \\ \text{sub-} \\ \text{problem} \end{array} \right\}$$

(we are searching for a new useful variable to be added)

- if $\bar{c} \geq 0$ (optimal of that) ≥ 0 , then there is no useful variable to add
- if $\bar{c} < 0$ (not nec. the optimal), then we add the variable represented by the d to the set J

Observations:

- choice of the initial set of variables / cols to has a strong impact
- for the pricing subproblem we can use heuristics, so we don't have to necessarily solve it at optimality
- CG method is very expensive and used in practice
- CG can be also included in a B&B (to branch and price becomes) framework.

3.10 LAGRANGIAN RELAXATION

Consider a generic LP in the form
 $\min \{ c^T x : D x \geq d, A x \geq b, x \in Z^n \}$
 competing constraints at least two combined in just having $x \in X \subseteq R^n$

Idea of Lagrangian relaxation: remove those competing constraints but add, for each of them, a penalty term (for their violation) in the objective function.

$z^* = \min_{x \in X} c^T x$ (2) original problem

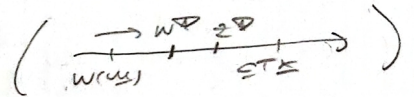
$W(\mu) = \min_{x \in X} c^T x + \mu^T (d - D x)$ (3) Lagrangian sub-problem

$w^* = \max_{\mu \geq 0} W(\mu)$ (a) Lagrangian dual

So we get that (3) is a relaxation of (2) for any multiplier vector $\mu \geq 0$. And (a) is the best we can do (we have the most restrictive bound, i.e. the closest to z^*). Otherwise there is a relaxation that is not bounded above and $w^* = z^*$.

Case (weak duality)

x feasible w.r.t. (2) $\Rightarrow W(\mu) \leq c^T x$



\Rightarrow if $W(\mu) = c^T \tilde{x}$, then \tilde{x} and μ are both optimal (for (2) and (a))

\Rightarrow if one problem is unbounded, the other is infeasible

If we relax some or equality constraints, we get the (a) with free variables μ , i.e. $\mu \geq 0$. This remains a problem:

- select a competing constraint we wish to remove
- use the dual multiplier it occurs (like "twice")
- introduce μ of continuity the above one (eg μ_i, μ_{EM})
- remove the constraint and update the obj. function

Prop. If $\mu \geq 0$ and

- $x(\mu)$ is an opt. set of (3)
 - $D x(\mu) \geq d$ (ie. unrelaxed constraints)
 - $[D x(\mu)]_i = d_i$ for each $\mu_i > 0$ (constraint not at equality) (or strictly positive μ_i)
- $\Rightarrow x(\mu)$ is also opt. for (2)

We also observe that the function $W(\mu)$ is concave (with the case of problems being min-max).

STRENGTH AND CHOICE OF LAG DUAL (a)

Problem (characterization in terms of an LP). Consider the problems (2), (3) and (a) with $X = \{ x \in Z^n : A x \geq b \}$. Then we have that

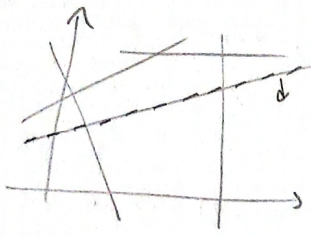
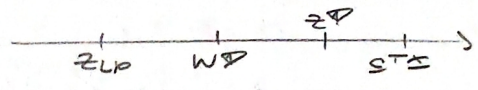
$w^* = \min_{x \in \text{conv}(X)} c^T x$ overall problem (with min and structure)

opt. set of the dual

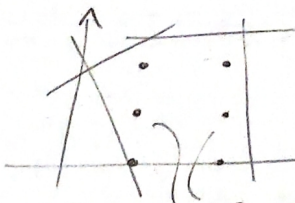
we relax the complex constraints staying in the convex hull of the remaining constraints ($A x \geq b$ and Z^n)

Con. Since $\text{conv}(X) = \text{conv}(\{x \in \mathbb{R}^n : A x \geq b\}) \subseteq \{x \in \mathbb{R}^n : A x \geq b\}$ we have

$\mathbb{Z}LP \subseteq W \subseteq \mathbb{Z}P$ — opt set of (2)
 — opt set of (a)
 — opt set of the LP relaxation of (2)
 — the set of all LP optima



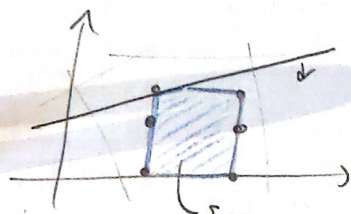
we see this and we are left with



all the removed constraints are $Ax \geq b$

these points are the set $X = \{x \in \mathbb{R}^n : Ax \geq b\}$

so we re-introduce it and we get



$\{x \in \text{conv}(X) : b \geq z\}$

- the set was first W or $\mathbb{Z}P$ could be
- removing $b \geq z$
- minimizing w.r.t STX
- over $\text{conv}(X)$ just could and the constraint $b \geq z$

Con. Since the theorem talks about optimizing on $\{x \in \text{conv}(X) : b \geq z\}$, the set of $\text{conv}(X)$ is equal to the LP relaxation of the original problem (2), we could ignore the $b \geq z$ constraint as well as the LP relaxation.

which constraint (a) should we re-introduce? we have to consider:

- the structure of the bound W
- the duality of value (3) and (a)

SOLVING LAG DUALS

We use a characterization of the subgradient method (see Ch 4 exercises) to convert recursive CT ones.

In general, the subgradient method is:

for min fct at $x \in \mathbb{R}^n$

- start from initial z_0
- at k-th iteration consider $g_k \in \partial f(x_k)$ and update $z_{k+1} = z_k - \alpha_k g_k$ ($\alpha_k > 0$)
- we don't orientate with g_k since for not all C^1 functions the direction $-g_k$ is not nec a descent one

under some assumptions (f convex, unbounded $\|x\| \rightarrow \infty$, the $\alpha_k \rightarrow 0$ but not too fast, i.e. $\sum \alpha_k = \infty$), we have that the subgradient method

- terminates after a finite # of iterations and converges to $\mathbb{Z}P$
- or admits a subsequence $\{x_{k_j}\}$ that converges to $\mathbb{Z}P$

All subgradient dual ones: min $W(x)$ s.t. $x \geq z$
 with $W(x)$ concave and piecewise linear.

How do we find subgradients of $W(x)$?
 This is a simple result:

Proof Consider $\tilde{x} \geq 0$ and $X(\tilde{x})$ is the set of optimal sets of (3)

$$W(\tilde{x}) = \min_{x \in X \cap \mathbb{R}^n} \{c^T x + \tilde{u}^T (b - Dx)\}$$

- \Rightarrow
- For each $x \in X(\tilde{x})$, the vector $(b - Dx(x)) \in \partial W(\tilde{x})$ is the convex subdifferential vector in a subdifferential of $W(\tilde{x})$.
 - The subdifferentials formed in this way span all the possible subdifferentials of $W(\tilde{x})$ at \tilde{x} .

