



Introduction to Optimization and Geoscience Applications

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Outline

- 1 B1: Fundamental of optimization
- 2 B2: Introductory examples in logistics optimization
- 3 A1: LP-QP-MILP
- 4 A2: Geoscience Applications
- 5 A3: Regression problems in geoscience
- 6 A4: Convex optimization applications
- 7 A5: Optimization case studies by PTTEP

How to read this handout

- 1 topics starting with **B** refer to **basic** lecture focusing on problem description and applications
- 2 topics starting with **A** refer to **advance** lecture that contain mathematical details of the optimization
- 3 the examples are presented according to application focus, not its mathematical problem type

Outline

1 B1: Fundamental of optimization

- What is optimization?
- Introductory examples: LP/MILP/Model estimation
- Problem setting
- Optimality of unconstrained problems
- Problem types
- Numerical tools
- Optimization workflow and modeling

2 B2: Introductory examples in logistics optimization

- Introduction to logistics optimization
- Traveling salesman problem (TSP)
- Facility location problem
- Inventory optimization

3 A1: LP-QP-MILP

- Linear programming
- Quadratic Programming
- Mixed integer programming

What is optimization?

Anatomy of optimization

definition: choosing the **best** element from a set of available alternatives. It involves finding the input values that result in the minimum or maximum value of a specific objective function while satisfying a given set of constraints.

essential elements of an optimization:

- 1 **objective:** a quantitative measure of success (e.g., profit, energy efficiency, or error rate).
- 2 **variables:** the 'knobs' you can turn or decisions/mechanism you can make
- 3 **constraints:** real-world limits—resources, physics, or legal requirements—that define the "feasible region."
- 4 **problem parameters:** parameters required to be set in the problem statement

Example: Diet problem



description:

- given n meals; each has different price and nutrient details
- design a diet plan to meet the nutrient requirements with the lowest cost

- 1 **variables:** the quantity of each meal to consume
- 2 **objective:** total cost of meals
- 3 **constraints:**
 - quantities of meals must be non-negative
 - consumed carb/protein/vitamin/fat must be within a recommended threshold
- 4 **problem parameters:** price and nutrients of each food, the required quantity of each nutrient

Diet problem: formulation

variables: x_1, x_2, x_3 quantities of milk, beans, meat
problem parameters

food	cost (\$/unit)	protein (g/unit)	calorie (kcal/unit)
milk	2.0	8	120
beans	1.5	12	200
meat	5.0	25	250

requirements (constraints)

- protein at least 60g
- calories at least 1800 kcal

diet optimization problem:

$$\begin{aligned} &\text{minimize} && 2x_1 + 1.5x_2 + 5x_3 \\ &\text{subject to} && x_1, x_2, x_3 \geq 0, \\ & && 8x_1 + 12x_2 + 25x_3 \geq 60, \\ & && 120x_1 + 200x_2 + 250x_3 \geq 1800 \end{aligned}$$

the objective and constraint functions are linear; called a linear program (LP)

Structure of diet problem

- each item can be decomposed to contain several entities (each food contain a set of nutrients)
- the role of cost and nutrient can be swapped
- one can maximize the total nutrient while the cost is within a limit
- if we only care about cost, we eat 'cheap' food; if we care about health, we eat 'clean' food

Example: Knapsack problem



description:

- given a backpack that can only hold up to 15 kg
- each item has a specific weight and a specific importance value
- decide which items to take to maximize total value without breaking the bag

- 1 **variables:** binary decision of each item (1 if taken, 0 if not taken); you cannot take 'half' of the camera
- 2 **objective:** maximize sum of total **value** of items you pack
- 3 **constraints:** the sum of the weights of selected items must be ≤ 15 kg
- 4 **problem parameters:** backpack weight limit, value of each item

Knapsack: formulation

zero-one knapsack problem

maximize $c^T x$ subject to $w^T x \leq K$, $x_j \in \{0, 1\}$, $j = 1, 2, \dots, n$

setting:

- given n items; each has weight w_j and value c_j
- given a bound K on the total weight that can be carried in a knapsack


goal: decide to select items to maximize the total value

Introductory examples: LP/MILP/Model estimation

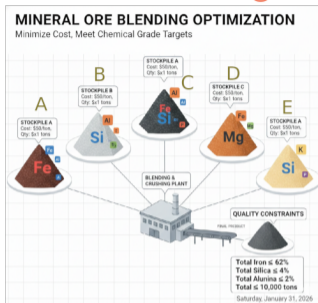
Energy economic dispatch



description:

- given power plants (solar, wind, natural gas, coal); each has different cost and CO₂ emission value
 - decide how much power to draw from each plant to meet the city's electricity demand with minimum operating cost
- 1 **variables:** generation's power outputs
 - 2 **objective:** minimize the total cost
 - 3 **constraints:**
 - total power must meet the demand
 - power from a plant has its physical limit
 - CO₂ emission must be below a limit
 - 4 **problem parameters:** 

Mineral ore blending



description:

- given multiple stockpiles of ore; each has different concentrations of minerals (iron, silica, alumina)
- final blending must meet the strict chemical grade requirement
- decide how to mix these stockpiles to minimize the cost of extraction and transport

- 1 **variables:** the quantity taken from each ore stockpile
- 2 **objective:** minimize the production cost
- 3 **constraints:**
 - total iron must be $\geq 62\%$; total silica must be $\leq 4\%$ and alumina $\leq 2\%$
 - sum of quantities must equal total shipment size
 - we cannot take more ore from a stockpile than is physical limit
- 4 **problem parameters:**

NASA Example: bring equipments to a satellite

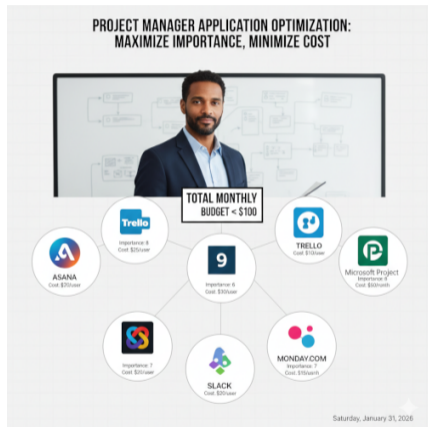


description:

- given a backpack having a limit of 50 kg
- each item has a specific weight and a specific importance value
- decide which items to take to maximize total value within the weight limit

- 1 **variables:**
- 2 **objective:**
- 3 **constraints:**
- 4 **problem parameters:**

Project management: select softwares



description:

- given a total monthly budget of 100 USD
- each software has a value and running cost
- decide which softwares to launch that maximize its importance within the budget

1 variables:

2 objective:

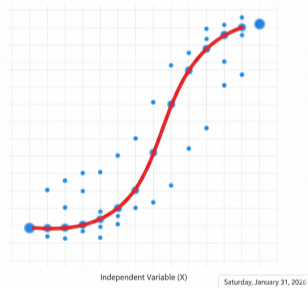
3 constraints:

4 problem parameters:

Curve fitting

NON-LINEAR CURVE FITTING

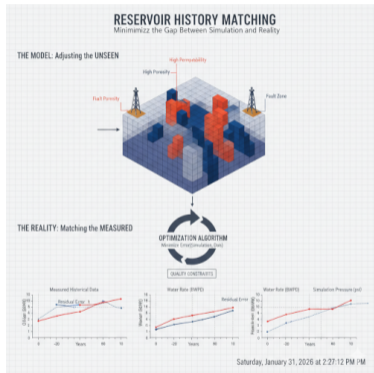
Minimizing Error for Complex Relationships



description:

- given N data points $\{(t_i, x_i)\}_{i=1}^N$, and a function description to fit (here, sigmoid function)
 - find the best function parameters that minimize the error
- 1 **variables:** function parameter θ :
$$f(x; a, b, c) = a / (1 + e^{-c(x-b)})$$
 - 2 **objective:** minimize the sum of squared errors
 - 3 **constraints:** -
 - 4 **problem parameters:** data points $\{(t_i, x_i)\}_{i=1}^N$

Reservoir history matching



description:

- a reservoir simulation model has thousands of uncertain parameters, such as local permeability and porosity
- adjust these parameters until the model's predicted oil, water, and gas production rates match the actual historical data from the wells

- 1 **variables:** model parameters
- 2 **objective:** minimize the sum of squared errors
- 3 **constraints:** depends on the model
- 4 **problem parameters:** data points

Reservoir history matching: formulation

let $g(t, x)$ be the **reservoir simulator** at time t for a given parameter x

- x contains permeability and porosity
- g usually is complex PDEs (Darcy's law and mass balance)

variable: model parameter x

problem: minimize error between the model prediction and observed data, while regularizing the estimated parameter

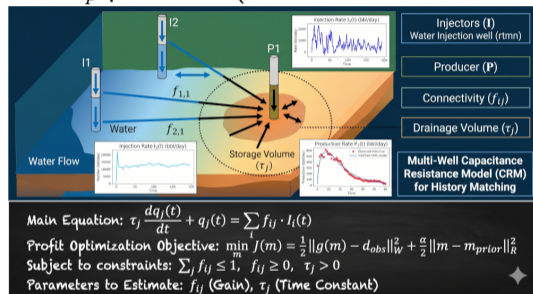
$$\underset{x}{\text{minimize}} f(x) := \sum_{t=1}^N \|g(t_i, x) - y(t)\|^2 + \gamma \|x - x_{\text{prior}}\|_2^2 \quad \text{subject to } x_{\text{min}} \preceq x \preceq x_{\text{max}}$$

proxy model: a radial flow model based on pressure data

$$g(t, x) = \frac{150(\log(t) + s)}{k}, \quad s = \text{skin factor}, \quad k = \text{permeability}$$

Reservoir matching: CRM (capacitance resistance model)

a reservoir field with N_i injectors (wells where we pump water in to maintain pressure) and N_p producers (wells where we extract oil/water)



- $f_{ij} \geq 0$ is a flow from injector i to reach producer j (connectivity)
- $\sum_{j=1}^{N_p} f_{ij} \leq 1$ (sum of all gains from an injector i must be less than 1)
- q_j is total fluid production rate (oil+water) from producer j
- I_j as the injection rate (input)

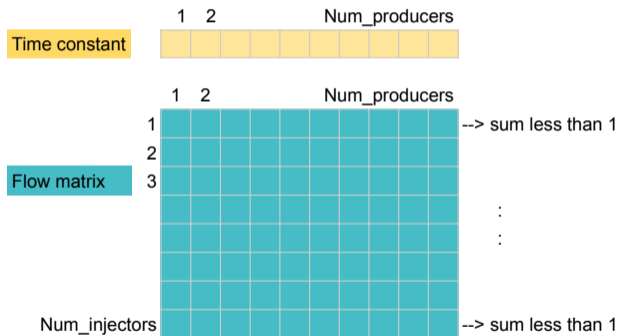
CRM model:
$$\tau_j \frac{dq_j(t)}{dt} + q_j(t) = \sum_{i=1}^{N_i} f_{ij} I_i(t), \quad j = 1, 2, \dots, N_p$$

τ_j is time constant, q_j is a response of first-order differential equation to injectors

CRM model estimation

given observed production rate q ,

estimate time constant τ and flow matrix $F = [f_{ij}]$ in CRM model to match q



- both τ and F are non-negative
- each row of F sums up to one

CRM parameter optimization

problem: given signals q_j^{obs} for $j \in [N_p]$ and I_i for $i \in [N_i]$ we aim to estimate τ_j and f_{ij} for all i, j

variables: $x = (\tau_j, f_{ij})$ for $j \in [N_p]$ and $i \in [N_i]$

optimization: minimize error between observed value and CRM model output

$$\underset{\tau_j, f_{ij}}{\text{minimize}} \sum_{j=1}^{N_p} \sum_{t=1}^T \left(q_j^{\text{obs}}(t) - q_j(t, f_{ij}, \tau_j) \right)^2 \quad \text{subject to} \quad f_{ij} \geq 0, \sum_{j=1}^{N_p} f_{ij} \leq 1, \tau_j \geq 0$$

- CRM model can be discretized using Euler method to simulate q_j

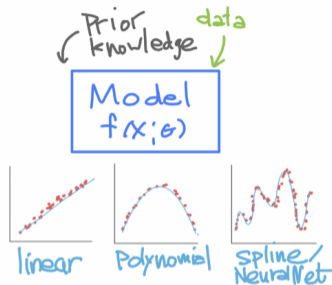
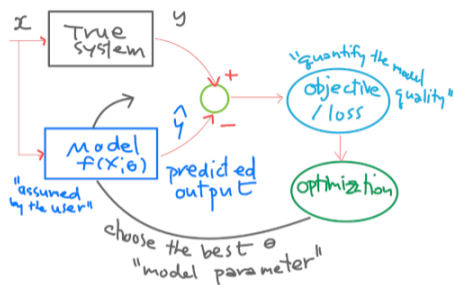
$$\tau_j \frac{(q_j[t] - q_j[t - 1])}{\Delta t} = \sum_i f_{ij} I_i[t] - q_j[t - 1]$$

CRM model estimation

observations on the optimization

- with the constraint $\sum_j f_{ij} \leq 1$, we optimize f_{ij} for all i, j (without it, the optimization is separable in j) – so f is a matrix variable, and τ is a vector
- treating CRM model output as nonlinear function of τ_j, f_{ij} , the optimization problem is nonlinear least-squares
- using modeling techniques can cast the discretized model as an autoregressive with exogenous input (ARX) and the linear least-squares technique can be applied

Structure of model estimation problem



- 1 variables:** model parameters
- 2 objective:** the concept of loss function; depend of model architecture/statistical assumption of estimation problem
- 3 constraints:** depend on model assumptions
- 4 problem parameters:** data points (x, y)

Problem setting

Problem setting

(mathematical) optimization problem

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & h_i(x) = 0, \quad i = 1, \dots, p \end{array} \quad (\text{P1})$$

- $x = (x_1, \dots, x_n)$: optimization variable
- $f_0 : \mathbf{R}^n \rightarrow \mathbf{R}$: objective function
- $f_i : \mathbf{R}^n \rightarrow \mathbf{R}, i = 1, \dots, m$: inequality constraint functions
- $h_i : \mathbf{R}^n \rightarrow \mathbf{R}, i = 1, \dots, p$: equality constraint functions

constraint set: $\mathcal{C} = \{x \in \mathbf{R}^n \mid f_i(x) \leq 0, i = 1, \dots, m, h_i(x) = 0, i = 1, \dots, p\}$

domain of the problem: $\mathcal{D} = \bigcap_{i=0}^m \text{dom } f_i \cap \bigcap_{i=1}^p \text{dom } h_i$

Optimal value

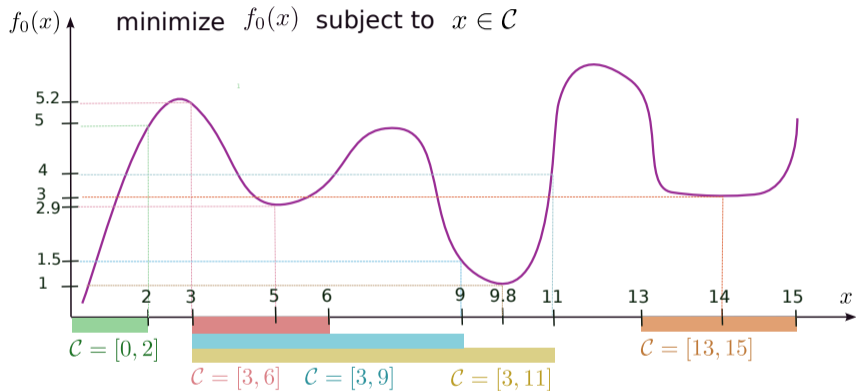
$$p^* = \inf \{ f_0(x) \mid f_i(x) \leq 0, i = 1, \dots, m, h_i(x) = 0, i = 1, \dots, p \}$$

- we say x is **feasible** if $x \in \text{dom } f_0(x)$ and $x \in \mathcal{C}$
- $p^* = \infty$ if the problem is **infeasible**
- $p^* = -\infty$ if the problem is unbounded below
- a feasible x is called **optimal** if $f_0(x) = p^*$; there can be many
- x is **locally optimal** if $\exists \epsilon > 0$ such that x is optimal for

$$\begin{array}{ll} \text{minimize} & f_0(z) \\ \text{subject to} & z \in \mathcal{C}, \quad \|z - x\|_2 \leq \epsilon \end{array}$$

in other words, a locally optimal point is the best solution in a neighborhood

Example



find achievable objective values, p^* and x^* for each \mathcal{C}

Optimality of unconstrained problems

assumption: f is twice continuously differentiable (smooth objective)

■ **1st-order necessary condition:**

if x^* is a local minimizer of f then $\nabla f(x^*) = 0$

■ **2nd-order necessary condition:** if x^* is a local minimizer of f then $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succeq 0$ (positive **semidefinite**)

■ **2nd-order sufficient condition:** if $\nabla f(x^*) = 0$ and $\nabla^2 f(x^*) \succ 0$ (pdf)

then x^* is a strict local minimizer of f

local minimizers can be distinguished from other stationary points by examining positive definiteness of $\nabla^2 f$

example: $f(x) = x^4$ has $x^* = 0$ as a local minimizer; $\nabla^2 f(x^*) = 0$ (hence, 2nd-order sufficient condition fails)

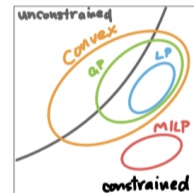
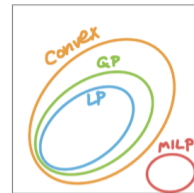
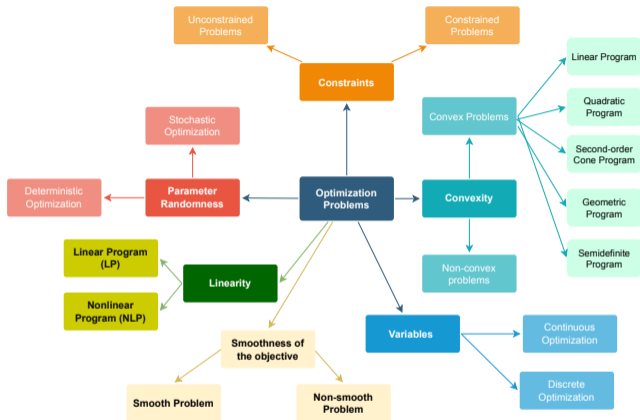
Problem types

Problem types

we can categorize optimization problems by

- **constraints**
 - unconstrained problem
 - constrained problems
- **variable types**
 - continuous optimization
 - discrete optimization
- **linearity of objective and constraints**
 - linear program
 - nonlinear program
- **convexity of objective and constraint set**
 - convex problem
 - non-convex problem
- **smoothness of the objective**
 - smooth problem
 - non-smooth problem
- **parameter randomness**
 - stochastic optimization
 - deterministic optimization

a numerical method generally is tailored to a specific problem type



other specific problem types are integer programming, vector optimization

Numerical tools

Numerical tools



- software tiers:
 - modeling languages/wrapper (describe the problem and connect with solvers): AMPL, cvxpy, Google OR-tools
 - solvers (computational engine): Gurobi, CPLEX
 - library/toolbox (bundle both modeling and solvers): MATLAB, Scipy
- commercial vs open source
- domain specificity: e.g. cvxpy is for convex problems

Modeling language and wrappers

- these tools allow us to describe what the problem is (objective and constraint) without worrying about how the computer solves it
 - **declarative modeling:** AMPL and CVXPY: we can write $Ax \leq b$ and the softwares builds the mathematical tree
 - **procedural modeling:** Google OR tools: it builds the model row-by-row (one constraint at a time); it is more of an **API** than a language
- acts as a middle man to translate our Python/math code to a format the computational engine can read

Solvers

this is the computational engine that runs the actual algorithms (simplex, interior point, branch and bound, etc.)

- **commercial (high performance):** Gurobi, CPLEX, and MOSEK; generally the fastest but require licenses
- **open source:**
 - GLOP/PDLP/CP-SAT: inside OR-tools
 - HiGHS: high-performance softwares to solve large-scale LP, MIP and QP
 - OSQP: solve QP problem using splitting method
 - SCS: solve large-scale convex cone problems
 - ECOS: solve second-order cone programming
 - SCIP: constraint integer programs (MIP and MINLP)

and more

Library and toolbox

provide a complete environment that includes both a way to model problems and built-in solvers

- **MATLAB:** uses optimization toolbox (`linprog`, `quadprog`) and provides a self-contained ecosystem
- **SciPy:** the `scipy.optimize` module includes basic solvers (like HiGHS for LP) and a functional interface
- **PyTorch/TensorFlow:** while primarily for AI, they are essentially *optimization libraries* for unconstrained problems using stochastic gradient descent.