For the procedure we:

- select initial y_0 and set $k=0$.
- solve (3) to get $W(y_k)$.
- if $x(y_k)$ opt set in (3) and $(b - Dx(y_k))$ is a subdifferential of $W(y_k)$ at y_k .
- update subdifferential multipliers as

$$y_{k+1} = \arg \min (0, y_k + \alpha_k (b - Dx(y_k)))$$
 (component-wise)
- set $k=k+1$ and repeat.

UNCONSTRAINED NONLINEAR OPT

Q. 2-2 OPTIMALITY CONDITIONS

We have a convex problem:

$$\min_{\xi \in S} f(\xi) \quad \text{with } S \subseteq \mathbb{R}^n, f: S \rightarrow \mathbb{R}, f \in C^k, k \geq 0$$

Def. $\xi \in \mathbb{R}^n$ is a feasible direction at $\xi \in S$ $(\Rightarrow) \exists \alpha > 0; \xi + \alpha d \in S \forall \alpha \in (0, \bar{\alpha}]$

(1st order) $f \in C^1(S)$ ξ local min $(\in S)$ $\Rightarrow \nabla f(\xi) \cdot d \geq 0$ \forall feasible direction at ξ ,
 \Rightarrow all feasible directions have to be ascent (nondecreasing) directions

(2nd order) $f \in C^2(S)$ ξ local min $(\in S)$ \Rightarrow (1) $\nabla f(\xi) \cdot d \geq 0 \forall$ feasible dir d at ξ
 (2) if $\nabla f(\xi) \cdot d = 0$ then (a) that d
 (3) $d^T D^2 f(\xi) d \geq 0$

Cor. $f \in C^2(S)$ ξ local min event $(\in S)$ \Rightarrow (1) $\nabla f(\xi) = 0$ (classical first condition)
 (2) $D^2 f(\xi)$ is positive semi-definite

(SUF) $f \in C^2(S)$ ξ event $(\in S)$ is not local min, ie $\nabla f(\xi) = 0$ and $D^2 f(\xi)$ is not definite $\Rightarrow \exists$ no a strict local min, ie $f(\xi) = f(x) \forall x \in N_\epsilon(\xi) \cap S$

CONVEX PROBLEMS

Now the problem is convex is:

$$\min_{\xi \in C} f(\xi) \quad \text{with } C \subseteq \mathbb{R}^n \text{ convex set } f: C \rightarrow \mathbb{R} \text{ convex function}$$

(NEC & SUF) f convex, C convex, $f \in C^1(C)$

$$\xi^* \text{ is a (global) min of } f \text{ on } C \quad (\Leftrightarrow) \quad \nabla f(\xi^*) \cdot (\xi - \xi^*) \geq 0 \quad \forall \xi \in C$$

The proof relies on the previous general result we stated above about 1st order NEC and the characterization of convex function for SUF.

There is also this

Property: f convex, C convex bounded and closed.

$$f \text{ has finite maximum over } C \quad (\Rightarrow) \quad \exists \text{ an optimal extreme point of } C$$

Q. 3-4 ITERATIVE METHODS & CONVERGENCE

now consider a general nonlinear optimization problem:

$$\min_{\xi \in S} f(\xi) \quad \text{at } g_i(\xi) \leq 0 \quad i=1, \dots, m \quad \xi \in S \subseteq \mathbb{R}^n$$

f and $g_i \in C^1$ at least
 $X = \{\xi \in S : g_i(\xi) \leq 0 \quad i=1, \dots, m\}$ is the feasible region

Most NO methods are iterative, ie:

- start from a certain $\xi_0 \in X$
- generate a sequence $\{\xi_k\}_{k=0}^{\infty}$ that converges (in some sense) to a point $\xi \in \mathbb{R}^n$ the set of desired sets (by points satisfying the above NEC optimality conditions)

We care about iterative methods because
 (1) Robust, where we want global convergence.

Def. A method is globally convergent if we reach $\|x_k - x^*\| \leq \epsilon$.
 Otherwise, if $\|x_k - x^*\| \geq \epsilon$ for $\forall k \in \mathbb{N}$ with $\epsilon > 0$, it is not globally conv.

(2) Efficient, ie fast overall.
Def. We say that $\{x_k\}$ converges to x^* with order $p \geq 1$ $\Leftrightarrow \exists \eta > 0$ (the noise) and $k_0 \in \mathbb{N}$ st $\|x_{k+1} - x^*\| \leq \eta \cdot \|x_k - x^*\|^p \quad \forall k \geq k_0$
 \Rightarrow we look for the largest p and smallest k_0

About the rate p we know that convergence (of $p=1$) is
 - linear w/ $p=1$
 - sublinear w/ $p < 1$
 - superlinear w/ $p > 1$ (actual) but with $p_k \rightarrow 0$ as $k \rightarrow \infty$.

LINE SEARCH METHODS

now consider an unconstrained opt problem
 $\min_{x \in \mathbb{R}^n} f(x)$ with $f: \mathbb{R}^n \rightarrow \mathbb{R}, C^1$ or C^2 and bounded below

The general scheme of these methods is:
 - select x_0 and $\epsilon > 0$, set $k=0$.
 While (termination criterion is not satisfied)
 - choose search direction $d_k \in \mathbb{R}^n$
 - determine step-length α_k along d_k such to
 $\min_{\alpha \geq 0} \phi(\alpha) = f(x_k + \alpha d_k)$
 - update $x_{k+1} = x_k + \alpha_k d_k$ and $k=k+1$
 end

where the termination criterion is by mean $\| \nabla f(x_k) \| \leq \epsilon$ or $|f(x_k) - f(x_{k+1})| \leq \epsilon$ or $\|x_{k+1} - x_k\| \leq \epsilon$.

About the search direction d_k we would like it to be a descent direction, and not a general structure is

$$d_k = -D_k \nabla f(x_k) \quad \text{with } D_k \text{ pos def (a matrix } n \times n)$$

About the step length α_k is sufficient to solve approximately, that one could make α_k smaller, or larger. So we get the following

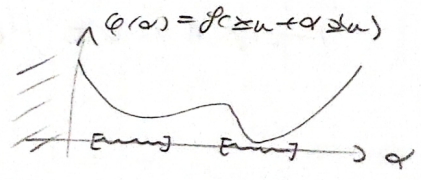
$\phi(\alpha) \leq \phi(0) + c_1 \alpha \phi'(0)$	(1)	Wolfe conditions (strong w/ (2) and (1) on the LHS)
$\phi(\alpha) \geq c_2 \phi'(0)$	(2)	

$\Rightarrow f(x_k + \alpha_k d_k) \leq f(x_k) + c_1 \alpha_k \nabla f(x_k) \cdot d_k$
 $\alpha_k \nabla f(x_k + \alpha_k d_k) \geq c_2 d_k \cdot \nabla f(x_k)$

with $0 < c_1 < c_2 < 1$

The idea is that

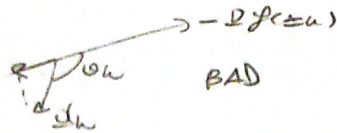
- (1) ensures that α_k makes f decrease sufficiently
- (2) ensures that α_k makes the slope $\nabla f(x_k)$ to decrease sufficiently



have this assurance that we can indeed find (under reasonable assumptions) some an intuitive choice conditions, and also an entirely new steps.

small, about global convergence, we have a result showing it can be guaranteed under suitable α_k and d_k .
 Consider $\cos(\theta_k) = \left(\frac{\text{angle between } d_k \text{ and } -\nabla f(x_k)}{\|d_k\| \cdot \|\nabla f(x_k)\|} \right) = \frac{(-\nabla f(x_k)) \cdot d_k}{\|d_k\| \cdot \|\nabla f(x_k)\|}$

usually the global convergence results when Δu is not too big and even the steepest descent direction $-\nabla f(x_k)$. The first $\cos^2(\theta_k) \geq \delta > 0$ we $\theta_k \leq \pi/2$ we Δu not \perp to $-\nabla f(x_k)$



Sub (Zwischenw.) Lemma

- or) the search method with descent Δu and α_k satisfying the conditions
- f bounded below in \mathbb{R}^n , C^1 on N open set containing $L = \{x \in \mathbb{R}^n : f(x) \leq f(x_0)\}$ and $\nabla f(x)$ is Lipschitz continuous on N

then

$$\Rightarrow \sum_{k=0}^{\infty} \cos^2(\theta_k) \cdot \|\nabla f(x_k)\|^2 < +\infty$$

(\Rightarrow) $\Delta u \rightarrow 0$ if $\cos^2(\theta_k) \geq \delta > 0$ (as to error term $\alpha_k \Delta u$ for $\alpha_k \rightarrow 0$)

and this can lead to larger step size more requirements on the matrix B_k of the Δu update

9.5 GRADIENT METHOD

Problem: Given $f: \mathbb{R}^n \rightarrow \mathbb{R}$, C^1 , look for a stationary point.
 Gradient method: with exact α_k search we

```

choose  $x_0$ , set  $k=0$ 
while (!criterion met)
    set direction  $\Delta u = -\nabla f(x_k)$ 
    find  $\alpha_k: \min_{\alpha} f(x_k + \alpha \Delta u)$ 
    update  $x_{k+1} = x_k + \alpha_k \Delta u$ ,  $k = k+1$ 
end
    
```

Remark: if α_k search is exact, successive directions are orthogonal Δu makes the method a bit slow.

What to monitor as criterion? the decrease on the x -values or on the values w is usually symmetric:

Prop. If $f(x) \in \mathbb{R}$ is μ times diff (strongly conv),

$$\|x_k - x^*\| \text{ converges (linearly) to } \leq \delta \iff \text{it converges on the value with } |f(x_k) - f(x^*)| < \delta$$

QUADRATIC STRICTLY CONVEX FUNCTIONS

$$f(x) = \frac{1}{2} x^T Q x - b^T x \quad \text{with } Q \text{ symm pos def}$$

$$(\nabla f(x) = Qx - b)$$

How choose the α_k exact search method (as α_k is easy) and we get

$$\alpha_k = \frac{\nabla f(x_k)^T \nabla f(x_k)}{\nabla f(x_k)^T Q \nabla f(x_k)} = \frac{\Delta u^T \Delta u}{\Delta u^T Q \Delta u}$$

Prop. For these functions, with exact α_k search, for $\delta > 0$ we have that $x_k \rightarrow x^*$ (is globally convergent) with linear speed and a rate dependent on condition number of Q :

$$\|x_{k+1} - x^*\|_Q^2 \leq \left(\frac{\lambda_{\max} - \lambda_{\min}}{\lambda_{\max} + \lambda_{\min}} \right)^2 \|x_k - x^*\|_Q^2 \quad (\|z\|_Q^2 = z^T Q z)$$

method is:	+ computationally cheap
	+ globally convergent
	- slow convergence

ARBITRARY FUNCTIONS

Def. If $f \in C^2$, we use exact 1D search, and we converge to $\pm \phi$ at $H(\pm \phi)$ w/o root of f (here $H(\pm \phi)$ under the role of ϕ above) then we have a similar result but involving the f' terms:

$$f(\pm u + \epsilon) - f(\pm \phi) \approx \left(\frac{\lambda_{\min} - \lambda_{\max}}{\lambda_{\min} + \lambda_{\max}} \right)^2 \cdot (f(\pm u) - f(\pm \phi))$$

9.6 NEWTON METHOD

Problem: as above but now f w/o C^2 .

(pure) Newton method: let $H(\pm) = \nabla^2 f(\pm)$.

- choose the quadratic approx of $f(\pm)$ at $\pm u$:

$$g_u(\pm) := f(\pm u) + \nabla f(\pm u) \cdot (\pm - \pm u) + \frac{1}{2} (\pm - \pm u)^T H(\pm u) (\pm - \pm u)$$

- choose $\pm u + \epsilon$ as stationary point of $g_u(\pm)$:

$$\nabla g_u(\pm) \stackrel{!}{=} 0 \quad (\Rightarrow) \quad \nabla f(\pm u) + H(\pm u) (\pm - \pm u) \stackrel{!}{=} 0$$

$$\Rightarrow \quad \pm u + \epsilon = \pm u + \underbrace{H(\pm u)^{-1}}_{\Delta u} (-\nabla f(\pm u))$$

no C^2 w/o exact search

also method is well defined if $H(\pm u)$ is invertible, and that Δu will be descent direction only if it is also root of f . There could be a Δu , but for pure Newton we have such Δu .

method w/o:	- extremely computationally
	- only locally convergent
	+ fast convergence
	+ convergent w/o affine coordinates transformations

Def. Suppose $f \in C^2$, $\pm \phi$ w/o at $\nabla f(\pm \phi) = 0$ and $H(\pm \phi)$ w/o root of and Lipschitz continuous. Then

Can $\pm \phi$ be reached close to $\pm \phi$ \Rightarrow (1) $\pm u \rightarrow \pm \phi$ quadratically, (2) $\|\nabla f(\pm u)\| \rightarrow 0$ quadratically

MODIFICATIONS AND EXTENSIONS

(1) If $\Delta u = \epsilon$ does not vanish, maybe continuous we can set ϵ w/o) with smallest search.

(2) To guarantee to have Δu well defined and a descent direction we could set

$$\text{not strictly} \quad \Delta u = H(\pm u)^{-1} (-\nabla f(\pm u))$$

$$\text{but rather} \quad \Delta u = (\epsilon u I + H(\pm u))^{-1} (-\nabla f(\pm u))$$

(3) Using trust regions: we could limit the search of Δu and Δu just on a region $B_r(\pm u)$ or which Δu is, approximate well $f(\pm)$.