- cvxpy is a modeling language that follows the rules of **Disciplined Convex Programming (DCP)**
- declarative modeling: we describe *what* the problem is using standard matrix algebra
- problem transformation: transform high-level math into a standard form that specialized solvers can understand
- solver independence: we can swap between different solver backends

Google OR tools

- solver interface (API): provides a bridge between high-level languages (Python, Java, C#) and low-level, high-performance C++ solvers like GLOP or CP-SAT
- multi-solver framework: a **wrapper** that can talk to many different types of engines. It has its own internal solvers but can also *plug in* to commercial ones like Gurobi or CPLEX
- procedural model building: unlike *declarative* modeling (where you describe what the math looks like), OR-Tools uses *procedural* building, where you tell the computer how to add each variable and constraint to the memory
- highly specialized for combinatorial and discrete optimization

Scope of problems solved by OR tools

specialized for combinatorial and discrete optimization

- 1 constraint programming (CP): handled by **CP-SAT** solver; problems with discrete variables and constraints can be non-linear or logical
- 2 linear programming (LP): solve by its internal **GLOP** engine or can interface with commercial solvers like Gurobi or CPLEX
- 3 mixed-integer programming (MIP)
- 4 bin packing and knapsack problems: packing items into containers with fixed capacities
- 5 vehicle routing (VRP): finding optimal routes for vehicles delivering to specified locations
- 6 graph and network flow: movement through a network

what is outside the scope of OR tools

- geneneral nonlinear programming
- general convex programming

Optimization workflow and modeling

Workflow

- 1 get problem statement from an application of interest
- 2 explore all elements: variables, constraint, objective
- 3 acquire all problem parameters
- 4 **formulate** the problem (require prior knowledge about the application)
- 5 use modeling language to **solve** the problem with example of problem data
- 6 **interpret** the solution; if not reasonable, check the root causes:
 - formulation structure
 - problem parameter values
- 7 reformulate the problem if needed
- 8 **implement** to solve the optimization ; select appropriate solver or softwares

Importance of problem formulation

the main reason why we need optimization techniques because

- the objective and constraints give non-trivial info to find optimal solutions

$$\text{P1: } \min 2x_1 + 3x_2 \text{ s.t. } x \succeq 0 \quad \text{P2: } \min 2x_1 + 3x_2 \text{ s.t. } -5 \leq x_1 + x_2 \leq 5$$

- the objective has coupled terms in x

$$\min (x_1 - 1)^2 + (x_2 - 3)^2 \quad \text{versus} \quad \min 4x_1^2 - 2x_1x_2 + 6x_2^2$$

- the constraints have coupled terms in x

$$\min (x_1 - 1)^2 + (x_2 - 3)^2 \quad \text{s.t.} \quad |x_1 + x_2| \leq 3$$

(versus constraint: $0 \leq x_1 \leq 2$ and $0 \leq x_2 \leq 2$)

conclusion: the resulting formulation should be non-trivial (avoid unbounded problem)

Importance of feasible set

when deriving constraints to be included in the problem, ensure that

- the feasible set is not empty (no point of optimizing in the first place)
- avoid redundant constraint functions

$$\text{C1: } |x| \leq 5 \quad \text{C2: } x^2 \leq 28$$

- equivalent constraint function is used when re-formulating

$$x_1^2 + x_2^2 \leq 3 \text{ is not equivalent to } |x_1|, |x_2| \leq \sqrt{3}$$

- if we have an equivalent feasible set from different constraint functions, choose a representation that is simple or suitable for the target problem type:

$$\text{C1: } |x| \leq 5 \text{ is equivalent to } \text{C2: } x^2 \leq 25$$

C1 can be framed as linear constraint (simpler), while C2 is quadratic

B2: Introductory examples in logistics optimization

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2 B2: Introductory examples in logistics optimization

- Introduction to logistics optimization
- Traveling salesman problem (TSP)
- Facility location problem
- Inventory optimization

3 A1: LP-QP-MILP

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Introduction to logistics optimization

Description

focus on the efficient movement of goods, the strategic placement of assets, and the minimization of operational costs

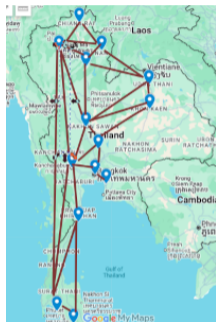
characteristics of problems:

- 1 combinatorial optimization: finding the best possible solution from a finite, but often overwhelming, set of options; in logistics, this usually means determining the best **ordering** or **sequencing** of stops to minimize distance or time
- 2 strategic or tactical planning: this group covers different layers of business decision-making

Traveling salesman problem (TSP)

TSP: problem statement

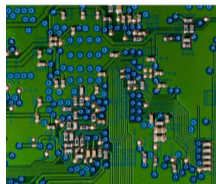
description:



- given n cities and the cost of every possible path from city j to i , $i = 1, 2, \dots, n$
 - visit n cities exactly once and return to the starting city
 - pick the **shortest/cheapest** possible route
- 1 **variables:** $x_{ij} \in \{0, 1\}$ the status of path from city j to i
 - 2 **objective:** minimize the total distance or cost associated with the path
 - 3 **constraints:** each city has one coming edge and outgoing edge
 - 4 **problem parameters:** cost of all connections

challenge: exact algorithm requires all possible combinations ($n!$); impractical for $n \geq 20$

TSP replica: Printed Circuit Board (PCB) Drilling

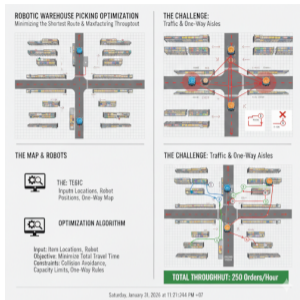


description:

- robotic drill must create hundreds of tiny holes on a circuit board at specific coordinates
- minimize the total distance the drill head travels to reduce manufacturing time and mechanical wear

- 1 **variables:** $x_{ij} \in \{0, 1\}$ the status of path from hole j to i
- 2 **objective:** minimize the total distance
- 3 **constraints:** each hole is drilled once; the drill starts and ends at home coordinate
- 4 **problem parameters:** coordinates of locations; distance of each pair of holes

TSP replica: Robotic warehouse picking

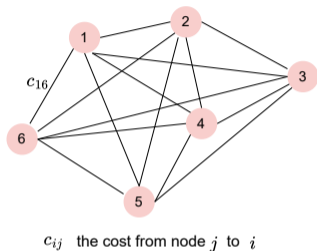


description:

- autonomous mobile robot (AMR) needs to collect items from n shelves to fulfill an order
- find the shortest loop (minimize time) to visit all shelves and return to the packing station
- unlike TSP, we can have many robots at the same time

- 1 **variables:** $x_{ij} \in \{0, 1\}$ the status of path from shelf j to i
- 2 **objective:** minimize the travel distance
- 3 **constraints:** for any location, only one robot can pick up and avoid collision; one-way aisle (robot only go forward) and many more constraints in real system
- 4 **problem parameters:** graph structure of shelves and distance

Structure of TSP



problem parameters:

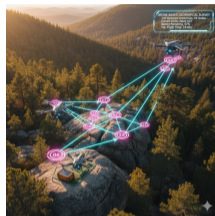
- a graph of n nodes
 - a path from node j to i has a cost of c_{ij} (given as an adjacency matrix)
 - graph can be directed (cost $c_{ij} \neq c_{ji}$) or undirected (symmetric)
-
- optimization solution is to determine $x_{ij} \in \{0, 1\}$ for all $1 \leq i \leq n$, where 1 if there is a path from j to i
 - the cost c_{ij} is not limited to distance; can reflect the fuel, terrain nature, or the difficulty of that path

TSP replica



- 1 power grid restoration:** a repair crew has 10 damaged substations or transformers that need to be inspected and fixed; minimize the total time the crew is on the road to restore power
- 2 seismic surveying:** companies need to collect data from thousands of geographic points (nodes) across difficult terrain; to predetermine *shot-points* where they either set off a small underground charge or use a *vibroiseis* truck to send sound waves into the earth
 - the cost is a combination of fuel, time, terrain difficulty (steep hill and downhill have different cost)
 - find the shortest and most fuel-efficient sequence to visit all shot-point

TSP replica



- 1 mineral exploration:** in remote areas (like the Australian Outback or the Canadian Shield), helicopters or off-road vehicles are used to move between sites; optimizing the flight path to drop off and pick up sampling teams at various outcrops to ensure maximum coverage before the sun sets or fuel runs out
- 2 drone survey:** drones have limited battery life; cannot simply fly a standard lawnmower pattern; TSP: calculating a path that visits all high-priority survey points in a single battery charge

TSP: Mixed-integer linear program

Miller-Tucker-Zemlin (MTZ) formulation

variable: x_{ij} binary status of a path from node j to i

objective function:

$$f(x) = \sum_{i=1}^n \sum_{j=1, j \neq i}^n c_{ij} x_{ij}$$

constraints:

- each city must be left and entered exactly once:

$$\sum_{j=1, j \neq i}^n x_{ij} = 1, \quad i \in [n]$$

- each city must be entered exactly once:

$$\sum_{i=1, i \neq j}^n x_{ij} = 1, \quad j \in [n]$$

TSP: Mixed-integer linear program

- the above two constraints are not enough as it could allow subtours like $1 \rightarrow 2 \rightarrow 1$ and $3 \rightarrow 4 \rightarrow 3$ separately
- subtour elimination constraint: create a time-stamp at each node

$$u_i - u_j + nx_{ij} \leq n - 1, \quad 2 \leq i, j \leq n, i \neq j$$

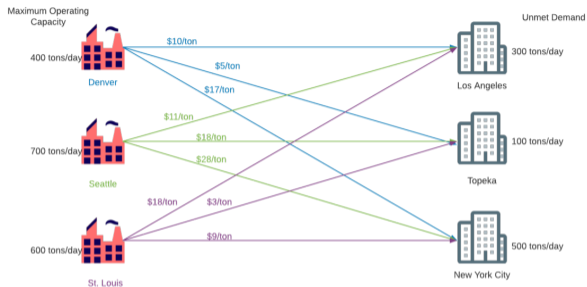
(if $x_{ij} = 1$ the constraint is $u_j \geq u_i + 1$; this forces the sequence to be strictly increasing; impossible in a closed loop)

- variable domain: $u_i \geq 0$ for $i = 2, \dots, n$

the problem can be hard to solve when n is large

Facility location problem

Basic description

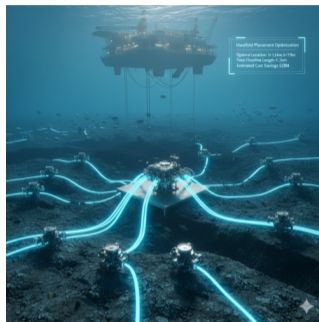


credit: <https://optimization.cbe.cornell.edu/>

given a set of potential facility locations and a set of demand points

- which facilities to open (incorporating a fixed **opening cost**)
- which demand points to assign to each open facility to minimize the **transportation cost**

Petroleum engineering: Manifold Placement



- in subsea oil field development, multiple wells are connected to a single **manifold** or gathering center
- find the geographic coordinates of the manifold that minimize the weighted sum of distances to all connected wellheads

Renewable energy: substation siting



- in a large-scale solar or wind farm, power from individual turbines/panels must be collected at a substation before being sent to the main grid
- placing the substation at the **geometric center** of the turbines to minimize electrical transmission losses (I^2R losses)

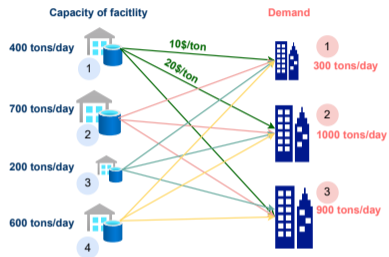
Logistics: disaster response



- placing emergency supply depots (food, water, medicine) in a region prone to natural disasters
- pick the locations that minimize the maximum distance any citizen has to travel to reach the depot after an event

(Capacitated) Facility location problem

given n facility locations indexed by i and m clients to be serviced indexed by j



- each client j has a demand d_j to be filled by selected facilities
- u_i is the capacity of facility i
- f_i is a fixed cost of opening facility i , while there is a cost c_{ij} of serving client j from facility i (\$/demand unit)

- 1 goal:** select a set of facility locations and assign each client to facilities that minimizes the total cost while meeting the targeted demand
- 2 variables:** $x_i \in \{0, 1\}$ for $i = 1, 2, \dots, m$ where $x_i = 1$ if facility i is open ; $y_{ij} \in \mathbf{R}$ represents the **fraction** of the demand d_j filled by facility i

(Capacitated) Facility location problem: formulation

minimize $\sum_{i=1}^n f_j x_i + \sum_{i=1}^n \sum_{j=1}^m c_{ij} d_j y_{ij}$

subject to $y_{ij} \geq 0, \quad i = 1, \dots, n, j = 1, \dots, m$ fractions are non-negative

$x_i \in \{0, 1\}, \quad i = 1, 2, \dots, n$ facility i is either open or closed

$\sum_{i=1}^n y_{ij} = 1, \quad j = 1, 2, \dots, m$ fractions of facilities to serve j sum to 1

$\sum_{j=1}^m d_j y_{ij} \leq u_i x_i, \quad i = 1, 2, \dots, n$ max capacity of facility i

force y_{ij} to be positive when $x_i = 1$

in matrix form: $C, Y \in \mathbf{R}^{n \times m}$ and $x, d, u \in \mathbf{R}^n$

■ cost: $f^T x + \mathbf{1}^T (C \odot Y) d$

■ constraints:

$$Y \geq 0, \quad x \in \{0, 1\}^n, \quad \mathbf{1}_n^T Y = \mathbf{1}_m, \quad Y d \leq u \odot x$$

(Uncapacitated) Facility location problem

when all facilities has ∞ capacity,

- capacitated: optimization solely selects the facility with the lowest cost
- change: modify $y_{ij} \in \{0, 1\}$ where $y_{ij} = 1$ if customer j is served by facility i

$$\text{minimize } \sum_{i=1}^n f_j x_i + \sum_{i=1}^n \sum_{j=1}^m c_{ij} d_j y_{ij}$$

$$\text{subject to } y_{ij} \in \{0, 1\}, \quad i = 1, \dots, n, j = 1, \dots, m$$

$$x_i \in \{0, 1\}, \quad i = 1, 2, \dots, n$$

$$\sum_{i=1}^n y_{ij} = 1, \quad j = 1, 2, \dots, m$$

$$y_{ij} \leq x_i, \quad i = 1, 2, \dots, n, j = 1, 2, \dots, m$$

binary value

facility i is either open or closed

to serve j only pick one facility i

use facility i only if it's open

force y_{ij} to be positive when $x_i = 1$

in matrix form: $C, Y \in \mathbf{R}^{n \times m}$ and $x, d \in \mathbf{R}^n$

- cost: $f^T x + \mathbf{1}^T (C \odot Y) d$

- constraints:

$$Y \in \{0, 1\}^{n \times m}, \quad x \in \{0, 1\}^n, \quad \mathbf{1}_n^T Y = \mathbf{1}_m, \quad Y \leq [x \ x \ \dots \ x]$$

Property of facility location problem

- a mixed integer linear programming (MILP)
- no of binary variable grows with number of clients
- fraction of demand filled by each facility grows with number of clients multiplied with number of locations
- can be solved by cvxpy or OR tools

Facility location: Petroleum engineering

an oil company identifies n sites for Gathering Centers (GC) and has m active oil fields

```
# 1. PROBLEM DATA
```

```
# Fixed costs for building 4 potential sites (Millions of USD)
```

```
f = np.array([20.0, 25.0, 18.0, 30.0])
```

```
# Capacities of the 4 sites (kbpd) kilo barrel per day
```

```
u = np.array([50.0, 60.0, 45.0, 80.0])
```

```
# Production Demands of 6 Oil Fields (kbpd)
```

```
d = np.array([15.0, 22.0, 18.0, 12.0, 25.0, 10.0])
```

```
# Transport Costs ($/bbl) from 4 Sites to 6 Fields
```

```
C = np.array([
    [1.20, 2.50, 3.10, 4.00, 5.20, 6.00],
    [3.50, 1.10, 2.00, 3.20, 4.10, 5.00],
    [5.00, 4.20, 1.50, 1.00, 2.80, 3.50],
    [6.50, 5.50, 4.00, 2.10, 1.20, 0.90]])
```

- minimize the total cost (fixed setup + transport costs) while serving the production demand
- find which site to be open and fraction allocation from each site to each oil field

Inventory optimization

Basic description



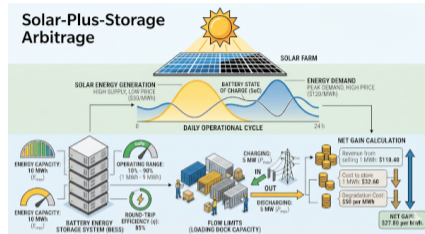
- the process of determining the right amount of stock to hold to meet demand while minimizing the total costs associated with ordering, holding, and shortages
- it depends on accurate demand forecasting, or predicting the quantity of goods that customers will purchase in the future

Petroleum engineering: drilling consumables



- a drilling rig in a remote location (offshore or desert) requires a constant supply of drill bits and casing pipes
- balancing the high cost of shipping equipment to a remote site (ordering cost) against the cost of storing bulky steel pipes on a space-constrained offshore platform (holding cost)

Renewable energy: battery storage



- in a wind or solar farm, energy (MWh) is an intangible inventory
- optimize the **state of charge** to ensure they have enough **stock power** to meet demand when the sun goes down, without building an unnecessarily large and expensive battery array
- MWh in battery are products on the shelf
- renewable generation is the supplier while grid/load is the customer

Costs involved in inventory models

- 1 **ordering and setup cost:** paperwork, billing, setting up/shutting down a machine
- 2 **unit purchasing cost:** variable cost associated with purchasing a single unit
- 3 **holding cost:** cost of carrying one unit of inventory for a time period (\$/unit/year)
- 4 **stockout or shortage cost:** demands can be back-ordered (customer accept delay delivery) or lost sales; both cases incur a cost

assumptions on the classic **Economic Order Quantity (EOQ) model**

- 1 repetitive ordering: ordering decision is repeated regularly
- 2 constant demand: demand occurs at a known, constant rate
- 3 constant lead time L : when an order is placed to the order arrives
- 4 continuous ordering: an order may be placed at any given time

Basic EOQ model

assumptions:

- 1 D : annual demand (units/year) occurs at a constant rate
- 2 K : setup cost (\$/order)
- 3 h : holding cost per unit per year (\$/unit/year)
- 4 q : order quantity (the decision variable)
- 5 p : per-unit purchasing cost (\$/unit)
- 6 I : inventory level (no. of units)
- 7 the lead time for each order is zero
- 8 no shortages are allowed

observations:

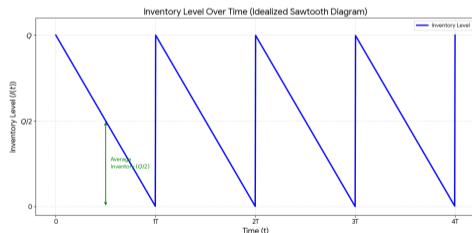
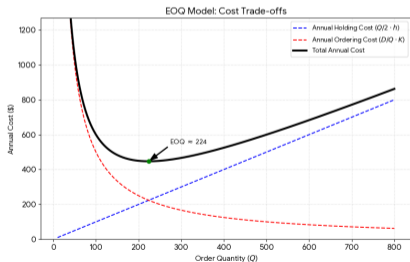
- we should never place an order when $I > 0$ (as it incurs a holding cost)
- we must place an order when $I = 0$ (to prevent a shortage from occurring)
- determine q units are ordered each time that $I = 0$ that minimizes the annual cost

Objective function and optimal quantity

total annual cost: sum of ordering cost, purchasing cost and holding cost

$$TC(q) = \frac{D}{q}K + pD + \frac{q}{2}h$$

(I drops linearly from q to 0, the average inventory is $q/2$)



Optimal order quantity

- TC is convex so the stationary point minimizes TC

$$\frac{dTC}{dq} = -\frac{DK}{q^2} + \frac{h}{2} = 0$$

- solving q gives the EOQ formula:

$$q^* = \sqrt{\frac{2DK}{h}} \quad (\text{units}), \quad \text{total of } \frac{D}{q^*} \text{ orders must be placed each year}$$

- observe effects of K and h on q^*
 - setup cost K increases then q^* increases
 - holding cost h increases then q^* reduces
 - if both K and h are doubled, q^* remains unchanged
- can be shown that if EOQ is ordered then holding cost = ordering cost (per year)