CONJUGATE GRADIENT METHOD

Def. Let Q a $n \times n$ non-singular matrix. Two vectors $z_1, z_2 \in \mathbb{R}^n$ are Q -conjugate w.r.t. $\langle z_1, z_2 \rangle = z_1^T Q z_2 = 0$.

If Q is sym \Rightarrow Def. A set of vectors z_1, \dots, z_n mutually Q -conj are also linear independent.

Consider the case of quadratic strictly convex functions, w $f(z) = \frac{1}{2} z^T Q z - b^T z$.

Def. Let z_0, \dots, z_{n-1} be n Q -conjugate directions.

\Rightarrow the seq z_k generated according to the usual line search scheme

$$z_{k+1} = z_k + \alpha_k z_k, \quad \alpha_k = - \frac{\nabla f(z_k) \cdot z_k}{z_k^T Q z_k}$$

terminate to the value of z_k at most n iterations
 $z^* = z_0 + \sum_{k=0}^{n-1} \alpha_k z_k$

Remark: The optimization is "incremental", in the sense that $z^* = z_k + \alpha_k z_k \Rightarrow$ the global optimum, at each of the z_k into the optimum.

- the full-variables are $\{z \in \mathbb{R}^n : z = z_k + \alpha z_k, \alpha \in \mathbb{R}\}$
- the full-variables space $\{z \in \mathbb{R}^n : z = z_0 + \sum_{k=0}^{n-1} \alpha_k z_k\} = \mathbb{R}^n$



$\Rightarrow \nabla f(z_k) \perp z_k$

How we derive Q -conjugate directions?

- initialization: $z_0, \alpha_0 = -\nabla f(z_0), h=0$
- iteration:

$$z_{k+1} = z_k + \alpha_k z_k$$

$$\alpha_k = \frac{-\nabla f(z_k) \cdot z_k}{z_k^T Q z_k}$$

(α_k can be chosen exact line search to minimize $f(z_k + \alpha_k z_k)$)
 $= \frac{z_k \cdot \nabla f(z_k)}{z_k^T Q z_k}$

two part resembles the local descent direction

$$\alpha_{k+1} = -\nabla f(z_k + \alpha_k z_k) \cdot z_k$$

$$\beta_k = \frac{\nabla f(z_k + \alpha_k z_k) \cdot (Q z_k)}{z_k^T Q z_k}$$

$$= (\beta_k) \frac{\|\nabla f(z_k + \alpha_k z_k)\|^2}{\|z_k\|^2}$$

$$= \frac{\nabla f(z_k + \alpha_k z_k)^T (\nabla f(z_k + \alpha_k z_k) - \nabla f(z_k))}{\|z_k\|^2}$$

method is: + no computational burden
 - requires exact/accurate Q search ($Q z_k$) to not lose Q -conjugacy
 - not invariant w.r.t. affine transformations
 (small α \rightarrow faster convergence w.r.t. gradient method)
 \rightarrow lower comp load w.r.t. Newton
 + can be accelerated recombination

CONJUGATE DIRECTION METHODS

now we are in the case of arbitrary functions.

- initialization: $z_0, \alpha_0 = -\nabla f(z_0), h=0$
- iteration

$$z_{k+1} = z_k + \alpha_k z_k$$

(α_k w.r.t. exact Q search)

$$\alpha_{k+1} = -\nabla f(z_k + \alpha_k z_k) \cdot z_k$$

$$\beta_k = \frac{\|\nabla f(z_k + \alpha_k z_k)\|^2}{\|\nabla f(z_k)\|^2}$$

Fletcher-Reeves

$$\beta_k = \frac{\nabla f(z_k + \alpha_k z_k) \cdot (\nabla f(z_k + \alpha_k z_k) - \nabla f(z_k))}{\|\nabla f(z_k)\|^2}$$

Polak-Ribiere

method us: + to be real - best choice for large n problems + even computationally cost + globally convergent if restart version (or even without)

QDM (Convergence, CQ): usually, the more we iterate (ie $k \uparrow$), the better and estimates we get.

$$\| \frac{z_{k+1} - z^*}{\|z_{k+1}\|} \|_2 \leq \left(\frac{\lambda_{\min} - \lambda_2}{\lambda_{\min} + \lambda_2} \right)^2 \| \frac{z_0 - z^*}{\|z_0\|} \|_2$$

($\lambda_1 \geq \dots \geq \lambda_n$ eigenvals of Q)

QDM (Convergence, CD): convergence is super-linear when n iterations (under $f \in C^2$, QR method, exact result; but will only hold for PR and exact result).

QUASI-NEWTON METHODS

Idea: rather than using $\nabla^2 f(z_k)$, we extract 2nd order information through variations of $\nabla f(z)$.

$z_{k+1} = z_k + \alpha_k \Delta_k \rightarrow$ Newton: $\Delta_k = (\nabla^2 f(z_k))^{-1} (-\nabla f(z_k))$
 \rightarrow Quasi-Newton: $\Delta_k = H_k (-\nabla f(z_k))$
 \Rightarrow we try to approximate $\nabla^2 f$ for 2nd order approx of the inverse of the Hessian

method us: + always well defined (and descent) directions + all involves 1st order derivatives + iteration cost $O(n^2)$ w/ $O(n^3)$ of Newton - requires storing / computing matrices (invariant w/ CQ or CD methods)

How do we characterize H_k ? ie how do we derive the 2nd order information?

$$f(z_k + \delta) \approx f(z_k) + \delta^T \nabla f(z_k) + \frac{1}{2} \delta^T \nabla^2 f(z_k) \delta$$

$$\frac{\partial}{\partial \delta} \rightarrow \nabla f(z_k + \delta) \approx \nabla f(z_k) + \nabla^2 f(z_k) \delta$$

\downarrow set $\Delta_k := z_{k+1} - z_k$

$$\Delta_k := \nabla f(z_{k+1}) - \nabla f(z_k) \approx \nabla^2 f(z_k) (\Delta_k)$$

$$\Delta_k \approx [\nabla^2 f(z_k)] \Delta_k$$

$$[\nabla^2 f(z_k)]^{-1} \Delta_k \approx \Delta_k$$

\Rightarrow recast (*) condition: $H_{k+1} \Delta_k = \Delta_k$

+ invariant w/... change + less sensitive to inexact 2D search

+ can end after closed form

But in this case we not yet determined H_{k+1} . So how do we update H_{k+1} ?