Example: Two-item inventory with storage constraint

setting:

- decide the quantities of drill bits (q_1) and casing pipes (q_2) to order
- in offshore drilling, we have the physical deck space: total area of $A = 5,000$ sq.ft

parameter	symbol	drill bits	casing pipes
annual demand	D_i	120 units	2,400 joints
ordering cost (per shipment)	K_i	\$5,000	\$15,000
holding cost (per unit/year)	h_i	\$300	\$1,200
storage area	a_i	2 sq.ft	40 sq. ft

optimization problem:

$$\begin{aligned} \text{minimize} \quad & \text{TC}(\mathbf{q}) = \sum_{i=1}^2 \left(\frac{D_i}{q_i} K_i + \frac{q_i}{2} h_i \right) \\ \text{subject to} \quad & a_1 q_1 + a_2 q_2 \leq A \end{aligned}$$

try EOQ solution $q_i = \sqrt{\frac{2D_i K_i}{h_i}}$ and find that it is infeasible; let's solve numerically

Example: Two-item inventory with storage constraint

- the problem is nonlinear programming (NLP) with two variables
- the problem is convex ($1/q$ is convex when $q \succ 0$)
- a constrained problem; define Lagrangian and multiplier

$$L(q_1, q_2, \lambda) = \sum_{i=1}^2 \left(\frac{D_i}{q_i} K_i + \frac{q_i}{2} h_i \right) + \lambda \left(\sum_{i=1}^2 a_i q_i - A \right)$$

- optimality conditions: zero gradient of L and complementary slackness

$$q_i(\lambda) = \sqrt{\frac{2D_i K_i}{h_i + 2\lambda a_i}}, \quad \lambda \cdot \left(A - \sum_{i=1}^2 a_i q_i \right) = 0$$

- solved by `scipy.optimize` or `cvxpy`

Storage arbitrage as inventory optimization

maximize revenue by storing energy during the day (low price/high supply) and selling it during the evening peak (high price/low supply), while managing the holding cost (battery degradation)

inventory	BESS equivalent	parameter
warehouse capacity	energy capacity	E_{\max} (MWh)
stock level	state of charge (SoC)	S_t (MWh or %)
restock rate	charging power	$P_{\text{chg},t}$ (MW)
sale rate	discharging power	$P_{\text{dchg},t}$ (MW)
perishability	self-discharge/loss	$\eta_{\text{chg}}, \eta_{\text{dchg}}$ (efficiency)
holding cost	degradation cost	C_{deg} (\$/MWh cycled)
external driver	electricity market price	Price_t (\$/MWh)

- price is the signal that dictates the flow of the inventory
- the battery is the warehouse and the energy is the stock
- the price acts as the external driver that determines when the warehouse should open its doors to restock (charge) or sell (discharge)

Storage arbitrage

variables: $P_{\text{chg},t}, P_{\text{dchg},t}, S_t$

objective function: maximize profit over a 24-hour horizon ($T = 24$)

$$\text{maximize } \Delta t \sum_{t=1}^T \text{Price}_t (P_{\text{dchg},t} - P_{\text{chg},t}) - C_{\text{deg}} (P_{\text{chg},t} + P_{\text{dchg},t})$$

constraints:

1 inventory balance: SoC dynamic

$$S_{t+1} = S_t + \left(\eta_{\text{chg}} P_{\text{chg},t} - \frac{P_{\text{dchg},t}}{\eta_{\text{dchg}}} \right) \Delta t$$

2 storage limit (physical warehouse): battery has operating range

$$S_{\min} \leq S_t \leq S_{\max}$$

3 flow limit (loading dock capacity): inverters limit how fast we can move

$$0 \leq P_{\text{chg},t} \leq P_{\max}, \quad 0 \leq P_{\text{dchg},t} \leq P_{\max}$$

A1: LP-QP-MILP

Outline

1 B1: Fundamental of optimization

- What is optimization?
- Introductory examples: LP/MILP/Model estimation
- Problem setting
- Optimality of unconstrained problems
- Problem types
- Numerical tools
- Optimization workflow and modeling

2 B2: Introductory examples in logistics optimization

- Introduction to logistics optimization
- Traveling salesman problem (TSP)
- Facility location problem
- Inventory optimization

3 A1: LP-QP-MILP

- Linear programming
- Quadratic Programming
- Mixed integer programming

Linear programming

- math standard setting
- feasibility, optimality
- common formulation techniques

Linear programming

a general linear program (LP) has the form

$$\begin{aligned} & \text{minimize} && c^T x \\ & \text{subject to} && Gx \preceq h \\ & && Ax = b \end{aligned}$$

where $G \in \mathbf{R}^{m \times n}$ and $A \in \mathbf{R}^{p \times n}$

- n optimization variables: $x = (x_1, \dots, x_n) \in \mathbf{R}^n$
- the objective function: $c^T x = \sum_{i=1}^n c_i x_i$
- the inequality constraint: $\sum_{j=1}^n g_{ij} x_j \leq h_i$ for $i = 1, 2, \dots, m$
- the equality constraint: $\sum_{j=1}^n a_{ij} x_j = b_i$ for $i = 1, 2, \dots, p$
- the objective function and constraint functions are *linear* in x

called **linear program (LP)** or **linear optimization problem**

Another standard form

LP can also be represented in another form

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax = b \\ & x \succeq 0 \end{array}$$

using the facts that

- any $x \in \mathbf{R}$ can be written $x = x^+ - x^-$
- $a^T x \leq b \iff a^T x + s = b, \quad s \succeq 0$

note: we assume A is fat and has full row rank

exercise: transform into the two general forms

$$\begin{array}{ll} \text{minimize} & 2x_1 - x_2 + x_3 \\ \text{subject to} & -3x_1 + x_2 - 5x_3 \leq 3 \\ & 2x_2 + 7x_3 \geq 10 \\ & 3x_2 + 4x_3 = 2 \end{array}$$

Mixed integer programming

if $x \in \mathbf{Z}^n$ (integers) the problem on page 215 is called an **integer linear programming (ILP)**

if some components of x are integers and some are real numbers, the problem is called a **mixed integer linear programming**

examples of integer programming:

- x represents quantities, countable units (pieces)
- number of sale products
- number of persons assigned on a work schedule
- $x \in \{0, 1\}$: **binary integer programming**
- x is status of a functioning unit in factory, '1' is on, '0' is off

Geometrical interpretation

- hyperplane: solution set of a linear equation with coefficient vector $a \neq 0$

$$\{x \mid a^T x = b\}$$

- halfspace: solution set of a linear inequality with coefficient vector $a \neq 0$

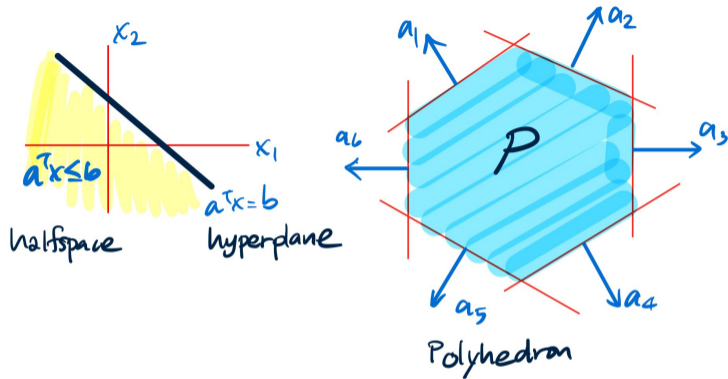
$$\{x \mid a^T x \leq b\}$$

we say a is the **normal vector**

- polyhedron: solution set of a finite number of linear inequalities

$$\{x \mid a_1^T x \leq b_1, a_2^T x \leq b_2, \dots, a_m^T x \leq b_m\} = \{x \mid Ax \preceq b\}$$

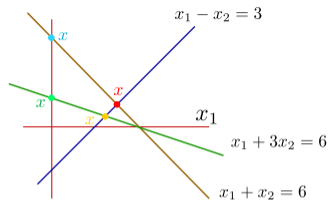
intersection of a finite number of halfspaces



extreme point of \mathcal{C}


a vector $x \in \mathcal{C}$ is an extreme point (or a vertex) if we cannot find $y, z \in \mathcal{C}$ both different from x and a scalar $\alpha \in [0, 1]$ such that $x = \alpha y + (1 - \alpha)z$

Solving LPs graphically



$$\begin{aligned} \text{minimize} \quad & c^T x \\ \text{subject to} \quad & x_1 + x_2 \leq 6 \\ & x_1 - x_2 \leq 3 \\ & x_1 + 3x_2 \geq 6 \\ & x_1, x_2 \geq 0 \end{aligned}$$

- the gradient of $c^T x$ is c
- the objective increases along direction c
- the level set: $\{x | c^T x = \alpha\}$ is the line \perp to c

- feasible set is a bounded polyhedron 
- find the level set: $c^T x = \alpha$ with smallest α that intersects with the feasible set
- find the optimal solution for a given c

$$c = (0, 1), x^* = \quad c = (-1, 0), x^* = \quad c = (-1, 1), x^* = \quad c = (1, 3), x^* =$$

- solving graphically is for conceptual understanding; for 2-dimensional problems

Simple linear programs

minimize $c^T x$ over each of these simple sets

we can derive an explicit solution of these LPs

- **box constraint:** $l \preceq x \preceq u$
- **probability simplex** (or budget allocation): $\mathbf{1}^T x = 1, x \succeq 0$
- **not all budget is used:** $\mathbf{1}^T x \leq 1, x \succeq 0$
- **halfspace:** $a^T x \leq b$

draw the constraint set and inspect the solution for a given c

Properties

refer to the standard form on page 86

- an LP may not have a solution (constraints are inconsistent or the feasible set is unbounded)
- we assume A is full row rank; if not, considering $Ax = b$
 - depending on A , the system could be inconsistent (hence, no extreme points), or
 - $Ax = b$ contains redundant equations, which can be removed
- if a standard LP has a finite optimal solution then

a solution can always be chosen from among the vertices of the feasible set

(called **basic feasible solutions**)

- the dual of an LP is also an LP
- solutions of some simple LPs can be analytically inspected

Common patterns in modeling

- piecewise linear functions
- problems involving absolute values
- problems involving l_1 or l_∞ norms

these problems can be cast as an LP

Problems involving absolute values

using the properties of $|\cdot|$,

linear inequality of absolute-valued function can be cast as linear inequality

- for $x \in \mathbf{R}$, $|x| \leq u \iff -u \leq x \leq u$
- for $x \in \mathbf{R}^n$, $\sum_i^n |x_i| \leq t \iff \exists u \in \mathbf{R}^n, -u \preceq x \preceq u, \mathbf{1}^T u \leq t$
- **ℓ_1 -norm:** $\|Ax - b\|_1 \leq t \iff \exists u \in \mathbf{R}^n, -u \preceq Ax - b \preceq u, \mathbf{1}^T u \leq t$

minimization of a function involving $|\cdot|$ can be cast as an LP (in variables x, u)

$$\text{minimize}_x \|Ax - b\|_1 \iff \begin{array}{l} \text{minimize}_{x,u} \mathbf{1}^T u \\ \text{subject to} \quad -u \preceq Ax - b \preceq u \end{array}$$

Problems involving max of linear functions

recall the fact that

$$\max(f_1(x), f_2(x)) \leq t \iff f_1(x) \leq t, f_2(x) \leq t$$

max of linear functions can be reformulated as linear inequalities

■ for $x \in \mathbf{R}^n$, $\max(0, x) \leq t \iff 0 \preceq t, x \preceq t\mathbf{1}$

■ **piece-wise linear function:**

$$\max(a_1^T x + b_1, a_2^T x + b_2, a_3^T x + b_3) \leq t \iff a_i^T x + b_i \leq t, i = 1, 2, 3$$

■ **l_∞ -norm:**

$$\|x\|_\infty \leq t \iff \max_i |x_i| \leq t \iff |x_i| \leq t, \forall i, \iff -t\mathbf{1} \preceq x \preceq t\mathbf{1}$$

Quadratic Programming

Quadratic Programming

a **quadratic program (QP)** is in the form

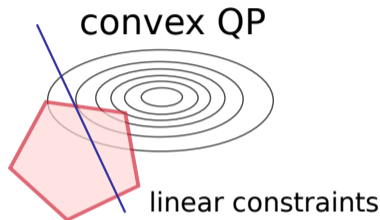
$$\begin{aligned} &\text{minimize} && (1/2)x^T P x + q^T x \\ &\text{subject to} && Gx \preceq h \\ &&& Ax = b, \end{aligned}$$

where $P \in \mathbf{S}^n$, $G \in \mathbf{R}^{m \times n}$ and $A \in \mathbf{R}^{p \times n}$

example: constrained least-squares

$$\begin{aligned} &\text{minimize} && \|Ax - b\|_2^2 \\ &\text{subject to} && l \preceq x \preceq u \end{aligned}$$

QP has **linear** constraints



Properties of QP

- an unconstrained QP is unbounded below if P is not positive definite
- an unconstrained QP has a unique solution: $x = -P^{-1}q$ when $P \succ 0$
- a QP is a convex problem if P is positive semidefinite
 - if $P \succeq 0$ then a local minimizer x^* is a global minimizer (by convexity)
 - if $P \succ 0$ then x^* is a *unique* global solution (by strictly convexity)
- the feasible set (polyhedron) may be empty (hence, the problem is infeasible)
- the feasible set can be unbounded (but if $P \succ 0$ it implies boundedness)
- solution of a QP may not be at a vertex
- the dual of a QP is also a QP

Mixed integer programming

Mixed integer linear programming

a general mixed integer linear programming (MILP) has two general forms

$$\begin{array}{ll} \text{minimize} & c^T x + d^T y \\ \text{subject to} & Ax + By = b \\ & x, y \succeq 0, \\ & x \text{ is integer} \end{array}$$

$$\begin{array}{ll} \text{minimize} & c^T x + d^T y \\ \text{subject to} & Gx + Fy \preceq h \\ & Ax + By = b \\ & x \text{ is integer} \end{array}$$

- $x = (x_1, \dots, x_n)$ where $x_i \in \mathbf{Z}$ (integer variables)
- $y = (y_1, \dots, y_p) \in \mathbf{R}^p$ (real-valued variables)
- the objective function: $c^T x + d^T y = \sum_{i=1}^n c_i x_i + \sum_{i=1}^p d_i x_i$
- the objective function and constraint functions are *linear* in x and y

Common patterns in modeling

- binary choice (zero-one knapsack)
- forcing constraints (facility location problem)
- relation between variables
- disjunctive constraints
- restricted range of values
- arbitrary piecewise linear functions (set packing, set covering)
- sequencing problem with setup times

Binary choice

scenario: when to encode a choice between two alternatives, use binary variables

zero-one knapsack problem

maximize $c^T x$ subject to $w^T x \leq K$, $x_j \in \{0, 1\}$, $j = 1, 2, \dots, n$

setting:

- given n items; each has weight w_j and value c_j
- given a bound K on the total weight that can be carried in a knapsack

goal: decide to select items to maximize the total value

Forcing constraints

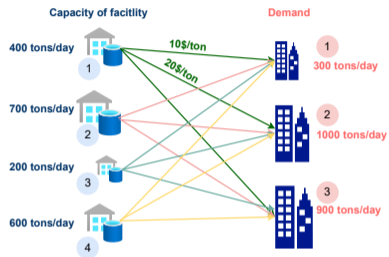
scenario: some variables are dependent; decision A can be made only if decision B has been made

modeling:

- introduce binary variables x, y corresponding to decision A and B, respectively
- set x to equal to 1 if A is chosen and 0 otherwise
- the dependence of the two decisions can be modeled using the constraint: $x \leq y$
- if $y = 0$ (decision B is not made), then $x = 0$ (decision A is not made)

(Capacitated) Facility location problem

given n facility locations indexed by i and m clients to be serviced indexed by j



- each client j has a demand d_j to be filled by selected facilities
- u_i is the capacity of facility i
- f_i is a fixed cost of opening facility i , while there is a cost c_{ij} of serving client j from facility i (\$/demand unit)

- 1 goal:** select a set of facility locations and assign each client to facilities that minimizes the total cost while meeting the targeted demand
- 2 variables:** $x_i \in \{0, 1\}$ for $i = 1, 2, \dots, m$ where $x_i = 1$ if facility i is open ; $y_{ij} \in \mathbf{R}$ represents the **fraction** of the demand d_j filled by facility i

(Capacitated) Facility location problem: formulation

$$\begin{array}{ll} \text{minimize} & \sum_{i=1}^n f_j x_i + \sum_{i=1}^n \sum_{j=1}^m c_{ij} d_j y_{ij} \\ \text{subject to} & y_{ij} \geq 0, \quad i = 1, \dots, n, j = 1, \dots, m \\ & x_i \in \{0, 1\}, \quad i = 1, 2, \dots, n \\ & \sum_{i=1}^n y_{ij} = 1, \quad j = 1, 2, \dots, m \\ & \sum_{j=1}^m d_j y_{ij} \leq u_i x_i, \quad i = 1, 2, \dots, n \end{array}$$

fractions are non-negative
facility i is either open or closed
fractions of facilities to serve j sum to 1
max capacity of facility i
force y_{ij} to be positive when $x_i = 1$

in matrix form: $C, Y \in \mathbf{R}^{n \times m}$ and $x, d, u \in \mathbf{R}^n$

■ cost: $f^T x + \mathbf{1}^T (C \odot Y) d$

■ constraints:

$$Y \geq 0, \quad x \in \{0, 1\}^n, \quad \mathbf{1}_n^T Y = \mathbf{1}_m, \quad Y d \leq u \odot x$$

Either-Or

we want at least one of the two constraints is satisfied

$$f(x_1, \dots, x_n) \leq 0, \quad g(x_1, \dots, x_n) \leq 0$$

we can introduce $y \in \{0, 1\}$ and a big number M and force

$$f(x_1, \dots, x_n) \leq My, \quad g(x_1, \dots, x_n) \leq M(1 - y)$$

If-Then constraints

we want to ensure that

$$f(x) > 0 \quad \text{implies} \quad g(x) \geq 0$$

- introduce $y \in \{0, 1\}$ and a big number M_f

$$f(x) \leq M_f \cdot y \quad \text{if } f(x) > 0 \text{ then } y \text{ must be 1}$$

(if $f(x) \leq 0$ then y can be 0 or 1)

- link the 'then' part: $y = 1 \Rightarrow g(x) \geq 0$

$$g(x) \geq -M_g(1 - y) \quad \text{if } y = 1 \text{ then } g(x) \geq 0$$

(if $y = 0$ this constraint does nothing as $-M_g$ is very small)

in conclusion, we formulate

$$f(x) \leq M_f y, \quad g(x) \geq -M_g(1 - y)$$

Fixed-charge problem

scenario: there is a cost associated with performing an activity at a nonzero level that does not depend on the level of activity

a fixed cost of operating machine A when there is an order of product A (but the cost does not depend on the units of A)

modeling:

- introduce binary variable y and let $x \in \mathbf{R}$ be the level/number of units of such activity
- goal: set y to 1 whenever x is nonzero
- use the constraint: $x \leq My$ where M should be set equal to the maximum of x that can attain

Relations between variables

scenario: when at most one of binary variables can be 1

modeling:

- at most one of the variables x_j can be one

$$\mathbf{1}^T x \leq 1$$

- exactly one of the variables x_j should be one

$$\mathbf{1}^T x = 1$$

Disjunctive constraints

scenario: given two constraints $a^T x \geq b$ and $c^T x \geq d$ where $a, c \succeq 0$, we would like to have at least one of the two constraints are satisfied

modeling: define a binary y and impose

$$a^T x \geq yb, \quad c^T x \geq (1 - y)d, \quad y \in \{0, 1\}$$

general scenario: given m constraints: $a_i^T x \geq b_i$, for $i = 1, \dots, m$ where $a_i \succeq 0$, we require at least K of them are satisfied

modeling:

$$a_i^T x \geq b_i y_i, \quad i = 1, 2, \dots, m, \quad \mathbf{1}^T y \geq K, \quad y_i \in \{0, 1\}$$

Restricted range of values

scenario: aim to restrict x to take values in a set $\{a_1, a_2, \dots, a_m\}$

modeling: define $a = (a_1, a_2, \dots, a_m)$ and a binary variable $y \in \mathbf{R}^m$ such that

$$x = a^T y, \quad \mathbf{1}^T y = 1, \quad y_j \in \{0, 1\}$$

Constraint Programming

Constraint programming

constraint programming (CP) is based on identifying feasible solutions, rather than minimizing some objective

CP may or may not have an objective function

examples:

- employee scheduling: create work schedules for employees over a horizon
- job shop problem: design schedule of multiple jobs processed on several machines

CP problems can be solved by CP-SAT solver in Google OR-Tools

Nurse scheduling problem

a problem of finding an optimal way to assign employees to shifts with a set of hard constraints

employee scheduling problems are defined by three key elements:

- 1 **resources:** the *entities* being scheduled; here, the nurses/employees
- 2 **tasks/slots:** time intervals needed to be filled; day and night shifts over an N -day horizon
- 3 **constraints:** rules of scheduling
 - capacity constraint: (3 people per shift)
 - temporal constraint: (no double-shifts, 12-hour recovery after nights)
 - distribution constraint: (min 3/ max 5 shifts per week)

scheduling is often treated as a **constraint satisfaction problem (CSP)**

unlike trying to minimize an objective, the primary challenge is simply finding *any* valid schedule that does not violate constraints

solver CP-SAT in Google OR-Tools can be used to solve this problem

Numerical tools

Solver overview (1)

Solver	LP	QP	MILP	Convex	w/ cvxpy	w/ OR-Tools	Notes
Gurobi	Yes	Yes	Yes	Yes	Yes	Yes	Leading commercial solver; offers the highest performance across all problem types
CPLEX	Yes	Yes	Yes	Yes	Yes	Yes	IBM's high-performance commercial solver; a standard in industrial-scale optimization
HiGHS	Yes	Yes	Yes	Partial	Yes	Yes/installed	A high-performance, modern open-source software for sparse linear optimization; support convex QP, not SOCP; currently, not implemented with solving QP within MathOpt interface in OR-Tools
SCIP	Yes	Yes	Yes	Yes	Yes	Yes/installed	A powerful global optimizer that handles MINLP and non-convex problems; fast non-commercial solvers available

Solver overview (2)

Solver	LP	QP	MILP	Convex	w/ cvxpy	w/ OR-Tools	Notes
ECOS	Yes	Yes	No	Yes	Yes/installed	No	A lightweight high precision interior-point solver specialized for LP, QP, SOCP
SCS	Yes	Yes	No	Yes	Yes/installed	No	ADMM (splitting methods); solve very large problems to moderate accuracy; for all conic problems
OSQP	Yes	Yes	No	Yes	Yes/installed	Yes	the operator splitting QP solver; currently the default and fastest open-source choice for convex QP
Clarabel	Yes	Yes	No	Yes	Yes/installed	No	all conic types; robust, modern implementation with strong numerical stability

Solver overview (3)

Solver	LP	QP	MILP	Convex	w/ cvxpy	w/ OR-Tools	Notes
PDLP	Yes	Yes	No	Yes	No	Yes/installed	Google's primal-dual hybrid gradient solver; built for massive-scale LP and convex diagonal QP
GLOP	Yes	No	No	No	No	Yes/installed	Google's primary first-party LP solver ; highly optimized for speed in pure LP tasks
CP-SAT	Yes	No	Yes	No	No	Yes/installed	Google's flagship solver of OR-tools ; a hybrid solver using Lazy Clause Generation that combines Constraint Programming, SAT, and LP; world-class for combinatorial problems

Solver overview (4)

Solver	LP	QP	MILP	Convex	w/ cvxpy	w/ OR-Tools	Notes
CBC	Yes	No	Yes	No	Yes	Yes	open-source MILP solver from the COIN-OR project; robust for discrete linear problems
GLPK	Yes	No	No	No	Yes	Yes	part of the GNU project; a reliable, widely-used engine for pure LP
GLPK_MI	Yes	No	Yes	No	Yes	No	MILP interface for GLPK
CVXOPT	Yes	Yes	No	Yes	Yes	No	legacy Python-based library for convex optimization that uses interior-point methods

Outline

1 B1: Fundamental of optimization

- What is optimization?
- Introductory examples: LP/MILP/Model estimation
- Problem setting
- Optimality of unconstrained problems
- Problem types
- Numerical tools
- Optimization workflow and modeling

2 B2: Introductory examples in logistics optimization

- Introduction to logistics optimization
- Traveling salesman problem (TSP)
- Facility location problem
- Inventory optimization

3 A1: LP-QP-MILP

- Linear programming
- Quadratic Programming
- Mixed integer programming

Examples on Geoscience

Example list

- l_1 - and l_∞ -norm approximation
- capturing geologic fold
- gas production allocation
- asset portfolio risk management
- rig scheduling
- pipeline network design
- fuel distribution

some compact notations: we always deal with vectors $x \in \mathbf{R}^n$

- for an integer n , $[n] = \{1, 2, \dots, n\}$
- $c \odot x$ (Hadamard product) is a vector of (c_1x_1, \dots, c_nx_n)
- $c^T x$ is a scalar returning $\sum_{i=1}^n c_i x_i$
- $\mathbf{1}^T x$ is a scalar returning $\sum_{i=1}^n x_i$

ℓ_1 -norm and ℓ_∞ -norm approximations

given $A \in \mathbf{R}^{m \times n}$ and $b \in \mathbf{R}^m$

- ℓ_1 -norm approximation: minimize $\|Ax - b\|_1$

equivalent LP:

$$\begin{aligned} & \text{minimize} && \mathbf{1}^T u \\ & \text{subject to} && -u \preceq Ax - b \preceq u \end{aligned}$$

with variable x and auxiliary variable u

- ℓ_∞ -norm (or Chebyshev) approximation: minimize $\|Ax - b\|_\infty$

equivalent LP:

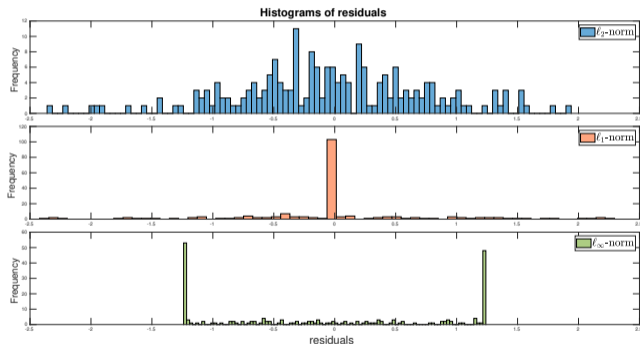
$$\begin{aligned} & \text{minimize} && t \\ & \text{subject to} && -t\mathbf{1} \preceq Ax - b \preceq t\mathbf{1} \end{aligned}$$

with variable x and auxiliary variable t

ℓ_1 - and ℓ_∞ -norm approximation results

compare histograms of residuals $Ax - b$ for

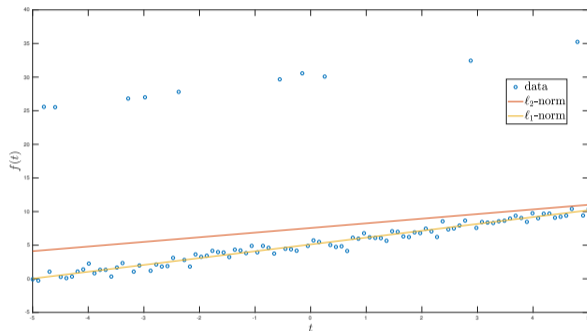
$$x_{1s} = \operatorname{argmin} \|Ax - b\|_2, \quad x_1 = \operatorname{argmin} \|Ax - b\|_1, \quad x_\infty = \operatorname{argmin} \|Ax - b\|_\infty$$



example of $A \in \mathbf{R}^{200 \times 100}$: residuals of 1-norm approximation is concentrated at zero

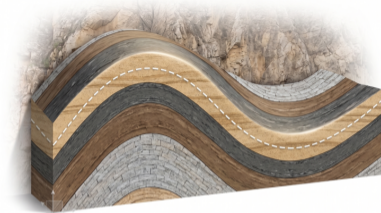
Estimation with outliers

fitting $f(t) = \alpha + \beta t$ to data containing 10% outliers



- ℓ_2 -norm approximation tends to reduce large residuals occurred from outliers
- ℓ_1 -norm has less penalty than ℓ_2 when residuals are large; it is more robust to outliers

Capturing geologic fold



the surface of a reservoir is rarely a flat plane

setting:

- to capture the actual curvature of rock layers, geoscientists represent the depth y as a function of geographic coordinates (easting d_e and northing d_n)

$$\hat{y} \approx x_0 + x_1 d_e + x_2 d_n + x_3 d_e^2 + x_4 d_n^2 + x_5 d_e d_n$$

- data y may contain noisy outliers (from seismic reflection and well-log data)

goal: estimate parameter x that gives $\hat{y} \approx y$ while avoiding sensitivity to outliers

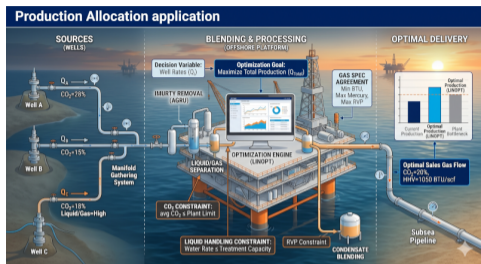
Capturing geologic fold

modeling: apply ℓ_1 -norm approximation where $x = (x_0, x_1, x_2, x_3, x_2)$

$$\hat{y} = [1 \quad d_e \quad d_n \quad d_e^2 \quad d_n^2 \quad d_e d_n] x$$

- note that \hat{y} is nonlinear in coordinate data but linear in x (parameter)
- frame as $\hat{y} = Ax$ and minimize $\|y - Ax\|_1$ to suppress the influence from outliers
- treat the problem as a convex, or reformulate as an LP (this lecture)

Gas production allocation



- n wells production gas with different CO₂
- gas must be blended before it enters the pipeline to meet the Sales Gas Agreement (SGA)

- **variables:** flow rate from each well, choke size (discrete), well status (on/off)
- **objective:** maximize total gas production (revenue)
- **constraints:**
 - CO₂ removal from all wells must be limited
 - heating value (HHV): gas must be hot enough but not so rich
 - liquid handling: limit how much gas you can draw from each well
 - daily contract quantity (DCQ): deliver a minimum amount to avoid penalty

Gas production allocation

assume no binary well status variable

- **variables:** flow rate $q \in \mathbf{R}^n$ (unit = MMscf/day)– Million standard cubic feet
- **objective:** maximize total revenue minus cost

$$\text{revenue} = \sum_{i=1}^n p_i q_i = p^T q, \quad p = \text{price} = \text{gas price} + \text{CGR} \cdot \text{condensate price}$$

$$\text{opex cost} = \sum_{i=1}^n \text{opex}_i q_i$$

$$\text{objective} = f(q) = (p - \text{opex})^T q \triangleq c^T q \quad (\text{unit} = \$)$$

notes:

- 1 price coefficients vary with wells
- 2 gas contains condensate (light oil) and has higher value than dry gas
- 3 the cost may additionally contain some penalty on impurities

Gas production allocation: Constraints

constraints:

1 $0 \preceq q \preceq q_{\max}$ (well capacity)

2 $\mathbf{1}^T q \leq \text{capacity}$ (total volume has a limit)

3 a limit for total mass of CO_2

$$\frac{\sum_{i=1}^n \text{CO}_{2,i} q_i}{\sum_{i=1}^n q_i} \leq \text{LCO}_2 \implies (\text{CO}_{2,i} - \text{LCO}_2)^T q \leq 0$$

4 liquid handling: $\sum_{i=1}^n \text{WGR}_i q_i \leq \text{LW}$ WGR = water gas ratio

5 SGA: Heating value must be in a range

$$\text{HHV}_{\min} \leq \frac{\sum_{i=1}^n \text{HHV}_i q_i}{\sum_{i=1}^n q_i} \leq \text{HHV}_{\max} \implies \begin{aligned} (\text{HHV} - \text{HHV}_{\min})^T q &\geq 0 \\ (\text{HHV} - \text{HHV}_{\max})^T q &\leq 0 \end{aligned}$$

Gas production allocation: Impurities

effect: increasing q makes the pressure drop near the wellbore increases and cause:

- water coning: higher rate pull water into the well, increasing WGR
- composition change: higher flow may draw gas from different layers that have higher CO_2

impurity modeling:

- concentration of impurity: % CO_2 or bbl/MMscf of water
 - each well has its own impurity model (assume linear)

$$c_i(q) = a_i q_i + b_i, \quad i = 1, 2, \dots, n$$

- a_i is the sensitivity of impurity to the flow rate
- b_i is the baseline impurity level at minimum flow
- total impurity function: can be put in the objective or as constraints

$$g(q) = \sum_{i=1}^n c_i(q) q_i = \sum_{i=1}^n a_i q_i^2 + b_i q_i = q^T A q + b^T q \quad (\text{quadratic function})$$

(unit = MMscf of CO_2 per day, or bbl/d for water)

Gas production allocation: Impurities

impurity model as **constraint**: replace the limit of CO₂ constraint with

$$g(q) = q^T Aq + b^T q \leq \text{Limit} \sum_{i=1}^n q_i$$

(total CO₂ mass entering must be \leq a limit multiplied by the total volume of gas)

impurity model as **objective**: minimize

$$\text{cost of impurity} = \lambda \cdot g(q) = \lambda(q^T Aq + b^T q)$$

(λ is the penalty coefficient: unit = \$ per MMscf of CO₂)

Gas production allocation: Optimizations

net cost = OPEX cost - revenue

default constraints = defined on page 131

- 1 P1: minimize net cost with default constraints
- 2 P2: minimize net cost + impurity cost with default constraints
- 3 P3: minimize net cost with default + impurity constraints

LP

QP

QCQP

Asset portfolio risk management

setting:

- n wells with different risk profiles and value; some has low decline, low risk but expensive to operate, while others are volatile but cheaper
- given production rate's average and covariance calculated from historical data

goal: determine the production rate for each well to meet a total demand while minimizing the total risk of the production

modeling:

- $x \in \mathbf{R}^n$: percentage of the total demand production from n wells
- $\Sigma \in \mathbf{S}^n$: covariance of the production rate (mmCFD²)
- $x^T \Sigma x$: the risk or volatility of the total gas supply
- μ : expected production rate (mmCFD) decline curve analysis (DCA)
- $\mu^T x$: weighted average production

Asset portfolio risk management: Covariance

- diagonals (variance): individual uncertainty of each well
- off-diagonals (covariance): Σ_{ij} is the covariance between well i and j
 - positive: if two wells are in the same reservoir layer, they likely have high positive covariance (some technical issues in that layer would cause both to decrease simultaneously)
 - low/zero: two wells are uncorrelated, providing the diversification for minimizing the overall risk

Asset portfolio risk management: Optimization

variable: x (allocation of production rate)

objective: $(1/2)x^T \Sigma x$ (the risk)

constraints:

- 1 allocation constraints: $0 \preceq x \preceq \mathbf{1}, \mathbf{1}^T x = 1$
- 2 demand requirement: $\mu^T x \geq D$ where D is the total required demand
- 3 physical capacity limit: $0 \preceq x \cdot D \preceq C$ where $C \in \mathbf{R}^n$ is the maximum capacity

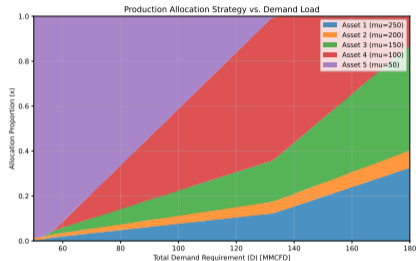
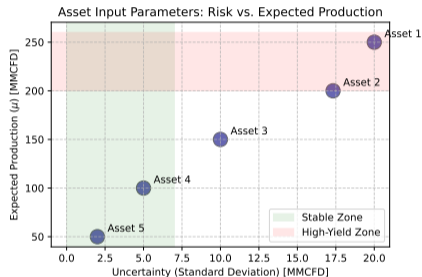
optimization: quadratic program (QP)

$$\begin{aligned} & \text{minimize} && (1/2)x^T \Sigma x \\ & \text{subject to} && 0 \preceq x \preceq \mathbf{1}, \mathbf{1}^T x = 1 \\ & && \mu^T x \geq D, \quad 0 \preceq x \cdot D \preceq C \end{aligned}$$

with variable $x \in \mathbf{R}^n$

Asset portfolio risk management: Results

example: five wells with different uncertainty and yield



- vary D (demand) and observe the portion of allocation
- for low D , invest all in well no. 5 (low risk)
- for high D , invest distributedly in well no. 1,2,3,4

Asset portfolio risk management: as an insurance policy

the formulation on page 223 is essentially an insurance policy model

- by setting D as a hard constraint, meeting the national gas demand is non-negotiable
- by minimizing $x^T \Sigma x$, we are looking for the *quietest* way to meet that demand—the allocation that is least likely to result in a supply shock if one of the wells underperforms

Asset portfolio risk management: Variance and production trade-off

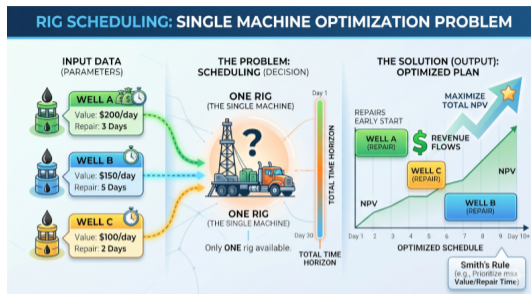
if we add the average production to the objective:

$$\begin{aligned} & \text{minimize} && (1/2) x^T \Sigma x - \lambda \mu^T \mathbf{x} \\ & \text{subject to} && 0 \preceq x \preceq \mathbf{1}, \mathbf{1}^T x = 1 \\ & && \mu^T x \geq D, \quad 0 \preceq x \cdot D \preceq C \end{aligned}$$

with variable $x \in \mathbf{R}^n$

- $\lambda > 0$ is **risk aversion parameter**: trade-off between *stable* and *cheap* production
- adding $\mu^T x$ to the objective seems redundant but it changes the behavior of the optimal solution within the feasible region
 - with only the constraint ($\mu^T x \geq D$): the solver finds the allocation x that minimizes risk and merely satisfies the demand D ; likely to hit the boundary where $\mu^T x = D$
 - with both ($\lambda \mu^T x$ in objective + constraint): the solver minimizes risk but is also *rewarded* for exceeding the demand D ; if there are assets that are both stable and high-producing, the solver may choose an allocation that results in $\mu^T x > D$ because the *benefit* of the extra production outweighs the marginal increase in risk.

Rig scheduling: single machine scheduling



setting:

- n wells require repair time and offers different production gain
- a workover rig can repair one well at a time
- a total available repair time is given

goal: find a schedule that maximize the total cumulative value after recovery

- fix the most productive wells as early as possible
- maximize the total value recovered presented as NPV

Rig scheduling: NPV

we prioritize fixing high-value wells as early as possible

- a well only begins generating revenue after the repair is complete
- if the repair of well i is finished at day c_i , the well will produce revenue for the remaining days $(T - c_i)$
- for well i , NPV (net present value) is the sum of discounted daily revenue:

$$\text{NPV}_i = \sum_{t=c_i+1}^T \frac{v_i}{(1+r)^t}, \quad r \text{ is the discount rate}$$

note: c_i is a function of x_{it} , and NPV appears to be a function of x

Rig scheduling: NPV

as $x_{it} = 1$ at day t and 0 otherwise, we can arrange a NPV matrix ($n \times T$) to be the sum starting from t to T :

$$\text{NPV}_{it} = \sum_{i=1}^n \left(\sum_{k=t}^T \frac{v_i}{(1+r)^k} \right)$$

the objective is to maximize the NPV that only counts after finishing the repair

$$\underset{x}{\text{maximize}} \quad \sum_{i=1}^n \sum_{t=1}^T x_{it} \cdot \text{NPV}_{it}$$

which has a linear objective

Rig scheduling: minimum lead time constraint

the sum of all *finish* possibilities for days earlier than the duration must be zero

$$\sum_{t=1}^{d_i-1} x_{i,t} = 0$$

example: if well i requires 4 days of work

$$x_{i1} = x_{i2} = x_{i3} = 0$$

Rig scheduling: non-overlap constraints

example: two wells where well 1 takes 2 days, and well 2 takes 3 days to finish

- 1 if the rig is working on well 1 on day $\tau = 4$ then $\text{active}_{1,4} = x_{1,4} + x_{1,5}$
 - it could finish at the end of day 4 (started day 3)
 - it could finish at the end of day 5 (started day 4)
- 2 if the rig is working on well 2 on day $\tau = 4$ then $\text{active}_{2,4} = x_{2,4} + x_{2,5} + x_{2,6}$
 - it could finish at the end of day 4 (started day 2)
 - it could finish at the end of day 5 (started day 3)
 - it could finish at the end of day 6 (started day 4)
- 3 the constraint on day $\tau = 4$ says that the sum across all wells must be ≤ 1

$$(x_{1,4} + x_{1,5}) + (x_{2,4} + x_{2,5} + x_{2,6}) \leq 1$$

example: $x_{1,4}$ and $x_{2,4}$ cannot be 1 at the same time; that would mean the rig is active on well 1 during day 3,4 while being active on well 2 during 2,3,4, creating an impossible overlap

Rig scheduling optimization

we can now present the optimization problem as IP:

maximize _{x} NPV
subject to minimum lead time constraint
non-overlap constraint

with variable $x \in \{0, 1\}^{n \times T}$

explain the solution outcomes under these considerations:

- when T is less than the total repair time, not all wells can be fixed
- what if the value does not decrease over time (not using NPV assumption), would the scheduling plan change?