- rank 1 update: $H_{k+1} = H_k + \alpha_k \gamma_k \gamma_k^T$

(*) $\Rightarrow H_k \Delta_k + \alpha_k \gamma_k \gamma_k^T \Delta_k = \Delta_k$
 $\alpha_k \gamma_k (\gamma_k^T \Delta_k) = \Delta_k - H_k \Delta_k$

measure $\gamma_k^T \Delta_k$ on both sides

$\alpha_k = \frac{1}{\gamma_k^T \Delta_k}$ we can not throw away Δ_k

Eventually this procedure will reach the true value (with $H_n = Q^{-1}$) but this rank 2 does not converge to Δf for us more than

rank 2 update: $H_{n+1} = H_n + \alpha_n \Delta y \Delta y^T + \beta_n \Delta y \Delta y^T$

$$(\Phi) \Rightarrow H_n \Delta u + \alpha_n \Delta y \Delta y^T \Delta u + \beta_n \Delta y \Delta y^T \Delta u = \Delta u$$

$$\frac{\alpha_n \Delta y (\Delta y^T \Delta u)}{\Delta y^T \Delta u} + \frac{\beta_n \Delta y (\Delta y^T \Delta u)}{\Delta y^T \Delta u} = \Delta u - H_n \Delta u$$

$$\alpha_n = \frac{1}{\Delta y^T \Delta u} = \frac{1}{\Delta u^T \Delta u} \quad \beta_n = \frac{-1}{\Delta y^T \Delta u} = \frac{-1}{(H_n \Delta u)^T \Delta u} = \frac{-1}{\Delta u^T H_n \Delta u}$$

We get in this way the DFP method.
 Prop. of this exists:

curvature (B) condition: $\Delta u^T B \Delta u > 0 \quad \forall \Delta u \neq 0 \Rightarrow$

DFP method preserves pos def of H_n (we if 40 was done the search dir will be 1)

But this condition is easy to come, so we see error.

if Δu search vectors satisfy conditions \Rightarrow (B) holds $\forall \Delta u \neq 0$

Forwards BFGS method, the idea is now to construct approximations (series) of the Hessian (rather than with inverse) but in a way that could be easily inverted.

So now for (Φ) we ask $B_n = B_n + \alpha_n \Delta u$ and again we can check w/ incremental search rank 2 updates.

Like the (Φ) inversion case from a result of lines above due to Sherman and Morrison.

BFGS has most of the same properties of DFP, but it's more robust in numerical terms.

Once we invert the BFGS matrix we can also compare w/ directly with the DFP one to describe the Broyden class of methods:

$$H_{n+1} = (1-\rho) H_{n+1}^{DFP} + (\rho) H_{n+1}^{BFGS}$$

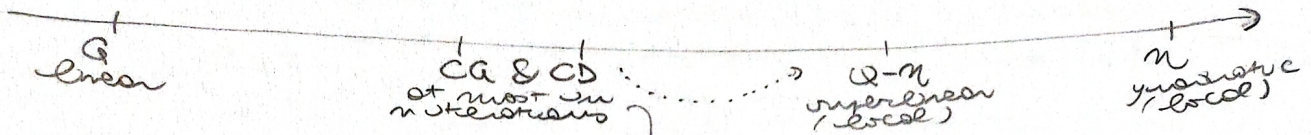
CONVERGENCE

Like (Dennis and Moré) (Moré), we can prove convergence of Δu (technical part, of EC3, B_n pos def, $\Delta u = \alpha \Delta u$, $\neq \Phi$ iterations) point is $\Delta f(\pm \Phi) = 0$ and local opt is $\Delta f(\pm \Phi)$ and def) the accuracy of B_n w/ the real Hessian $\Delta f(\pm \Phi)$ increases in the direction over Δu :

$$\lim_{k \rightarrow \infty} \frac{\| (B_k - \Delta f(\pm \Phi)) \Delta u \|}{\| \Delta u \|} = 0$$

Def. Under more assumptions, we can have global convergence even in the worst case.

velocity of convergence:

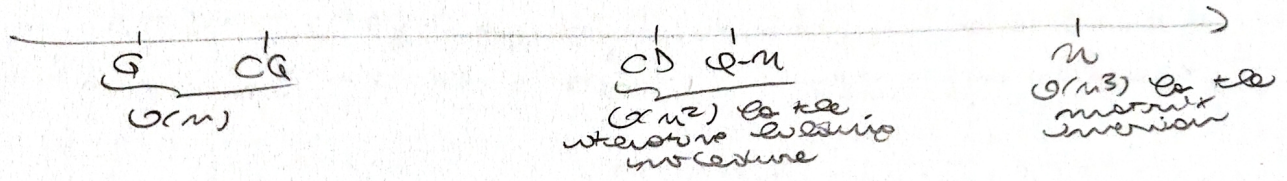


velocity of convergence:



but slow for Q-n we can characterize global conv under some assumptions

Computational load:



CONSTRAINED NONLINEAR OPTIMIZATION

5.1 NEC OPT CONDITIONS

Consider the problem structure

$$\min_{\mathbb{R}^n} f(x) \quad \text{s.t. } g_i(x) \leq 0 \quad \forall i \in I = \{1, \dots, m\}, \quad \begin{matrix} f, g \in C^1 \\ \mathbb{S} \text{ is convex} \\ \text{feasible} \end{matrix}$$

Def. 4. For $\bar{x} \in \mathbb{S}$ let

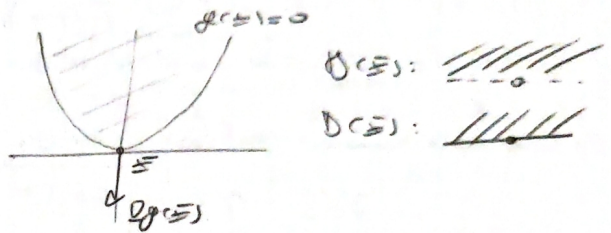
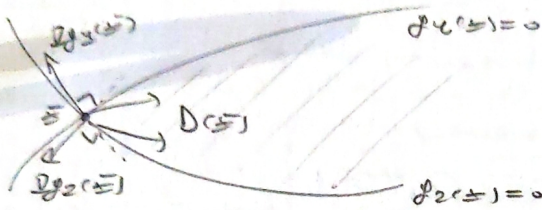
$$\mathcal{D}(\bar{x}) = \{d \in \mathbb{R}^n : \exists \alpha > 0 : \bar{x} + \alpha d \in \mathbb{S} \forall d \in \mathcal{D}(\bar{x})\} =$$

= cone of the feasible directions

$$I(\bar{x}) = \{i \in I : g_i(\bar{x}) = 0\} = \text{set of the active constraints (i.e. the constraints violated at } \bar{x})$$

$$D(\bar{x}) = \{d \in \mathbb{R}^n : \nabla g_i(\bar{x}) \cdot d \leq 0 \quad \forall i \in I(\bar{x})\} =$$

= cone of the directions ^{not the feasible!} $\nabla g_i(\bar{x}) \cdot d \leq 0$ the gradients of the active constraints



Propert. $D(\bar{x}) \supseteq \overline{D(\bar{x})} \quad \forall \bar{x} \in \mathbb{S}$.

(4.1.1) NEC $f \in C^1$ $\bar{x} \in \mathbb{S}$ loc. min $\Rightarrow \nabla f(\bar{x}) \cdot d \geq 0 \quad \forall d \in D(\bar{x})$
 \Rightarrow all feasible directions are ascent directions

not all vectors $d \in D(\bar{x})$ are feasible directions, which are the ones of $\overline{D(\bar{x})}$. However, this is sufficient to characterize. So we can see the following:

Def (CQ, constraint qualification, Karush) \Rightarrow $D(\bar{x}) = \overline{D(\bar{x})}$

CQ condition holds at $\bar{x} \in \mathbb{S} \Leftrightarrow D(\bar{x}) = \overline{D(\bar{x})}$ if CQ on \bar{x} does not hold, then KKT are not nec

Def (KKT, nec opt conditions) Suppose $f \in C^1, g \in C^1, CQ$ on $\bar{x} \in \mathbb{S}$ (a feasible point).

$$\bar{x} \text{ is loc. min of } f \text{ on } \mathbb{S} \Rightarrow \begin{cases} \exists \text{ KKT multipliers } \mu_1, \dots, \mu_m \geq 0 \text{ s.t.} \\ \nabla f(\bar{x}) = \sum_{i \in I(\bar{x})} (-\mu_i) \nabla g_i(\bar{x}) \quad \leftarrow \text{active constraints} \\ \mu_i g_i(\bar{x}) = 0 \quad \forall i = 1, \dots, m \quad \leftarrow \text{all constraints} \end{cases}$$

If we will impose these conditions plus the ones of \bar{x} naturally, we can have feasible candidate optimum points.

How can we ensure that these CQ on \bar{x} holds?

- Prop (suff conditions for CQ)
- (1) g_i are linear $\forall i$, OR \bar{x} is a vertex of \mathbb{S} $\Rightarrow CQ$ holds $\forall \bar{x} \in \mathbb{S}$
 - (2) $\nabla g_i(\bar{x})$ are linearly independent $\forall i \in I(\bar{x})$ (active constraints) $\Rightarrow CQ$ on \bar{x} holds at $\bar{x} \in \mathbb{S}$

Now the next result shows how the KKT conditions become up for convex problems.

Def (KKT nec and suf, convex problems). Suppose $f \in C^1$, convex, $g \in C^1$ convex, and we have Slater cond (for CQ).

$f \in S$ is a local min $\Rightarrow \exists u_1, \dots, u_m \geq 0$ st

$$\begin{cases} \nabla f(x^*) = \sum_{i=1}^m (-u_i) \nabla g_i(x^*) \\ \sum_{i=1}^m u_i g_i(x^*) = 0 \quad \forall i = 1, \dots, m \end{cases}$$

GENERAL CASE WITH EQUALITY CONSTR

usually the equality constr will be always active constr, and then KKT multiplier will be $\in \mathbb{R}$ (not in \mathbb{R}_+).

min $f(x)$
 st $g_i(x) \geq 0 \quad i \in I$
 $h_j(x) = 0 \quad j \in E$
 $x \in X \subseteq \mathbb{R}^n$

$f, g_i, h_j \in C^1$
 S is feasible region

Due to equality, we usually set $\lambda_j \in \mathbb{R} = \mathbb{R}_+$, as we extend it into a new definition.

Def. $\mathcal{L}(x) = \left\{ \lambda \in \mathbb{R}^m : \lambda = \gamma \cdot \lim_{h \rightarrow 0} \frac{g(x+h) - g(x)}{\|x+h-x\|}, \gamma \geq 0, \gamma \neq 0 \right\}$
 = closed cone of the tangents at x

Def (CQ, constraint qualification, active)

CQ condition holds at $x \in S \Leftrightarrow \mathcal{D}(x) = \mathcal{D}(S) \cap H(x)$

$\mathcal{D}(x) = \left\{ \lambda : \nabla g_i(x) \cdot \lambda \geq 0 \quad \forall i \in I(x) \right\}$ (active inequality constraints)
 $H(x) = \left\{ \lambda : \nabla h_j(x) \cdot \lambda = 0 \quad \forall j \in E \right\}$ (active equality constraints)

Def (KKT, nec and suff conditions, general case) Suppose $f \in C^1, g \in C^1, h \in C^1, \mathcal{D} \in C^1$ and CQ on holds at $x \in S$.

$f \in S$ is a local min of f on $S \Rightarrow \exists u \geq 0 \quad \forall i \in I(x), \lambda \in \mathbb{R} \quad \forall j \in E$ st

$$\nabla f(x) = \sum_{i \in I(x)} (-u_i) \nabla g_i(x) + \sum_{j \in E} (-\lambda_j) \nabla h_j(x)$$

Prop (suff cond for CQ).

- (1) f is convex, f is linear over $S \Rightarrow$ CQ on holds at $x \in S$
- (2) $\nabla g_i(x) \cdot \lambda \geq 0 \quad \forall i \in I(x)$ and $\nabla h_j(x) \cdot \lambda = 0 \quad \forall j \in E \Rightarrow$ CQ on holds at $x \in S$

5.2 SUP OPT CONDITIONS

min $f(x)$
 st $g_i(x) \geq 0 \quad i \in I = \{1, \dots, m\}$ (P)
 $x \in X \subseteq \mathbb{R}^n$ even discrete

Def The Lagrangian function associated to problem (P) is $L(x, \lambda) = f(x) + \sum_{i \in I} u_i g_i(x)$ ($x \in X, u_i \geq 0$)

same penalization as we saw in DOPT

A point (x^*, λ^*) with $x^* \in X, \lambda^* \geq 0$ (or feasible for L) is a candidate point of

$F = \max_{x \in X} L(x, \lambda^*)$ & $\lambda^* = \arg \max_{\lambda \geq 0} L(x^*, \lambda)$

Prop (characterization)

- (x^*, λ^*) with $x^* \in X, \lambda^* \geq 0$ is a candidate pt of $L \Leftrightarrow$
- (1) $L(x^*, \lambda^*) = \max_{x \in X} L(x, \lambda^*) \checkmark \Rightarrow$ min
 - (2) $g_i(x^*) \geq 0 \quad \forall i \in I \checkmark \Rightarrow$ feasible
 - (3) $u_i g_i(x^*) = 0 \quad \forall i \in I \checkmark$ (complementarity)

Def (out constraints).

$$(\bar{x}, \bar{y}) \text{ is a saddle point of } L(x, y) \Rightarrow \bar{x} \text{ is a global min of problem } (P)$$

It ensures also nec for convex problems, where it also ensures a connection to the KKT multipliers.

with the caveat that for non-convex problems a saddle point may not exist

Def. Suppose f is convex, g are linear (conv sets F or interval double point). Then, (\bar{x}, \bar{y}) is a saddle point.

$$(P) \text{ has an optimal val } z^* \Leftrightarrow \exists \bar{x} \geq 0 \text{ s.t. } (\bar{x}, \bar{y}) \text{ is a saddle point of } L(\bar{x}, \bar{y})$$

(necessary + suff)