Rig scheduling: the effect of using NPV

effect on a scenario where a well with a high value also has a long repair duration
setup: $T = 10$, two wells: $v = (500, 200)$ and $d = (5, 2)$

case 1: $r = 0$

- option 1: fix well A before well B, finished on day 5 and then 7

$$\text{revenue} = A + B = (10 - 5) \times 500 + (10 - 7) \times 200 = 3100\$$$

- option 2: fix well B before well A, finished on day 2 and then 7

$$\text{revenue} = B + A = (10 - 2) \times 200 + (10 - 7) \times 500 = 3100\$$$

areas under the revenue curve are the same: the solver is indifferent
the sequence of choosing well to be fixed is not relevant

Rig scheduling: the effect of using NPV

setup: $T = 10$, two wells: $v = (500, 200)$ and $d = (5, 2)$

case 2: $r = 0.001$ a dollar on day 1 is worth more than on day 10

- option 1: fix well A before well B (high value first)
 - well A starts generating revenue on day 6 (\$500/day), which is more valuable than well B (\$200/day)
 - choose well A first if r is relatively low (discount penalty is low as compared to value generating)
- option 2: fix well B before well A (short duration first)
 - well B finishes fast (day 2) and generate revenue immediately
 - if the discount rate r is high enough, the solver might prefer starting the smaller \$200 on day 3, rather than waiting until day 6 for \$500 option

when $r > 0$, its value and (v, d) affect the sequence of scheduling

the solver feels *pressure* to finish high-value wells early to avoid losing value over time

Rig scheduling: connection to other problems

without NPV: the actual value is $v_i \times$ remaining days

the problem share similarities to knapsack and bin packing problems

- knapsack goal: choose subset of wells that fits into the time slot (as capacity) to maximize the total value from the subset you pick
- bin packing goal: focus on space utilization (arrange wells so there is no idle time for the rig)

Rig scheduling: as a single machine scheduling

in general, a single machine scheduling has several objectives: *e.g.*,

- minimize the sum of completion times
- minimize the cost of lateness
- minimize the profit of earliness

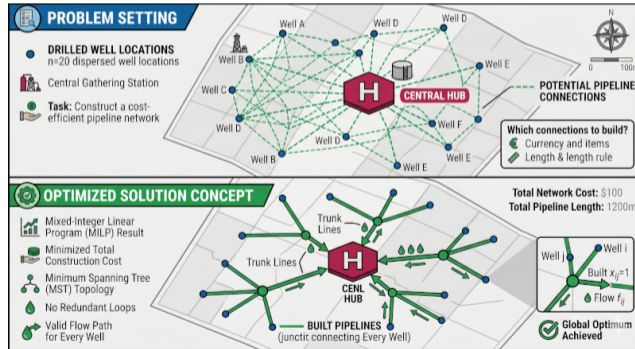
the smith's rule (weighted shortest processing time, WSPT) is optimal algorithm for **infinite horizon**

with NPV or a fixed T , smith's rule is a heuristic (provide a good starting point) but not optimal

Pipeline network design

setting:

- n newly drilled wells across a field and one central station
- aim to connect every well to the station using minimum cost
- ensure that every well has a valid flow path to the destination



Pipeline network design: Variables and Objective

variables:

- $x_{ij} \in \{0, 1\}^{n \times n}$: $x_{ij} = 1$ if a pipeline is constructed from node j to node i
- $f_{ij} \geq 0$: the amount of fluid flowing from node j to node i

objective:

$$\text{minimize} \quad \sum_{1 \leq i, j \leq n} c_{ij} x_{ij}$$

example of the cost coefficient: c_{ij} can be the distance between location i and j

once x and f are solved, we can represent the network using **graph** concept

- a set of nodes indexed by $1, 2, \dots, n$
- a set of edges connected between node i and j ; here, using x as the adjacency matrix to determine the edges

an edge connected between from node j to node i if $x_{ij} = 1$

Pipeline network design: Constraints

- **flow balance:** for each node i , the net flow (total flow out - total flow in) must equal the production

$$\sum_k f_{ki} - \sum_j f_{ij} = b_i \quad (\text{production})$$

(f_{ki} is flow out of i to k , and f_{ij} is flow from j into i)

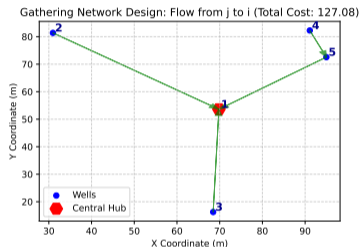
- if $b_i > 0$, the node i is a generator or a source
 - if $b_i < 0$, the node i is a sink (or load), e.g., the station
- **capacity link:**

$$f_{ij} \leq M \cdot x_{ij}, \quad M \text{ is a large number}$$

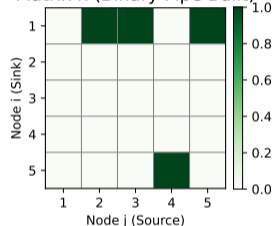
this ensures flow can only exist from j to i if the pipe x_{ij} is built

Pipeline network design: Results

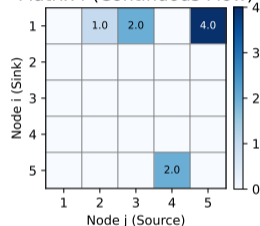
the optimization is MILP



Matrix x (Binary Pipe Built)



Matrix f (Continuous Flow)



- node 1 is the hub: row 1 has nonzero entries on column 2,3,5 (from nodes 2,3,5)
- link from node 4 to node 5: row 5 has a nonzero entry on column 4
- sum of row 1: sum of flows to the hub

Pipeline network design: extension

some relevant constraint in a more realistic setting

- 1 pressure drop and nonlinear flow

$$f_{ij}|f_{ij}| = C_{ij}^2 \sqrt{P_j^2 - P_i^2} \quad (C_{ij} \text{ is a pipeline constant})$$

the flow is proportional to the square root of the difference of squared pressures (this is nonlinear; require some more math technique to re-formulate)

- 2 define an auxiliary variable: $\pi_i = P_i^2$ and use a **relaxation**

$$f_{ij}^2 \leq C_{ij}^2 (\pi_j - \pi_i) \quad (\text{relax to inequality})$$

- 3 this can be rewritten as a **second-order cone** form:

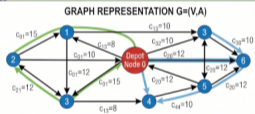
$$2 \left(\frac{f_{ij}}{C_{ij}} \right)^2 + 2\pi_i \leq 2\pi_j \quad \implies \quad \left\| \begin{array}{c} \sqrt{2} \frac{f_{ij}}{C_{ij}} \\ \pi_j - \pi_i - 1 \end{array} \right\|_2 \leq \pi_j - \pi_i + 1$$

the problem is a mixed-integer second-order cone program (MISOCP)

Fuel distribution

a central terminal (depot) must supply a set of gas stations using a fleet of trucks

EXPLORING THE FUEL DISTRIBUTION VRP (VEHICLE ROUTING PROBLEM)



KEY VRP PROPERTIES
V: Vertex Set (Nodes {0..N})
A: Arc Set (Directed edges (i,j))
 c_{ij} : Cost matrix (Distance, Time, Fuel)
 d_i : Station demand
 Q_k : Vehicle Capacity

network: a directed graph $G = (V, A)$

- $V = \{0, 1, \dots, n\}$: set of nodes (node 0 is the depot and nodes $1, \dots, n$ are delivery points)
- $A = \{(i, j) \mid i, j \in V, i \neq j\}$: an ordered pair (i, j) implying a direction from node i to j

- **depot:** a single starting and ending point for all vehicles
- **customers:** n gas stations, each with a known fuel demand d_i
- **fleet:** K identical tanker trucks, each with a maximum fuel capacity Q
- **travel cost:** c_{ij} (distance or time) is the cost from location i to j

Fuel distribution: Variables

- $x \in \{0, 1\}^{(n+1) \times (n+1) \times K}$: travel status

$x_{ijk} = 1$ if vehicle k travels directly from node i to node j

- $u \in \mathbf{R}^{(n+1) \times K}$: cumulative load variable

u_{ik} represents the total load carried by vehicle k after visiting node i
(to track capacity and prevent sub-tours)

Fuel distribution: Objective

the goal is to minimize the total operational cost of the fleet.

$$\text{minimize } \sum_{k=1}^K \sum_{i=0}^n \sum_{j=0}^n c_{ij} \cdot x_{ijk}$$

this minimizes the sum of all segments traveled by all active tanker trucks

indices i, j starts at **0** referring to the depot index and $1, \dots, n$ for customers

Fuel distribution: Constraints

notation: $V = \{0, 1, \dots, n\}$ and $[n] = \{1, \dots, n\}$

every station is serviced without exceeding truck limits

- 1 service guarantee:** each gas station must be visited exactly once by one truck

$$\sum_{k \in [K]} \sum_{i \in V} x_{ijk} = 1, \quad \forall j \in [n]$$

(this is assign constraint to gas station, so j runs from 1, not 0)

- 2 flow conservation:** if a truck enters a gas station (node i), it must also leave that station to go to the next node or return to the depot

$$\sum_{i \in V} x_{ipk} - \sum_{j \in V} x_{pjk} = 0, \quad \forall p \in V, \forall k \in [K]$$

(go from i to p and then go from p to j)

Fuel distribution: Constraints

- 3 **depot continuity:** every truck used must start its route at the depot and return to the depot after its final delivery

$$\sum_{j \in [n]} x_{0jk} = 1, \quad \forall k \in [K], \quad \sum_{i \in [n]} x_{i0k} = 1, \quad \forall k \in [K]$$

- 4 **capacity constraint:** for any vehicle k , the sum of demands d_j for all stations on its route cannot exceed the tanker's capacity Q_k

$$\sum_{i \in V} \sum_{j \in [n]} d_i \cdot x_{ijk} \leq Q_k \quad \forall k \in [K]$$

- 5 **sub-tour elimination:** ensure the solution is one continuous loop per truck rather than several disconnected small cycles

Fuel distribution: Sub-tour elimination

a common approach is the **Miller-Tucker-Zemlin (MTZ)** formulation:

$$\text{MTZ 1: } u_{ik} - u_{jk} + Q_k x_{ijk} \leq Q_k - d_j, \quad \forall (i, j) \in A, j \neq 0, \forall k \in [K]$$

$$\text{MTZ 2: } d_i \leq u_{ik} \leq Q_k, \quad \forall i \in [n], \forall k \in [K]$$

how it works: the constraint MTZ 1 is binding only when traveling from i to j

- if travel from $i \rightarrow j$ ($x_{ijk} = 1$): constraint reduces to

$$u_{jk} \geq u_{ik} + d_j \quad \Rightarrow \quad \text{force } u_{jk} \text{ to strictly increase}$$

creating a logical flow that cannot loop back on itself

example: consider a loop $1 \rightarrow 2 \rightarrow 3 \rightarrow 1$

1 for $1 \rightarrow 2$: $u_{2k} \geq u_{1k} + d_2$

2 for $2 \rightarrow 3$: $u_{3k} \geq u_{2k} + d_3 \implies$

3 for $3 \rightarrow 1$: $u_{1k} \geq u_{3k} + d_1$

take the sum of three inequalities

we get a **contradiction**

$$0 \geq d_1 + d_2 + d_3$$

therefore, **no such loop can exist** in a feasible solution

Fuel distribution: Sub-tour elimination

- if not travel from $i \rightarrow j$ ($x_{ijk} = 0$): constraint reduces to

$$u_{ik} - u_{jk} \leq Q_k - d_j, \quad \Rightarrow \quad \text{easily satisfied by any load value (loose constraint)}$$

meaning u_{jk} is free to be any value that fits the rest of the route's logic

Fuel distribution: Optimization

the problem is MILP and regarded as a **capaciated vehicle routing (CVRP)** problem

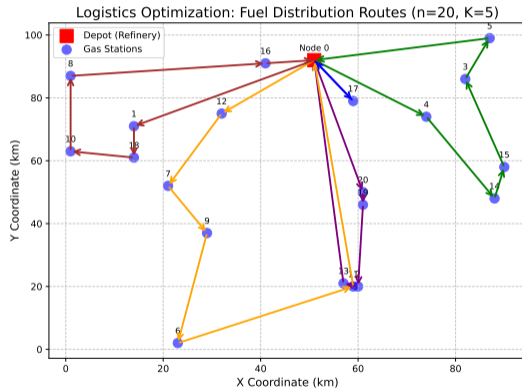
minimize travel cost
subject to service guarantee
flow conservation
depot continuity
capacity constraint
sub-tour elimination

with variables $x \in \{0, 1\}^{(n+1) \times (n+1) \times K}$ (travel status) and $u \in \mathbf{R}^{(n+1) \times K}$ (cumulative load variable)

can be solved by routing library in Google OR tools

Fuel distribution: Results

example: $n = 20$, $K = 5$, $Q = (25, 25, 25, 25, 25)$, random coordinates and demand, cost is the distance



the solver naturally groups gas stations that are geographically close to each other

essentially a collection of TSP with added constraints

- for one vehicle with infinite capacity, CVRP simplifies to a standard TSP
- since TSP is NP-hard¹, CVRP must also be NP-hard
- MILP formulations can be used for small-to-medium problems but for large-scale logistics, we often rely on specialized heuristics
- OR-tools use metaheuristics (guided local search, GLS) in routing problem
- CVRP introduces elements of bin packing problem as we must decide which gas stations (demand) fit into which truck (bins of capacity)
- CVRP is a VRP with a capacity constraint; if we set infinite capacity ($Q = \infty$), it becomes multi-vehicle VRP

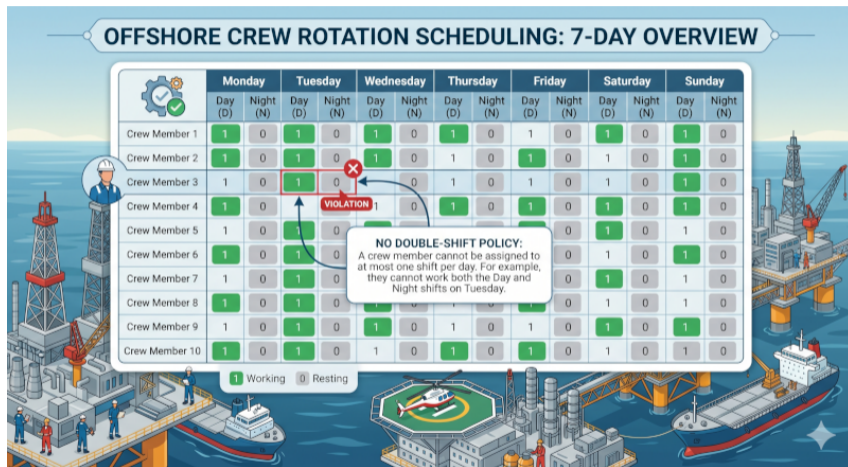
¹(non-deterministic polynomial-time hard; it is at least as difficult as the hardest problems in NP)

Shift assignment

an offshore gas platform operates two 12-hour shifts (Day and Night) per day. You must assign a pool of 10 crew members to these shifts over a 7-day rotation period while satisfying strict safety and labor regulations.

- 1 minimum skill coverage:** each shift (day and night) must have exactly 3 crew members assigned; no more, no less
- 2 no double-shift rule:** a crew member can be assigned to at most one shift per day; they cannot work both the day and night shifts
- 3 recovery period:** if a crew works a night shift, they cannot work the day shift immediately following it; need at least 12 hours of rest
- 4 fair work-life balance:** over 7-day period, every member must work at least 3 shifts but no more than 5 shifts total

Shift assignment: Example of results



Project scheduling

goal: to schedule a set of n maintenance activities during a planned facility shutdown

- maintenance list: valve replacement, sensor calibration, pressure vessel inspection
- the platform has limited specialized personnel (divers, welders) and equipment (heavy-lift cranes)
- each task has a known duration, but some tasks cannot start until others are finished

variables:

- start time: S_i an integer showing when task i begins for $i \in [n]$
- end time: E_i an integer showing when task i finishes for $i \in [n]$
- presence: P_i a boolean (if a task is optional, though in shutdowns, most are mandatory)
- interval: I_i a logical object that link start, end, and duration ($E_i = S_i + \text{duration}$)

Project scheduling: Logic constraints

- 1 precedence constraints: task B cannot start until task A is complete: $S_B \geq E_A$
- 2 resource capacity (cumulative): the total number of welders required by all active tasks at any hour t cannot exceed the 5 welders currently offshore

$$\sum_i \text{welders}_i \leq \text{available welders}$$

- 3 disjunctive constraints (no-overlap): two specific tasks cannot happen at the same time because they share the same physical space or tools

$$I_A \text{ and } I_B \text{ must not overlap}$$

- 4 fixed windows: the flare tip replacement must be during daylight hours for safety

$$S_{\text{flare}} \geq 06:00 \text{ and } E_{\text{flare}} \leq 18:00$$

Project scheduling: Objective

minimize the maximum E_i (the finish time of the very last task)

this translate to minimizing lost production revenue

CP-SAT uses interval variables and cumulative functions designed specifically to handle blocks of time efficiently

Project scheduling: Example

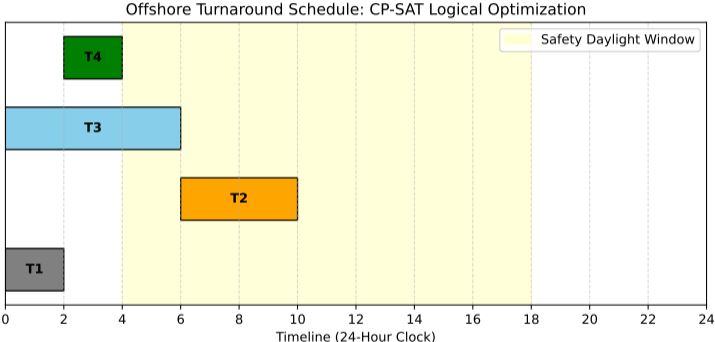
horizon: 24-hour to complete all the tasks

Task	Work	Duration (h)	Resource
T1	scaffold	2	2 workers
T2	flare removal	3	3 workers + crane
T3	pipe welding	6	2 workers
T4	crane calibration	2	1 worker + crane

logic constraints:

- 1 precedence: we must scaffold before removing the flare tip (T2)
- 2 resource capacity: T2 and T3 must require the workers to stays ≤ 4
- 3 no-overlap: T2 and T4 both require the single crane
- 4 fixed window: T2 (flare removal) must occur during 6:00-18:00

Project scheduling: Result



Outline

1 B1: Fundamental of optimization

- What is optimization?
- Introductory examples: LP/MILP/Model estimation
- Problem setting
- Optimality of unconstrained problems
- Problem types
- Numerical tools
- Optimization workflow and modeling

2 B2: Introductory examples in logistics optimization

- Introduction to logistics optimization
- Traveling salesman problem (TSP)
- Facility location problem
- Inventory optimization

3 A1: LP-QP-MILP

- Linear programming
- Quadratic Programming
- Mixed integer programming

Regression problem

Regression problem

setting: suppose $\{(x_i, y_i)\}_{i=1}^N$ are input/output data

- y (output/response variable) is a function of x (input/regressor)
- ground-truth: $y = g(x; \theta) + e$ where g is the actual relationship between x and y parametrized by θ but g is unknown
- we model $\hat{y} = f(x; \theta)$ and estimate θ such that $\hat{y} \approx y$

method: to quantify that $y \approx \hat{y}$, several choices of loss functions can be applied

- ℓ_2 -norm: $\ell(\theta) = (1/N) \|y - \hat{y}\|_2^2 = (1/N) \sum_{i=1}^N |y_i - f(x_i; \theta)|^2$
- ℓ_1 -norm: $\ell(\theta) = (1/N) \|y - \hat{y}\|_1 = (1/N) \sum_{i=1}^N |y_i - f(x_i; \theta)|$
- ℓ_∞ -norm: $\ell(\theta) = \|y - \hat{y}\|_\infty = \max_{i=1, \dots, N} |y_i - f(x_i; \theta)|$

other robust loss functions exist in literature (huber, median absolute deviation (MAD), etc.)

Regularized regression

we provide a concept of estimation with two objectives:

$$\underset{x}{\text{minimize}} \quad f(x) := g(x) + \gamma h(x)$$

- x is model parameter
- g is a loss function that indicates **model fitting**
- h is a **regularization function** that affects solution properties (aka **penalty**)
- $\gamma > 0$ is a penalty weight controlling a balance between model quality and regularization of x

g is typically a quadratic loss or log-likelihood function

the choice of h dictates the solution behaviour

ℓ_2 regularization

given x_r as a targeted solution (defined by the user)
we add the 2-norm penalty to the objective function

$$\underset{x}{\text{minimize}} \quad g(x) + \gamma \|x - x_r\|_2^2$$

- seek for a solution that minimizes $g(x)$ but also close to x_r
- the trade-off is controlled by $\gamma > 0$ (large value heavily forces $x \approx x_r$)
- also called **Tikhonov regularized least-squares** or **ridge regression**
- when $g(x)$ is the linear least-squares loss: $g(x) = \|Ax - y\|_2^2$, the ℓ_2 -regularized LS has the analytical solution for any $\gamma > 0$:

$$x^* = (A^T A + \gamma I)^{-1} A^T y$$

(no restrictions on shape, rank of A)

- interpreted as a MAP estimation with the log-prior of the Gaussian

ℓ_1 regularization

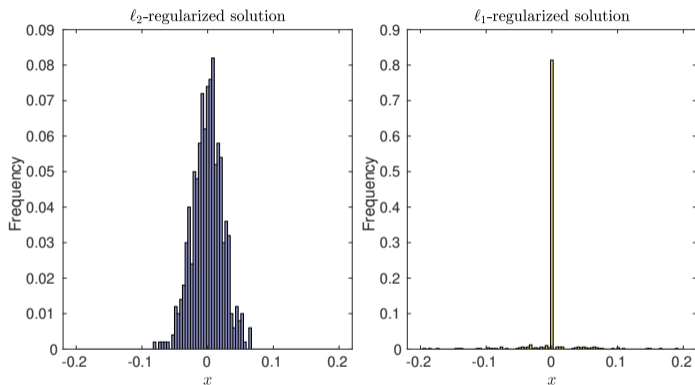
adding the ℓ_1 -norm penalty to the least-square problem

$$\underset{x}{\text{minimize}} \quad g(x) + \gamma \|x\|_1$$

- a convex heuristic method for finding a sparse x that also minimizes g
- also called **Lasso** or **basis pursuit**
- a nondifferentiable problem due to $\|\cdot\|_1$ term
- no analytical solution (even when g is linear LS loss), but can be solved efficiently
- interpreted as a MAP estimation with the log-prior of the Laplacian distribution
- find many applications known as **sparse** methods: sparse- logistic regression, PCA, SVM, Gaussian graphical model, etc.

Regularization: Example

solve linear LS with $h(x) = \|x\|_2^2$ and $h(x) = \|x\|_1$ using $\gamma = 0.2$



- solution of ℓ_2 regularization is more widely spread
- solution of ℓ_1 regularization is concentrated at zero

Quantile regression

suppose we model $y = f(x; \beta)$ where f can be any nonlinear mapping

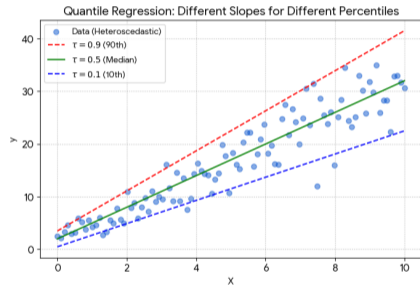
goal: find β_τ that makes $\hat{y} = f(x; \beta)$ match well with τ -quantile of y

$$\underset{\beta_\tau}{\text{minimize}} \quad (1/N) \sum_{i=1}^N \rho_\tau(y_i - f(x_i; \beta_\tau))$$

where ρ_τ is called the **pinball loss**

$$\rho_\tau(r) = \max(\tau r, (\tau-1)r) = \begin{cases} (\tau-1)r, & r < 0, \\ \tau r, & r \geq 0 \end{cases}$$

- can be shown that $\hat{y} = f(x; \beta_\tau)$ agrees with the sample τ -quantile of y
- if $f(x; \beta_\tau)$ is **linearly parametrized** in β_τ , the problem can be cast as an LP



LP formulation for quantile regression

when $f(x; \beta_\tau)$ is linearly parametrized in β_τ :

$$f(x; \beta_\tau) = \beta_{\tau,1}g_1(x) + \cdots + \beta_{\tau,s}g_s(x)$$

(a nonlinear model f is represented as a sum of s -basis functions g_k)

minimizing pinball loss can be cast as an LP

$$\begin{aligned} & \text{minimize}_{d, \beta_\tau} && \mathbf{1}^T d \\ & \text{subject to} && \tau(y_i - f(x_i; \beta_\tau)) \leq d_i, \quad i = 1, \dots, N \\ & && (\tau - 1)(y_i - f(x_i; \beta_\tau)) \leq d_i, \quad i = 1, \dots, N \end{aligned}$$

(by introducing $d \in \mathbf{R}^N$ as an upper bound of max function)

it can be an LP because $f(x; \beta_\tau)$ is linear function in $\beta_{\tau,1}, \dots, \beta_{\tau,s}$

Quantile regression: Multiple quantiles

when the goal is to find \hat{y}_τ associated with a list of τ -quantiles:

$$\tau \in \Gamma = \{\tau_1, \tau_2, \dots, \tau_m\} \quad \text{e.g., } \Gamma = \{0.1, 0.2, \dots, 0.9\}$$

- we must have separate coefficients β_τ for each τ
- mathematical fact: the value of $\hat{y}_\tau = f(x; \beta_\tau)$ is increasing as τ increase, e.g.,

$$\hat{y}_{0.1} \leq \hat{y}_{0.2} \leq \dots \leq \hat{y}_{0.9}$$

- the coefficients $\beta_{0.1}, \dots, \beta_{0.9}$ are linked to **non-crossing quantile** condition

quantile regression with non-crossing quantile constraint

$$\begin{aligned} & \text{minimize}_{\beta_\tau} && (1/N) \sum_{i=1}^N \sum_{\tau \in \Gamma} \rho_\tau(y_i - f(x_i; \beta_\tau)) \\ & \text{subject to} && f(x_i; \beta_{\tau_1}) \leq f(x_i; \beta_{\tau_2}) \leq \dots \leq f(x_i; \beta_{\tau_m}), \quad i = 1, \dots, N \end{aligned}$$

Examples in geoscience

- well test analysis
- decline curve analysis (DCA) and regularization
- quantile decline curve

Well test analysis

motivation:

- when we shut in a producing well, the pressure in the wellbore begins to rise as the surrounding reservoir fluids try to reach equilibrium
- how the pressure increases over time is a *unique* characteristic of the reservoir

problem setting: given N samples of t_i and ΔP_i (change in pressure) for $i \in [N]$

model the pressure change by

$$\Delta \hat{P}(t; kh, s) = \frac{162.6 \cdot q \cdot B \cdot \mu}{kh} \left[\log_{10} \left(\frac{kt}{\phi \mu c_t r_w^2} \right) - 3.23 + 0.869s \right]$$

where q (flow rate), B (formation volume factor), μ (viscosity), ϕ (porosity), c_t (compressibility), r_w (wellbore radius) are known constants

unknown parameters: $k \cdot h$ (permeability-thickness) and s (skin factor)

Well test analysis: as Nonlinear least-squares

we can group the terms: $A = 162.6 \cdot q \cdot B \cdot \mu$ and $D = \frac{1}{\phi \mu c_t r_w^2}$

$$\Delta \hat{P}(t; kh, s) = \frac{A}{kh} [\log_{10}(kDt) - 3.23 + 0.869s]$$

physical constraints: $kh > 0$ and $s \geq -5$ (physical limit for stimulated well)

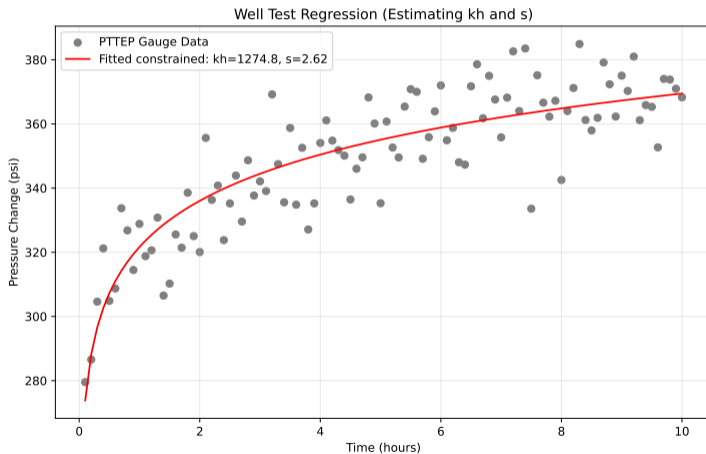
nonlinear least-squares:

$$\underset{kh, s}{\text{minimize}} \quad \frac{1}{N} \sum_{i=1}^n \left[\Delta P_i - \left(\frac{A}{kh} [\log_{10}(kDt_i) - 3.23 + 0.869s] \right) \right]^2$$

- we can try solving NLS with and without physical constraints
- note that if kh is known, the problem becomes linear LS in s

Well test analysis: Fitted result

given a fixed h , ground-truth value ($kh = 1250.0, s = 2.5$)



Decline curve analysis (DCA)

when open a well, the pressure is high, and the oil flows fast; as oil leaves the tank, the pressure drops, and the flow rate declines

questions to be explored:

- forecasting: how much oil will the well produce next month?
- EUR: Estimated uncertainty recovery: what is the total volume we will recover before the well dies?
- mine life: when will the well hit its economic limit where it costs more to run than it earns?

DCA: the Arps equations

J.J.Arps observed that the relative change in production rate follows

$$q(t) = \frac{q_0}{(1 + bD_0t)^{1/b}}, \quad t > 0 \quad t \text{ is time}$$

- q_0 : initial production rate when the well first starts
- D_0 : initial decline rate (how fast the production drops at the every beginning, e.g., 10% per year)
- b : the b-factor describes the **curvature** of the decline
 - $b = 0$ (exponential): decline by a constant percentage per year (take the limit $b \rightarrow 0$, we get $q(t) = q_0e^{-D_0t}$ using L'Hôpital's rule)
 - $0 < b < 1$ (hyperbolic): a common case where the rate itself slows down over time
 - $b = 1$ (harmonic): special case often seen in high-water-derive reservoirs

DCA: Linearized Arps equations

instead of viewing $q(t)$ as the response, we consider the relative change in production

$$\text{decline rate: } D(t) \triangleq -\frac{1}{q(t)} \frac{dq(t)}{dt} = \frac{D_0}{1 + bD_0t}$$

the reciprocal of $D(t)$ is linearly parametrized in b

$$\frac{1}{D(t)} = bt + \frac{1}{D_0} = [t \quad 1] \begin{bmatrix} b \\ \frac{1}{D_0} \end{bmatrix} \triangleq y = Ax$$

- by changing the response variable, we can use a linear model (the estimation part becomes easy)
- calculating dq/dt from raw data can be extremely noisy
- outlier: if dq/dt is near zero (during a temporary production spike or sensor error), the value $\frac{q}{dq/dt}$ goes to ∞

DCA: Nonlinear least-squares

for a single well, we observe data $(t, q(t))$, find $x = (q_0, D_0, b)$ that

$$\underset{x}{\text{minimize}} \sum_{t=1}^T (q(t) - \hat{q}(t; x))^2$$

where $\hat{q}(t; x)$ is the production from the assumed model

linear case: when $b = 0$, reduces to linear LS

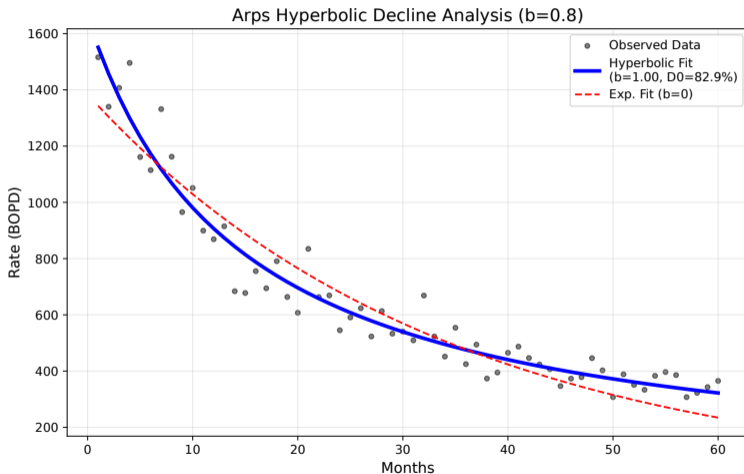
$$\log q(t) = \log(q_0) - D_0 t$$

practical issues:

- data may contain outliers due to shut-in period, adjusted choke
- well condition change (pump installation, water breakthrough); this may require refit the decline curve in multi-segment
- with a few samples, the optimization may return b factor that is unrealistic, e.g., $b = 2$ (may fix by posting a constraint)

DCA: Fit result

ground-truth: Arps equation with $b = 0.8$



fitted with `scipy.optimize.curve_fit`

DCA: ℓ_2 regularization

penalize the squared distance of the b factor from a known physical **anchor**, b_{prior} for a shale (unconventional reservoir), expect $b \approx 1 - 1.5$ during first 3-5 years


$$\ell_2\text{-regularized LS: } \underset{x}{\text{minimize}} \sum_{t=1}^T (y(t) - \hat{y}(t; x))^2 + \gamma(b - b_{\text{prior}})^2$$

- regularize on the nonlinear Arps model

$$y(t) = q(t), \quad \hat{y}(t; x) = \frac{q_0}{1 + bD_0t}, \quad x = (b, D_0)$$

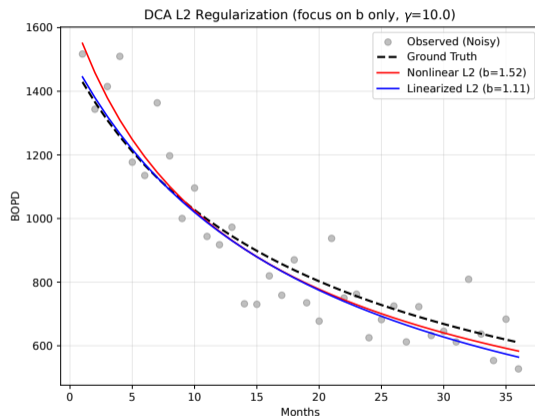
- regularize on the linearized Arps model

$$y(t) = \frac{1}{D(t)}, \quad \hat{y}(t; x) = bt + \frac{1}{D_0}, \quad x = (b, 1/D_0)$$

closed-form solution: $b = (A^T A + \gamma e_1 e_1^T)^{-1} (A^T y + \gamma e_1 b_{\text{prior}})$, $e_1 = (1, 0)$ 

DCA: Fit result of ℓ_2 regularization

ground-truth: Arps equation with $b = 1.4$ and set $b_{\text{prior}} = 1.3$



the performance depends on γ (penalty parameter) and the confidence in b_{prior}

Quantile decline curve

produce a family of curves $q_\tau(t)$ that define the probability space of well's performance

- P90 curve ($\tau = 0.1$): the **conservative profile**; there is a 90% chance that the actual production at any time t will be above this line
- P50 curve ($\tau = 0.5$): the **most likely profile**; the median expectation
- P10 curve ($\tau = 0.9$): the **upside potential**; only 10% of wells, given these x inputs, will perform this well

modeling:

- response y : production rate (q_t) at time t (STB/d)
- predictor t : time (months on production)
- predictor X :
 - controllable: lateral length, number of stages, total proppant
 - measured: porosity, initial reservoir pressure, depth
 - choke size setting

Quantile decline curve

assume the production rate follows a model $f(t, x; \beta)$

quantile regression minimizes the pinball loss: given quantile list $\Gamma = \{0.1, 0.5, 0.9\}$

$$\begin{aligned} &\text{minimize}_{\beta_\tau} \sum_{\tau \in \Gamma} \sum_{i=1}^{N_{\text{no. well}}} \sum_{t=1}^{T_i} \max(\tau(y_{i,t} - f(t, x_i; \beta_\tau)), (\tau - 1)(y_{i,t} - f(t, x_i; \beta_\tau))) \\ &\text{subject to} \quad \text{non-crossing quantile constraint} \end{aligned}$$

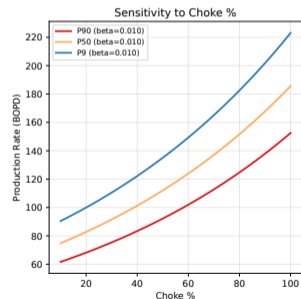
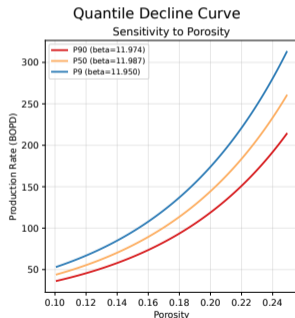
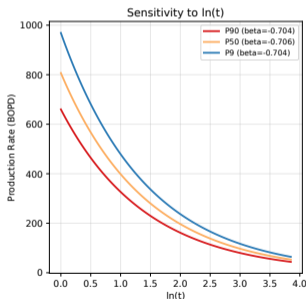
- some static predictors x_i that do not change over time
 - depth of well i
 - amount of proppant (sand) injected into well i during completion
 - geological coordinates of well i
- the time length T_i may vary between wells (well A has 24-month data, while well B has 6 month)
- coefficient β_τ is **global** across wells (represent physics applied to the entire field)

Quantile decline curve

data: 200 wells, $\tau = 0.1, 0.5, 0.9$

$$\log q(t) = \beta_0 + \beta_1 \log(t) + \beta_2 \cdot \text{porosity} + \beta_3 \cdot \text{choke}$$

(choke changes over time, but porosity is static)



(plotted in the original transform - reverse log back to expo)

Numerical tools

Python library

- nonlinear least-squares with constraints
 - `scipy.optimize.curve_fit`
 - `scipy.optimize.least_squares`
 - linear case: `np.linalg.lstsq`
- quantile regression
 - linear case: can be alternatively solved using LP formulation
 - `statsmodel` with `QuantReg` class
 - `Scikit-learn` with `QuantileRegressor` class
 - tree-based models such as `LightGBM`, `XGboost`, quantile regression forest
- quantile neural network (QRNN): we can use `PyTorch` implementation

other regression problems: depend on the problem type

if convex, we can use `cvxpy`

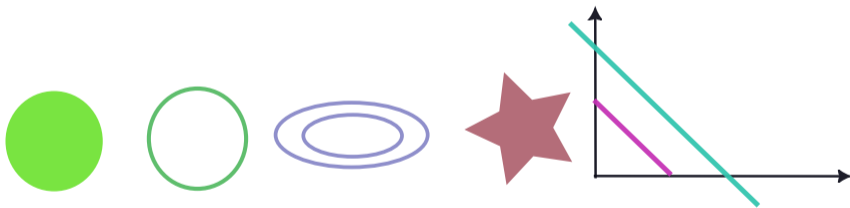
A4: Convex optimization applications

Convex sets

a set \mathcal{C} is said to be **convex** if for any $x, y \in \mathcal{C}$ we have

$$\theta x + (1 - \theta)y \in \mathcal{C}, \quad \text{for all } 0 \leq \theta \leq 1$$

which of the following sets are convex ?



fact: an intersection of convex sets is convex (even infinitely many number of intersections)

Convex sets: Examples

examples in \mathbf{R}^n

- hyperplane, halfspace
- polyhedron: $\{x \in \mathbf{R}^n \mid a_i^T x \leq b_i, i = 1, \dots, m, c_j^T x = d_j, j = 1, \dots, p\}$
- probability simplex: $\{x \mid x \succeq 0, \mathbf{1}^T x = 1\}$
- norm ball: $\{x \in \mathbf{R}^n \mid \|x\| \leq \alpha\}$ where $\alpha \geq 0$ is given
- norm cone: $\{(x, t) \mid \|x\| \leq t\} \subseteq \mathbf{R}^{n+1}$
- second-order cone: is the norm cone for the ℓ_2 -norm
- convex cone: C is a set that $x_1, x_2 \in C$ and $\theta_1, \theta_2 \geq 0$ we have $\theta_1 x_1 + \theta_2 x_2 \in C$