For convex problems, the KKT ensures that a point is optimal if $(\bar{x}, \bar{y}) \geq 0$, and the optimal val. turns out that

$$(KKT) = (\text{Karush-Kuhn-Tucker conditions})$$

$$L(x, y) = f(x) + \sum_{i \in I} \lambda_i g_i(x)$$

$$D_x L = 0 \Rightarrow Df(x) + \sum_{i \in I} (-\lambda_i) Dg_i(x) = 0$$

(KKT)

5.6 LAGRANGIAN DUALITY

What we do now in D.O.P. is take w that is a min problem (P) we can solve it by solving the dual problem, looking for a saddle point of the Lagrange function.

$$(P) \text{ min } f(x) \text{ s.t. } g(x) \leq 0 \text{ for } x \in \mathbb{R}^n$$

$$(D) \text{ max }_{\lambda \geq 0} \left(\text{min}_{x \in \mathbb{R}^n} L(x, \lambda) \right)$$

\Rightarrow we look for a saddle point

$$f(x) \leq w(\lambda) \leq f(x) \Rightarrow w(\lambda) \leq f(x)$$

under constraint, $f(x) = w(\lambda)$ \Leftrightarrow $\exists x$ opt of (P) \Leftrightarrow $\exists \lambda$ opt of (D)

$$\Leftrightarrow (\bar{x}, \bar{y}) \text{ is a saddle point}$$

So the method to solve the problem is:

- derive the Lagrange function
- minimize w.r.t x forming $w(\lambda)$ and maximize w.r.t λ
- we find λ function of w , and we then maximize the $L(x, \lambda)$ to get $w(\lambda)$, we can then maximize the $L(x, \lambda)$ to get $w(\lambda) = f(x)$
- if no dual exists we should get $w(\lambda) = -\infty$

When optimizing $w(\lambda)$ in the last point remember that
 (1) $w(\lambda)$ is concave
 (2) $f(x)$ is a upper bound of $w(\lambda)$ if we solve the min $L(x, \lambda)$

In general (D) is easier than (P) even if no saddle point exists. If saddle point \exists : we can derive λ optimal for (P) & the no-dual case and require constraint.

- if saddle point \exists : we can solve and λ is upper bound of $f(x)$ and the reverse of $L(x, \lambda)$ on the value $f(x)$, and we also create a reverse of λ as λ min $L(x, \lambda)$.

Under convex assumptions there is no dual case and there exists a saddle point.

5.5 2nd ORDER KKT CONDITIONS

$\min f(x)$
 s.t. $g_i(x) \leq 0 \quad \forall i \in I$
 $h_j(x) = 0 \quad \forall j \in E$
 $x \in \mathbb{R}^n$

$f, g_i, h_j \in C^2$
 X open set

$$\Rightarrow L(x, \lambda, \mu) = f(x) + \sum_{i \in I} \lambda_i g_i(x) + \sum_{j \in E} \mu_j h_j(x)$$

(2nd ORD)
NEC
KKT COND

\bar{x} local min
 $\exists \lambda, \mu \in \mathbb{R}^m$ are chosen
 s.t. $\lambda_i \geq 0 \quad \forall i \in I$

\exists some (λ, μ) s.t. \bar{x} satisfies the KKT conditions

$$\begin{aligned} \nabla_x L(\bar{x}, \lambda, \mu) &= 0 \\ \lambda_i g_i(\bar{x}) &= 0 \\ \lambda_i &\geq 0, \quad \forall i \in I \end{aligned} \quad \text{KKT}$$

$$\begin{aligned} h_j(\bar{x}) &= 0 \\ \mu_j & \text{ free} \end{aligned} \quad \text{Eqs}$$

Moreover, over \mathbb{R}^m at $\bar{x} \in I \cap E$
 $\nabla^2_x L(\bar{x}, \lambda, \mu) \cdot d = 0 \quad \forall d \in \mathbb{R}^n$
 $d \cdot \nabla^2_x L(\bar{x}, \lambda, \mu) \cdot d \geq 0$
 must satisfy

(2nd ORD)
SUF
KKT COND

\bar{x} satisfies with (λ, μ)
 the previous KKT cond
 $\forall d \in \mathbb{R}^n : d \cdot \nabla^2_x L(\bar{x}, \lambda, \mu) \cdot d > 0$

$$\forall d \in \mathbb{R}^n : \begin{aligned} \nabla g_i(\bar{x}) \cdot d &= 0 & \forall i \in I : \lambda_i > 0 \\ \nabla h_j(\bar{x}) \cdot d &= 0 & \forall j \in E : \mu_j < 0 \\ \nabla h_k(\bar{x}) \cdot d &= 0 & \forall k \in E \end{aligned}$$

\Rightarrow \bar{x} is a strict local min of f over X

5.6 QUADRATIC PROGRAMMING

$\min g(x) = \frac{1}{2} x^T Q x + c^T x$
 s.t. $a_i^T x \leq b_i \quad \forall i \in I$
 $a_j^T x = b_j \quad \forall j \in E$
 $x \in \mathbb{R}^n$

quadratic obj function
 linear constraints
 Q symm (n.b.s)

EX: minimizing (linear) SVM: find the hyperplane
 parallel to the data margin

$\min_{x \in \mathbb{R}^2} \frac{1}{2} \|w\|^2$
 s.t. $f_0(w) = (w^T x - b) - 1 \geq 0$
 $f_1(w) = w^T x - b - 1 \leq 0$



Since number of constr \Rightarrow we have equality

we need a 30 to be complementary or we are used to

$$\max_{\lambda \geq 0} \left(\min_{x \in \mathbb{R}^2} L(x = \begin{pmatrix} w \\ b \end{pmatrix}, \lambda) \right)$$

$$\left[\frac{1}{2} \|w\|^2 \right] + \sum_{i=0}^1 \lambda_i \left[- (w^T x - b) - 1 \right]$$

QP WITH ONLY EQUALITY CONSTR

so we just have $\min \{ \frac{1}{2} x^T Q x + c^T x : Ax = b \}$

we write the KKT conditions:

$\begin{cases} \lambda \geq 0 \\ \lambda^T (Ax - b) = 0 \end{cases}$

$\Rightarrow A = \begin{pmatrix} -c \\ -A \\ -b \end{pmatrix}$

$$\begin{cases} (Q \pm \epsilon) + \sum_{i=1}^m \lambda_i \begin{pmatrix} a_i \\ 0 \end{pmatrix} = 0 \\ \lambda_i \geq 0 \end{cases}$$

all variables from same in constr

$Ax = b$ — some rows are auto-matically rotated

which was needed to plus expanded linear system, derived from removing the constraints:

$$\begin{cases} Qz + \sum \omega_i u_i = -c \\ Az = b \end{cases} \Rightarrow \begin{pmatrix} Q & A^T \\ A & 0 \end{pmatrix} \begin{pmatrix} z \\ w \end{pmatrix} = \begin{pmatrix} -c \\ b \end{pmatrix}$$

Null space method: we can find z whose cols are here (A) and then we translate the variables as $z = z_0 + ZW$ with
 - z_0 a feasible pt
 - W an appropriate vector $\in \mathbb{R}^{n-m}$