Convex functions

convex function: $f : \mathbf{R}^n \rightarrow \mathbf{R}$ is convex if

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$$

for all x, y in the domain of f and $0 \leq \theta \leq 1$

loosely speaking, f is convex if it has an upward shape

examples on \mathbf{R} :

- affine: $ax + b$ for any $a, b \in \mathbf{R}$
- exponential: e^{ax} for any $a \in \mathbf{R}$
- powers of absolute value: $|x|^p$ for $p \geq 1$
- negative entropy: $x \log x$ on \mathbf{R}_{++}

Examples of convex functions on \mathbf{R}^n

- affine: $a^T x + b$
- norm functions: $\|x\|$
- norms of affine: $\|a^T x + b\|$
- quadratic: $x^T P x + q^T x$ when $P \succeq 0$
- negative entropy: $\sum_{i=1}^n x_i \log x_i$ on \mathbf{R}_{++}^n
- log-sum-exponential: $\log(\sum_{i=1}^m e^{x_i})$
- sum of K -largest entries: $x_{[1]} + \dots + x_{[K]}$ where $x_{[1]} \geq x_{[2]} \geq \dots \geq x_{[n]}$

fact: a α -sublevel set of a convex function f :

$$\mathcal{C}_\alpha = \{x \in \mathbf{R}^n \mid f(x) \leq \alpha\}$$

is a convex set

Connection between convex sets and convex functions

suppose a feasible set is described by inequality constraint functions:

$$\mathcal{C} = \{x \in \mathbf{R}^n \mid f_i(x) \leq 0, i = 1, 2, \dots, m \}$$

fact: \mathcal{C} is a convex set if all $f_i(x)$'s are convex functions

- the constraint of each $f_i(x) \leq 0$ corresponds to a convex set (sublevel set of convex function property)
- \mathcal{C} is the **intersection** of m convex sets, and hence is convex

First- and second-order conditions of convex functions

suppose f is differentiable; then f is convex if and only if

$$\mathbf{dom} f \text{ is convex and } f(y) \geq f(x) + \nabla f(x)^T(y - x), \quad \forall x, y \in \mathbf{dom} f$$

- the first-order Taylor approximation of f is a **global underestimator** of f if and only if f is convex
- if $\nabla f(x) = 0$ then for all $y \in \mathbf{dom} f$, $f(y) \geq f(x)$, i.e., x is a **global minimizer** of f

assume that $\nabla^2 f$ exists at each point in $\mathbf{dom} f$; then f is convex if and only if

$$\mathbf{dom} f \text{ is convex and } \nabla^2 f(x) \succeq 0, \quad \forall x \in \mathbf{dom} f$$

f is convex if and only if its Hessian matrix is positive semidefinite

Operations that preserve convexity

preserve convexity of a convex set

- intersection
- image (and inverse image) of affine mapping
- image (and inverse image) of perspective mapping

preserve convexity of a convex function

- non-negative weighted sum
- composition with affine mapping, composition rules
- pointwise maximum and supremum, minimization over one variable
- perspective of a function
- conjugate function (important role in duality theory)

Pointwise maximum

if f_1, \dots, f_m are convex then their pointwise maximum:

$$f(x) = \max\{f_1(x), f_2(x), \dots, f_m(x)\}$$

is also convex

example:

- piece-wise linear function:

$$f(x) = \max\{a_1^T x + b_1, a_2^T x + b_2, \dots, a_m^T x + b_m\}$$

Composition of convex with affine function

if $f(x)$ is convex then $f(Ax + b)$ is also convex

examples:

- $f(x) = \|Ax + b\|$ for any norm $\|\cdot\|$

- $f(x) = \log \left(\sum_{i=1}^m e^{a_i^T x + b_i} \right)$ (softplus, smooth approximation of max)

- $f(w) = \max(0, 1 - y_i(w^T x_i + b))$ (hinge loss in SVM)

Supremum over an infinite set of convex functions

if for each $y \in \mathcal{A}$, $f(x, y)$ is convex in x , then the function g , defined as

$$g(x) = \sup_{y \in \mathcal{A}} f(x, y)$$

is convex in x

- distance to farthest point of a set:

$$f(x) = \sup_{y \in C} \|x - y\| \quad \text{is convex}$$

(since $\|x - y\|$ is linear in x (hence, convex in x))

- support function of a set:

$$S_C(x) = \sup \{x^T y \mid y \in C\}$$

(since $x^T y$ is linear in x)

Convex programs

convex optimization problem is one of the form

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & f_i(x) \leq 0, \quad i = 1, \dots, m \\ & a_i^T x = b_i, \quad i = 1, \dots, p \end{array}$$

where

- objective and constraint functions are **convex**
- equality constraint functions $h_i(x) = a_i^T x - b_i$ must be **affine**

result: an optimal solution of a convex program is a **global** minimizer

Properties of convex problems

convex problems are of interest due to some desirable properties

- many operations preserve convexity of a convex set
 - intersection
 - image (and inverse image) of affine mapping
 - image (and inverse image) of perspective mapping
- many operations preserve convexity of a convex function
 - non-negative weighted sum
 - composition with affine mapping, composition rules
 - pointwise maximum and supremum, minimization over one variable
 - perspective of a function
 - conjugate function (important role in duality theory)
- KKT conditions are *sufficient* and *necessary* for optimality

many optimization problems in engineering are convex programs

LP and QP

a general **linear program** has the form

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Gx \preceq h \\ & Ax = b \end{array}$$

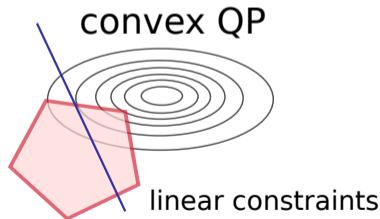
where $G \in \mathbf{R}^{m \times n}$ and $A \in \mathbf{R}^{p \times n}$

a **quadratic program (QP)** is in the form

$$\begin{array}{ll} \text{minimize} & (1/2)x^T Px + q^T x \\ \text{subject to} & Gx \preceq h \\ & Ax = b, \end{array}$$

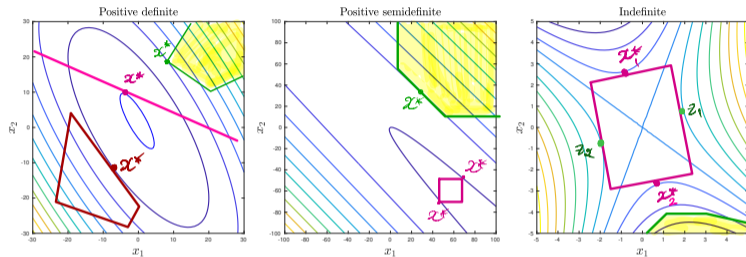
where $P \in \mathbf{S}^n$, $G \in \mathbf{R}^{m \times n}$ and $A \in \mathbf{R}^{p \times n}$

QP has **linear** constraints



Contour of quadratic objective

consider three cases of P and different feasible sets



verify the location of the optimal solution for each constraint set

- left: a bounded set, a line, an unbounded feasible set
- middle: bounded and unbounded feasible sets, while f is unbounded below
- right: a bounded feasible set, while f is unbounded below and above

a **quadratically constrained quadratic program (QCQP)** is in the form

$$\begin{aligned} & \text{minimize} && (1/2)x^T P_0 x + q_0^T x \\ & \text{subject to} && (1/2)x^T P_i x + q_i^T x + r_i \leq 0, \quad i = 1, \dots, m \\ & && Ax = b, \end{aligned}$$

where P_i 's are positive semidefinite, $G \in \mathbf{R}^{m \times n}$ and $A \in \mathbf{R}^{p \times n}$

QCQP has both **linear and quadratic** constraints

Second-order cone programming

SOCP is the problem:

$$\begin{aligned} & \text{minimize} && f^T x \\ & \text{subject to} && \|A_i x + b_i\|_2 \leq c_i^T x + d_i, \quad i = 1, \dots, m \\ & && Fx = g \end{aligned}$$

with variable $x \in \mathbf{R}^n$

we call a constraint of the form

$$\|Ax + b\|_2 \leq c^T x + d, \quad A \in \mathbf{R}^{k \times n}$$

a **second-order cone constraint** since it requires the affine function $(Ax + b, c^T x + d)$ to lie in the second-order cone in $k+1$

if $c_i = 0, i = 1, \dots, m$, the SOCP is equivalent to a QCQP

Common convex functions and convexity proof

we list some common convex functions and give simple proof

- estimation (regression, machine learning)
- risk measure
- conic problems

Convex functions in estimation

let $\ell(u)$ be a convex loss function where u is typically a residual error; if $u = y - \hat{y}(\theta)$ is linear in θ then $\ell(y - \hat{y}(\theta))$ is convex in θ

proof: a composition of convex with affine function is convex

example of convex loss function ℓ :

- negative log-likelihood of some distributions
- $\|\cdot\|_2^2$ or any norm: $\ell(\cdot) = \|\cdot\|$
- Huber loss

in which scenario is $\hat{y}(\theta)$ linear in θ ?

- $\hat{y}(\theta)$ is a sum of basis functions (polynomials, Fourier, etc.)
- $\hat{y}(\theta)$ is the output of feed-forward NN where all the weights in hidden layers are frozen, and only the weights in output layers are parameters

Sum of K -largest function

for $x \in \mathbf{R}^n$, denote $x_{[k]}$ the k^{th} largest entry with $x_{[1]} \geq x_{[2]} \geq \cdots \geq x_{[n]}$

the sum of K -largest function whered $1 \leq K \leq n$, defined as

$$f(x) = x_{[1]} + x_{[2]} + \cdots + x_{[K]}$$

is convex

- proof: $f(x) = \max\{x_{i_1} + x_{i_2} + \cdots + x_{i_r} \mid 1 \leq i_1 < i_2 < \cdots < i_r \leq n\}$
- f is the maximum of all possible sums of r different components (pointwise maximum of convex is convex)

more generally, $g(x) = \sum_{i=1}^K w_i x_{[i]}$ is convex provided that $w_1 \geq w_2 \geq \cdots \geq w_r \geq 0$

when $K = n$, g is called **ordered weighted ℓ_1 norm**

Sum of K -largest function

the function $f(x) = \sum_{i=1}^K x_{[i]}$ is the optimal value of the following LP with its dual:

$$\begin{array}{ll} \text{(P)} & \text{maximize}_y \quad x^T y \\ & \text{subject to} \quad 0 \preceq y \preceq \mathbf{1}, \\ & \quad \quad \quad \mathbf{1}^T y = K. \end{array} \qquad \begin{array}{ll} \text{(D)} & \text{minimize}_{t,z} \quad Kt + \mathbf{1}^T z \\ & \text{subject to} \quad t\mathbf{1} + z \succeq x, \\ & \quad \quad \quad z \succeq 0. \end{array}$$

- from the primal, $f(x) = \sup_{y \in C} x^T y$
- the pointwise supremum of linear function in x over y is convex (another convexity proof)
- from the dual, $f(x) \leq c$ is feasible if and only if the followings are feasible

$$Kt + \mathbf{1}^T z \leq c, \quad t\mathbf{1} + z \succeq x, \quad z \succeq 0$$

(the sum of K -largest constraint can be presented as linear constraints)

Asset portfolio risk management: Sum-of-largest- K

variable: x (allocation of production rate)

objective: $(1/2)x^T \Sigma x$ (the risk)

constraints:

- 1 allocation constraints: $0 \preceq x \preceq \mathbf{1}$, $\mathbf{1}^T x = 1$
- 2 demand requirement: $\mu^T x \geq D$ where D is the total required demand
- 3 physical capacity limit: $0 \preceq x \cdot D \preceq C$ where $C \in \mathbf{R}^n$ is the maximum capacity
- 4 **bound on K -largest allocations:** $\sum_{i=1}^K x_{[i]} \leq \gamma$ where $0 < \gamma \leq 1$

optimization: quadratic program (QP)

$$\begin{aligned} & \text{minimize} && (1/2)x^T \Sigma x - \lambda \mu^T x \\ & \text{subject to} && 0 \preceq x \preceq \mathbf{1}, \mathbf{1}^T x = 1 \\ & && \mu^T x \geq D, \quad 0 \preceq x \cdot D \preceq C \\ & && \sum_{i=1}^K x_{[i]} \leq \gamma \end{aligned}$$

with variable $x \in \mathbf{R}^n$

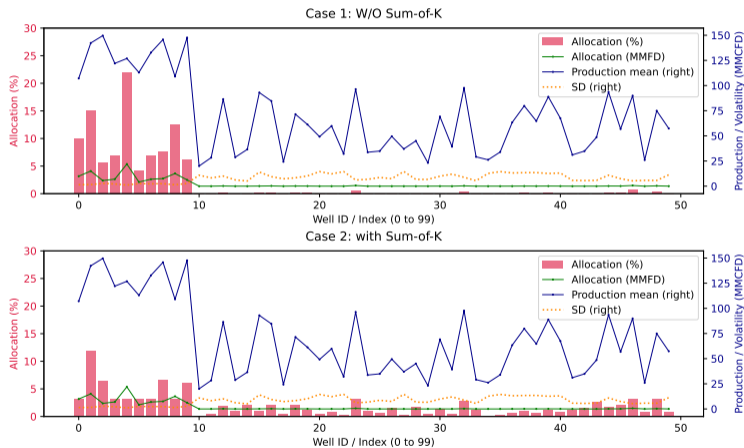
Asset portfolio risk management: Sum-of-largest- K

why should we worry about the K -largest allocations?

- **prevent high-consequence single points of failure:** if the portfolio dominantly allocates high fraction to just a few wells, when one of these wells faces an unplanned shutdown, it would significantly affect the total supply targets
- **reservoir depletion and management:** over-relying on the top few high-performing wells can lead to rapid localized pressure drops or premature water/gas coning in the reservoir 🖊 the sum-of- K -largest constraint prevents the optimization from aggressively draining the most attractive assets all at once

Asset portfolio risk management: Sum-of-largest- K result

$n = 50$ with 10 dominant wells, set $K = 10, \gamma = 0.5$



with sum-of- K -largest constraint, the portfolio is more diversified

Sum of K -largest: Connection to CVaR

from duality on page 222, the function can be represented as

$$\begin{aligned}\sum_{i=1}^K x_{[i]} &= \underset{t \in \mathbf{R}}{\text{minimize}} \left[K \cdot t + \mathbf{1}^T \max(0, x - t\mathbf{1}) \right] \\ &= \underset{t \in \mathbf{R}}{\text{minimize}} \left[K \cdot t + \sum_{i=1}^n (x_i - t)_+ \right]\end{aligned}$$

Conditional Value-at-Risk (CVaR)

in risk management, let X be a discrete RV representing a loss and with pmf p

definitions:

- **Value-at-Risk** (VAR_α) is the α -quantile of the loss distribution
- **CVaR** (aka Expected Shortfall) is the expected loss given that the loss exceeds VAR_α

CVaR at a confidence level α can be written using the Rockafellar-Uryasev formula:

$$\begin{aligned}\text{CVaR}_\alpha(X) &= \min_{t \in \mathbf{R}} \left[t + \frac{1}{1 - \alpha} \sum_{i=1}^n p_i (X_i - t)_+ \right] \\ &= \min_{t \in \mathbf{R}} \left[t + \frac{1}{n(1 - \alpha)} \sum_{i=1}^n (X_i - t)_+ \right] \quad (\text{assume } p_i = 1/n)\end{aligned}$$

Sum of K -largest: Connection to CVaR

for CVaR, multiply the constant factor $n(1 - \alpha)$:

$$n(1 - \alpha) \cdot \text{CVaR}_\alpha(X) = \min_{t \in \mathbf{R}} \left\{ \left[n(1 - \alpha) \right] \cdot t + \sum_{i=1}^n (X_i - t)_+ \right\}$$

by setting the vector of losses X equal to asset allocation vector x ,

$$K = n(1 - \alpha) \quad \implies \quad \alpha = 1 - \frac{K}{n} \quad \implies \quad \sum_{i=1}^K x_{[i]} = K \cdot \text{CVaR}_{1-K/n}(x)$$

- setting $\sum_{i=1}^5 x_{[i]} \leq 0.4$ means that

$$K = 5, \alpha = 1 - 5/100 = 0.95 \text{ (95\%)} \quad , \quad \text{CVaR}_{0.95}(x) \leq \frac{0.4}{5} = 0.08 \text{ (8\%)}$$

- the average allocation of our top 5% most heavily relied-upon wells cannot exceed 8% of the total target production

Robust LP: Uncertainty set approach on objective

consider an LP: minimize $c^T x$ subject to $Ax \preceq b$ but c is uncertain

goal: find a framework that the optimal solution is robust to c

- uncertainty set modeling: assume $c \in \mathcal{U}$ where prior knowledge about the structure of \mathcal{U} is assumed
- use the information of \mathcal{U} to consider the **worst-case** objective

$$w(x) = \sup_{c \in \mathcal{U}} c^T x$$

and define a robust LP as the minimization of the worst-case objective instead

$$\begin{array}{ll} \text{minimize}_x & \sup_{c \in \mathcal{U}} c^T x \\ \text{subject to} & Ax \preceq b \end{array}$$

the robust LP is convex because $w(x)$ is pointwise maximum of linear function in x
the problem structure of the resulting robust LP is determined by the set \mathcal{U}

Robust LP: Uncertainty set approach on objective

example 1: $\mathcal{U} = \{ \bar{c} + u \mid \|u\|_\infty \leq \delta \}$

- c has a nominal value plus a perturbation u with maximum magnitude of δ
- the worst-case objective can be derived as

$$c^T x = \bar{c}^T x + u^T x \quad \Rightarrow \quad \sup_{c \in \mathcal{U}} c^T x = \bar{c}^T x + \sup_{\|u\|_\infty \leq \delta} u^T x = \bar{c}^T x + \delta \|x\|_1$$

(using Holder inequality: $x^T y \leq \|x\|_\infty \|y\|_1$ and the inequality can be tight)

robust LP: minimize $\bar{c}^T x + \delta \|x\|_1$ subject to $Ax \preceq b$

the resulting problem can be further cast as an LP

Robust LP: Uncertainty set approach on objective

example 2: $\mathcal{U} = \{c \mid Fc \preceq g\}$

- the description of uncertainty set is generally described by a polyhedron
- e.g., c deviates less than 25% from its nominal and the average of c does not deviate more than 10% from the average of the nominal:

$$0.75\bar{c} \preceq c \preceq 1.25\bar{c}, \quad 0.9(\mathbf{1}^T \bar{c})/n \leq (\mathbf{1}^T c)/n \leq 1.1(\mathbf{1}^T \bar{c})/n$$

- apply duality theory to find the worst-case objective:

$$\text{primal: } \max_{c \in \mathcal{U}} c^T x \quad \text{dual: } \min_z g^T z \quad \text{subject to } -x + F^T z = 0, \quad z \succeq 0$$

(strong duality holds: primal and dual optimum are equal)

robust LP: the two minimizations can be merged into one over x, z

$$\begin{aligned} & \text{minimize}_{x,z} && g^T z \\ & \text{subject to} && -x + F^T z = 0, \quad z \succeq 0, \quad Ax \preceq b \end{aligned}$$

Robust LP: Uncertainty set approach on constraints

consider an LP: minimize $c^T x$ subject to $Ax \preceq b$ but A is uncertain

goal: find a framework that the optimal solution is robust to A

suppose the row vectors of A , a_i^T for $i = 1, 2, \dots, m$ are uncertain; each $a_i \in \mathcal{U}_i$ (belong to some uncertainty set)

robust LP: the worst-case of $a_i^T x$ should be still less than b_i :

the constraint $Ax \preceq b$ is replaced by

$$\sup_{a_i \in \mathcal{U}_i} a_i^T x \leq b_i, \quad i = 1, 2, \dots, m$$

the resulting robust LP depends on the characterization of the supremum

Robust LP: Uncertainty set approach on constraints

example: coefficient a belongs to a box uncertainty set

$$\mathcal{U}_i = \{ \bar{a}_i + u \mid \|u\|_\infty \leq \gamma_i \}$$

- use the fact that $y^T x \leq \|y\|_\infty \|x\|_1$ (tight when $y = \mathbf{sign}(x)$)