In this way the null space gets worked to an unconstrained QP
 $\min_{W \in \mathbb{R}^{n-m}} \left[\frac{1}{2} W^T (Z^T Q Z) W + (Q z_0 + c)^T Z W \right]$

QP WITH INEQUALITY CONSTR

Showing how the removal of variables can be done, the idea was this case is to:

- determine $I(z^*)$, the active set around the opt pt
- solve a sequence of QPs with only eq constr

Active set method: find an initial feasible z_0 and choose $W_0 = E \cup \{w \in I: z_0^T z_0 = b\} = E \cup I(z_0)$. then at iteration k :

- determine α_k solving

$$\min_{\{g \in E \cup I\}} \{g^T (z_k + \alpha) = b, w \in W_k\}$$

we minimize g along direction z (small stepsize all constr required α_k W_k)

$$\Rightarrow \min_{\{g \in E \cup I\}} \{g^T z = \alpha, w \in W_k\}$$

- based on α_k we determine α_k to update z_{k+1} as $z_k + \alpha_k z_k$, and to update W_{k+1} .

- if $\alpha_k \neq 0$ we end α_k as the largest step such that $z_k + \alpha_k z_k$ is feasible, all the (equality) constr, the ones outside W_k

$$\Rightarrow \alpha_k = \min \left(1, \min_{\substack{w \in W_k \\ z_k^T w > 0}} \frac{b - z_k^T w}{z_k^T w} \right)$$

$W_{k+1} = W_k \cup \{w\}$ with w the index of the constr because active at z_{k+1}

- if $\alpha_k = 0$ then z_k is the min over the W_k constr. We need to check if it is the loc opt of the full problem: we compute the KKT multipliers

$$(Q z_k + c) + \sum_{w \in W_k} u_w^k z_w = 0 \quad \text{with } u_w^k = \sum_{w \in W_k} (-u_w^k) z_w$$

actually, here the use of the opt computed in the system when minimizing $g(z_k + \alpha)$

$$\begin{cases} \text{if } u_w^k > 0 \text{ for } w \Rightarrow z_k \text{ is the loc opt of QP} \\ \text{if } \exists w: u_w^k < 0 \Rightarrow z_{k+1} = z_k \text{ and } W_{k+1} = W_k \setminus \{w\} \\ \text{with } w \text{ the most neg index} \end{cases}$$

5.7 PENALTY METHOD & AUGMENTED LAG

Penalty method: the idea was to

- remove a constr
- enforce its/their violation in the obj function
- solve a sequence of unconstrained (QP) problems

$$(P) \quad \min_{z \in \mathbb{R}^n} f(z) \text{ s.t. } c_j(z) = 0 \quad w \in E$$

idea: let $\gamma_k \rightarrow \infty$ and for each k let z_k minimize that $Q(z, \gamma_k)$

(quadratic penalty - exact method)

$$\min_{z \in \mathbb{R}^n} Q(z, \gamma) = f(z) + \frac{1}{2\gamma} \sum_{w \in E} c_w(z)^2$$

General scheme:

- (0) select $\epsilon > 0, y_0 > 0, \epsilon_k \rightarrow 0, \epsilon_3, k=0$
- (1) compute $\pm u$ approximate minimum of $Q(\pm u, y_k)$ starting from $\pm u_0$ and terminate when $\| \nabla Q(\pm u, y_k) \| \leq \epsilon_k$.
- (2) if overall termination criteria is met (e.g. $|f(\pm u) - f(\pm u)| < \epsilon$) then \rightarrow return $\pm u$
 else \rightarrow reduce $y_{k+1} \in (0, y_k)$, set $\pm u_{k+1} = \pm u, k = k+1$ and repeat from (1)

LEM (unrestricted)

$$\pm u \text{ glob. min of } Q(\cdot, y_k) \\ \text{th. (if } \epsilon_k = 0 \text{ th. } y_k \rightarrow 0)$$

\Rightarrow every limit point $\neq \emptyset$ is a local min of f and also a local min of P

LEM (more restrictive)

$$\epsilon_k \rightarrow 0 \\ y_k \rightarrow 0 \quad \Rightarrow$$

every limit point $\neq \emptyset$ of u is a local min of f and also a local min of P

Moreover, the sub-requirement defined by Q with $\epsilon_k \rightarrow 0$ is not

$$u_{\text{opt}} = \arg \min_{u \in \mathbb{R}^n} \frac{Q(u, y_k)}{y_k}$$

rather $y_k \rightarrow 0$ is a local min of f and also a local min of P

$$L(\pm, y) = f(\pm) - \sum u_i c_i(\pm) \Rightarrow \nabla_x L = \nabla f - \sum u_i \nabla c_i = 0$$

$$Q(\pm, y) = f(\pm) + \frac{1}{2y} \sum c_i(\pm)^2 \Rightarrow \nabla_x Q = \nabla f + \frac{1}{2y} \sum c_i(\pm) \nabla c_i = 0$$

However, as $y_k \rightarrow 0$ the quadratic penalty method becomes ill conditioned. In fact, it will be to move the quadratic penalization on the unconstrained function.

Just to conclude, we can employ this method also until we reach a term $1/2y \sum [c_i(\pm)]^2$, considering it as a term $c_i(\pm) \geq 0$ we can use other restrictions such as the quadratic one.

Augmented Lagrangian method: reduce all constrained problems to - moving the penalization on the unconstrained - introducing explicit estimates on the Lagrange multipliers

$$(P) \quad \min_{\pm \in \mathbb{R}^n} f(\pm) \\ \text{st } c_i(\pm) = 0 \quad \forall i \in I$$

see Evidencia

quadratic penalization term

$$(AP) \quad \min_{\pm \in \mathbb{R}^n} L(\pm, u, y) = f(\pm) - \sum_{i \in I} u_i c_i(\pm) + \frac{1}{2y} \sum_{i \in I} (c_i(\pm))^2$$

General scheme:

- (0) initialize $\epsilon > 0, y_0 > 0, \epsilon_k \rightarrow 0, \epsilon_3, y_0, k=0$.
- (1) determine error measure $\pm u$ of $L(\pm, y_k, y_k)$ starting from $\pm u_0$ until $\| \nabla_x L \| \leq \epsilon_k$. Note that

$$\nabla_x L(\dots) = \nabla f(\pm) - \sum_{i \in I} \left(u_i - \frac{c_i(\pm)}{y} \right) \nabla c_i(\pm)$$

there will exist to be the optimal u_i multiplier

- (2) if overall termination criteria is met then \rightarrow stop
 else \rightarrow update $u_{i+1} = u_i - \frac{c_i(\pm)}{y}$, reduce $y_{k+1} \in (0, y_k)$, set $\pm u_{k+1} = \pm u$ and loop.

LEM

\Rightarrow local min of u is a local min of f and also a local min of P and also a local min of f and also a local min of P

\Rightarrow

the method is well posed, defined (7) set $\pm u$ at step 1, we have good conv speed, ecc)