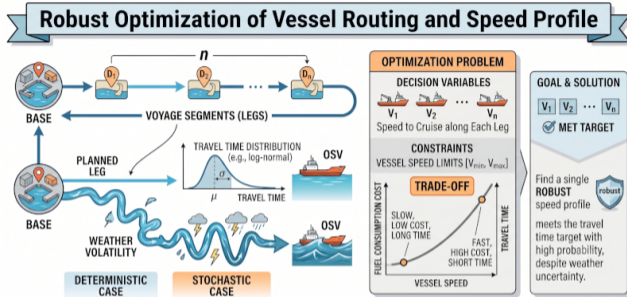
$$\sup_{a_i \in \mathcal{U}_i} a_i^T x = \bar{a}_i^T x + \sup_{\|u\|_\infty \leq \gamma_i} u^T x = \bar{a}_i^T x + \gamma_i \|x\|_1$$

(supremum holds when $u = \gamma_i \mathbf{sign}(x)$)

robust LP: can be further cast as an LP

$$\begin{aligned} & \text{minimize} && c^T x \\ & \text{subject to} && \bar{a}_i^T x + \gamma_i \|x\|_1 \leq b_i, \quad i = 1, 2, \dots, m \end{aligned}$$

Robust optimization of vessel routing



goal: decide the speed to cruise the vessel along each leg to meet the travel time target under vessel speed constraints and weather volatility information

- plan the speed of an offshore vessel that travel along a sequence of n voyage segments (legs) starting from base to each destination and back to base
- the vessel travels along each leg under different volatile weather conditions, making the travel time a random quantity
- the trade-off is between speed and fuel economy; increase the speed, finish the trip fast but consume more cost

Robust optimization of vessel routing: Variables

n : the number of legs (travel segments), e.g., base \rightarrow 1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow base ($n = 5$)

parameters:

- $d \in \mathbf{R}_+^n$: the distance vector of voyage segments
- σ_k^2 for $k \in [n]$: the variance of day per hour of transit (due to weather uncertainty)
- $T_{\max} \in \mathbf{R}_+$: hard deadline for the entire voyage loop (hours)
- $C \in \mathbf{R}_+$: fuel price factor (USD/consumption)

variables:

- $\tau \in \mathbf{R}_+^n$: planned nominal transit time per leg (hours)
- $\Gamma \in \mathbf{R}_+$: total voyage time standard deviation

Robust optimization of vessel routing: Modeling

- the fuel consumption rate per hour scales cubically with speed
- fuel versus time: since speed is $v_k = d_k/\tau_k$,

$$\text{fuel}_k = \text{rate} \times \text{time} \propto \left(\frac{d_k}{\tau_k}\right)^3 \times \tau_k = \frac{d_k^3}{\tau_k^2}$$

- for each leg k , assume there is a random delay ξ_k scales with the planned nominal transit time τ_k :

$$\xi_k = \sigma_k \cdot \tau_k \cdot Z_k \quad \text{where } Z_k \sim \mathcal{N}(0, 1)$$

(assume that ξ_k 's are uncorrelated)

- the travel time on leg k is $T_k = \tau_k + \xi_k$ and hence, $\text{var}[T_k] = \sigma_k^2 \tau_k^2$
- the total travel time is $T = T_1 + \dots + T_n$; hence, it is also Gaussian with mean $\sum_k \tau_k$ and the standard deviation of

$$\Gamma = \sqrt{\sum_{k=1}^n \sigma_k^2 \tau_k^2} \quad (\text{as } \xi_k \text{'s are uncorrelated})$$

Robust optimization of vessel routing: Objective and Constraints

objective: the economic cost of fuel consumption (\$): $f(\tau) = C \sum_{k=1}^n \frac{d_k^3}{\tau_k^2}$ (convex)

constraints:

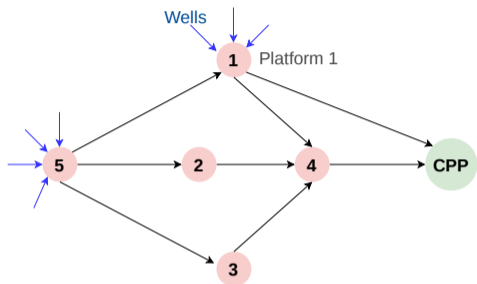
- 1 vessel speed limit: can be reflected in limit of travel time: $\tau_{\min} \preceq \tau \preceq \tau_{\max}$
- 2 chance-constrained deadline: $P(T \leq T_{\max}) \geq \alpha$ where α is a confidence level, e.g., 0.95 and use $T \sim \mathcal{N}(\mathbf{1}^T \tau, \Gamma^2)$

$$F(T_{\max}) \geq \alpha \quad \Leftrightarrow \quad T_{\max} \geq F_T^{-1}(\alpha) \quad \Leftrightarrow \quad \mathbf{1}^T \tau + z_{1-\alpha} \cdot \Gamma \leq T_{\max}$$

- 3 STD relaxation: relax $\sqrt{\sum_{k=1}^n \sigma_k^2 \tau_k^2} = \Gamma$ to an inequality in SOCP form:

$$\left\| \begin{bmatrix} \sigma_1 \tau_1 \\ \vdots \\ \sigma_n \tau_n \end{bmatrix} \right\|_2 \leq \Gamma \quad (\text{the inequality should be tight at optimum})$$

Production optimization with network constraints



setting:

- m wellhead platforms routes gas, condensate, and water through a central processing platform
- each platform has n_j wells

wells compete for limited processing capacity at the host platform while their individual performance is dictated by subsea network pressures

goal: maximize daily revenue while satisfying strict facility and reservoir security bounds

Variables

for a network of m platforms and one CPP: $n = \sum_{j=1}^m n_j$ is the number of all wells

- $j \in [m]$ is the platform index
- $i \in [n_j]$ is the well index
- $g \in \mathbf{R}_+^n$: gas production rate of well (MMCFD)
- $c \in \mathbf{R}_+^n$: condensate production rate of well (stb/d)
- $w \in \mathbf{R}_+^n$: water production rate of well (stb/d)
- $p \in \mathbf{R}_+^{m+1}$: nodal pressure at platform j (psig)

we model that condensate and water rates are functions of gas rate via

$$c_i = \text{GOR}_i \cdot g_i, \quad w_i = \text{WGR}_i \cdot g_i$$

(GOR = gas-oil ratio and WGR = water-gas ratio)

Objective

the objective is to maximize net daily asset revenue: maximize $f(g, p)$

- revenue = $R_{\text{gas}} \mathbf{1}^T g + R_{\text{cond}} \mathbf{1}^T c$
- environmental cost incurred from processing water: $C_{\text{water}} \mathbf{1}^T w$
- fuel consumption of compressor: offshore platforms do not have access to an onshore electrical grid; to run multi-megawatt compressors that boost gas, they burn a fraction of the produced natural gas as fuel in gas turbines suppose there are N_{comp} compressors and j is the compressor index

$$P_j(g) = a_j \left(\sum_{i \in W_j} g_i \right)^2 + b_j \left(\sum_{i \in W_j} g_i \right) + c_j$$

- W_j is the subset of wells routing into compressor j
- $a_j, b_j, c_j \geq 0$ are empirical quadratic coefficients derived from compressor's characteristics

Objective

option 1: neglect the fuel consumption

$$f_1(g) = \sum_{i=1}^n (R_{\text{gas}} + R_{\text{cond}} \cdot \text{GOR}_i - C_{\text{water}} \cdot \text{WGR}_i) g_i$$

the objective is linear in g

justification: 1) if the compressors are running at fixed speed, it consumes relatively constant fuel gas or 2) absorb this cost in lower revenue coefficient, R_{gas}

option 2: include the fuel consumption

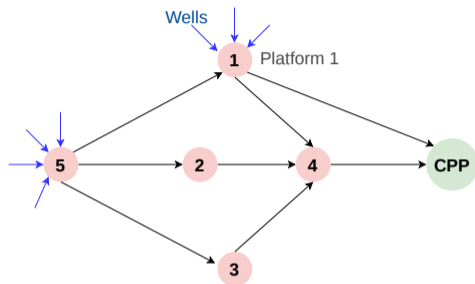
$$f_2(g) = f_1(g) - \sum_{j=1}^{N_{\text{comp}}} a_j \left(\sum_{i \in W_j} g_i \right)^2 + b_j \left(\sum_{i \in W_j} g_i \right) + c_j$$

the objective is quadratic in g

Constraints

- 1 total gas handling capacity: the export compressors cannot exceed a maximum throughput: $\sum_{i=1}^n g_i \leq Q_{\text{gas_max}}$
- 2 produced water disposal limit: $\sum_{i=1}^n \text{WGR}_i \cdot g_i \leq Q_{\text{water_max}}$
- 3 slug/liquid capacity: total liquid (condensate+water) entering the reception must not flood the system: $\sum_{i=1}^n (\text{GOR}_i + \text{WGR}_i) g_i \leq Q_{\text{liquid_max}}$
- 4 well operational limit: $G_{\text{min}} \preceq g \preceq G_{\text{max}}$
- 5 **pressure dictates the flow rates:** well's flow rate (g) and pressure (p) are bound together by the laws of fluid mechanics
- 6 **network flow:** the platform network topology defines the flow layout specifying the upstream and downstream sides and the mass balance constraint

Platform network



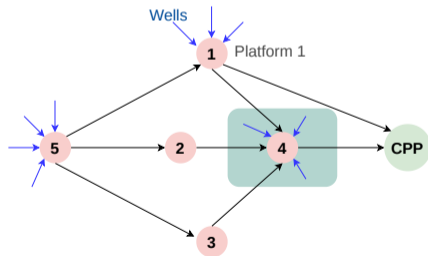
- $j \in [m]$ is the platform index
- each platform has n_j wells connected
- pipelines connect between platforms

- upstream and downstream are designated from the flow (high to low pressure)
- modeled as a directed graph of $m + 1$ nodes and pipelines are the set of direct edges from node i to j
- CPP (central processing platform) is the sink node, collecting all field production

Mass balance constraint

variable: pipeline flow variable

- g_{ud} is defined as the volumetric gas flow rate travelling *through* the specific pipeline that connects node u to node d
- g_{ud} is not the flow of a single well but the cumulative sum of all fluids passing through that pipe segment



Kirchhoff's current law for fluids:

at every node j which has n_j wells

$$\sum_{i \in [n_j]} g_i + \sum_{u \in \text{upstream}} g_{uj} = \sum_{d \in \text{downstream}} g_{jd}$$

Pressure/flow rate constraint

the Weymouth equation:

$$g_{ud}^2 = K_{ud} (p_u^2 - p_d^2)$$

- g_{ud} is gas flow rate from upstream to downstream
- K_{ud} is a constant based on pipeline diameter, length friction, and gas gravity
- p_u, p_d are upstream/downstream pressures

the quadratic equality constraints from Weymouth equation is **non-convex**

- for gas to flow from u to d , we need $p_u > p_d$; the bigger the pressure gap, the more gas the pipe can physically clear
- K_{ud} acts as a hydraulic conductivity; if the pipeline is long, K_{ud} is small, meaning that we need a high pressure difference to push the gas through

Pressure/flow rate SOCP relaxed constraint

apply a **convex relaxation**

$$g_{ud}^2 \leq K_{ud} (p_u^2 - p_d^2)$$

when the objective favors pushing large g to maximize the production, we hope the relaxation becomes tight at optimum

we further introduce auxiliary variables: $\phi_u = p_u^2$ and $\phi_d = p_d^2$ and re-arrange terms:

$$\left\| \begin{array}{c} g_{ud} \\ K_{ud}(\phi_u - \phi_d) - 1 \end{array} \right\|_2 \leq K_{ud}(\phi_u - \phi_d) + 1$$

this is a **second-order cone** constraint in variables g_{ud}, ϕ_u, ϕ_d

(use identity: $(2x)^2 + (y - 1)^2 \leq (y + 1)^2 \Leftrightarrow x^2 \leq y$ where $x = g_{ud}$ and $y = K\Delta\phi$)

Pressure physical constraints

- 1 the fixed boundary condition at CPP: p_{cpp} is fixed constant by facility valves
- 2 maximum pressure limits: $p_j \leq p_{\text{max},j}$ for $j \in [m]$ (metallurgical wall)
- 3 inflow performance relationship (IPR): the pressure at wellhead relates to reservoir pressure and flow rate by

$$p_{\text{wh},i} \leq P_{\text{reservoir},i} - \alpha \cdot g_i$$

(if g_i increases, $p_{\text{wh},i}$ drops because of reservoir depletion; the maximum pressure a well can ever hit is its static reservoir shut-in pressure, $P_{\text{reservoir},i}$)

for fluid to physically flow from well i into the platform manifold j , the wellhead pressure must be higher than (or equal to) the platform manifold pressure

$$p_j \leq p_{\text{wh},i} \Rightarrow p_j \leq P_{\text{reservoir},i} - \alpha \cdot g_i, \quad \Leftrightarrow \quad \sqrt{\phi_j} \leq P_{\text{reservoir},i} - \alpha \cdot g_i \quad j \in [m]$$

Production optimization with network constraints

combining all objective and constraints, we observe that

- the flow rate of one node affects the constraint of neighboring nodes and has to satisfy the Weymouth relaxation
- the problem parameters highly affect problem feasibility; if the values are not realistic, the mass balance constraints are hard to achieve
- even for a simple network where mass balance constraint can be achieved; however, the relaxation is not tight at optimum

Structured convex problems

some structures that are amenable for parallel and distributed algorithms

■ separable sum

$$\underset{x_1, \dots, x_m}{\text{minimize}} \quad f(x) := \sum_{i=1}^m f_i(x_i)$$

it is obvious that we can minimize over x_i independently

■ global consensus

$$\underset{x}{\text{minimize}} \quad f(x) := \sum_{i=1}^m f_i(x)$$

f_i is a local objective; x is the global variable

consensus form: add a consensus constraint that makes all local x_i 's agree

$$\underset{x_1, \dots, x_m}{\text{minimize}} \quad \sum_{i=1}^m f_i(x) \quad \text{subject to} \quad x_1 = x_2 = \dots = x_m$$

Structured convex problems

■ global exchange

$$\underset{x}{\text{minimize}} \quad \sum_{i=1}^m f_i(x_i) \quad \text{subject to} \quad \sum_{i=1}^m x_i = 0$$

interpretation: x_i 's are quantities of commodities exchanged among m agents

goal: minimize **total social cost** subject to the **market clearing**

■ allocation

$$\underset{x}{\text{minimize}} \quad \sum_{i=1}^m f_i(x_i) \quad \text{subject to} \quad x_i \geq 0, \quad \sum_{i=1}^m x_i = b$$

interpretation: x_i 's are non-negative resources allocated to m activities

goal: minimize each activity cost while the total resource is limited to a budget

Distributed model fitting

a problem of fitting y using a linear model Ax using a loss function l

$$\underset{x}{\text{minimize}} \quad l(Ax - y) + r(x)$$

$l(Ax - y) = \sum_{i=1}^N l_i(a_i^T x - y_i)$ represents the model cost due to error $Ax - y$

r is a separable function representing **regularization**, e.g., $\|\cdot\|_1, \|\cdot\|_2^2$

this is an example of global consensus

a common model parameter x that makes the model fits with *all* data samples

Scalarized multi-objective optimization

a common form of multi-objective problem: for a given $\gamma > 0$,

$$\text{minimize } f(x) + \gamma g(x)$$

- we desire both f and g to be small but they are weighed in by a given weight, γ (or often called **penalty parameter**)
- as γ is higher, we penalize more on g , then the minimized g is smaller; in this case, we care less about f
- appear in model performance evaluation where two different metrics are desired to be small
- example 1: minimize model error + model complexity
- example 2: minimize system tracking error + input power

Multi-objective optimization

setting: minimizing $f_0 : \mathbf{R}^n \rightarrow \mathbf{R}^m$ (vector-valued function) over a feasible set

$$\begin{array}{ll} \text{minimize} & f_0(x) \\ \text{subject to} & x \in \mathcal{C} \end{array}$$

a vector optimization has a **vector-valued** objective function

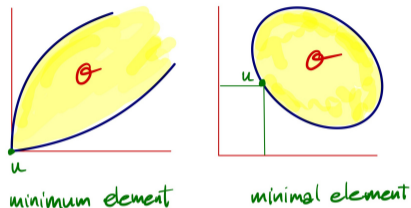
- example: $f_0(x) = (\text{fuel}, \text{time})$ the energy used and time spent of a vehicle parameter x
- require a generalized inequality definition for comparing any two vectors of $f_0(x)$

$$\begin{bmatrix} 5 \\ 2 \end{bmatrix} \preceq \begin{bmatrix} 10 \\ 3 \end{bmatrix} \quad \text{but} \quad \begin{bmatrix} 5 \\ 2 \end{bmatrix} \not\preceq \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$

here, for $f_0(x) \in \mathbf{R}^n$, we typically use the **non-negative orthant** to define \preceq

Achievable objective values

define $\mathcal{O} = \{f_0(x) \mid x \in \mathcal{C}\}$ the set of objective values of feasible points



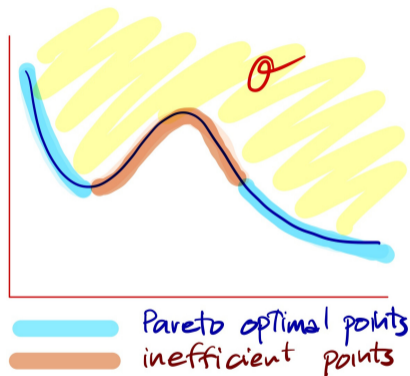
- u is said to be the **minimum** element of \mathcal{O} if $u \preceq v$, for every $v \in \mathcal{O}$
- u is said to be a **minimal** element of \mathcal{O} if $v \in \mathcal{O}$, $v \preceq u$ only if $v = u$
- if \mathcal{O} has a minimum point (then it is unique) and

\exists feasible x such that $f_0(x) \preceq f_0(y)$, for all feasible y

then we say x is **optimal**

Pareto optimal points

consider when \mathcal{O} does not have a minimum element



- x is called **Pareto optimal** (or efficient) if $f_0(x)$ is a minimal element of \mathcal{O}
- a technique to extract pareto optimal points: scalarization (more on this later)

Overview of available methods

- unconstrained problems: gradient descent, Newton, quasi Newton, trust-region
- convex programs: interior point, gradient projection, ellipsoid method
- convex programs of certain structures: proximal methods
- linear programming: simplex, interior point
- quadratic programming: interior point, active set, conjugate gradient, augmented Lagrangian

MATLAB: *cvx*

- CVX is a MATLAB-based modeling system for convex optimization
- <http://cvxr.com/cvx/>

Python

- **CVXPY**: Python-embedded modeling language for convex optimization problems available at <https://www.cvxpy.org/> by Stephen Boyd group
- **CVXOPT**: Python-based package for convex optimization available at <http://cvxopt.org/> by M. Andersen, J. Dahl and L. Vandenberghe

References

- 1 S. Boyd and L. Vandenberghe, *Convex Optimization*, Cambridge, 2004
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A5: Optimization case studies by PTTEP

Optimal location of wellhead platform

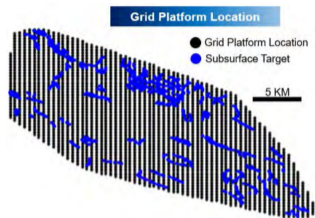


Figure 3—Grid Platform location to cover subsurface target

Platform / Well	W1	W2	W3	W4	W5	W6
P1	1	1	0	0	1	0
P2	0	0	1	1	1	0
P3	0	1	1	0	0	0
P4	1	0	0	0	1	0
P5	0	0	0	0	1	1
P6	1	0	0	0	0	0
P7	0	0	0	0	0	1

source: <https://onepetro.org/SPEAPOG/proceedings-abstract/21APOG/21APOG/D011S009R004/470152>

setting:

- there are P platforms and W wells connected by a coverage matrix
- each well has different hydrocarbon resources and distance to the connected platform
- each platform's total gas resource must pass the minimum cutoff constraint

goal: K platforms that maximize the hydrocarbon resource with smallest total distance

Variables

variables:

- $A \in \{0, 1\}^{P \times W}$: assignment matrix where a_{ij} shows that the well j is assigned to platform i
- $w \in \{0, 1\}^W$: $e_i = 1$ if the well i is selected
- $p \in \{0, 1\}^P$: $p_i = 1$ if the platform i is selected

parameters:

- $K \in \mathbf{Z}_+$: a target number of platforms
- $g \in \mathbf{R}^W$: the reserve coefficient vector (hydrocarbon value)
- $D \in \mathbf{R}^{P \times W}$: distance matrix with d_{ij} the distance from well j to platform i
- $N_{\text{well}} \in \mathbf{Z}^P$: number of wells in the platform can handle
- $\text{OGIP}_{\text{cut-off}}$: original gas in place threshold

Constraints

- 1 target number of platforms: $\mathbf{1}^T p = K$
- 2 platform coverage: $\sum_{i=1}^P C_{ij} p_i \geq w_j, \quad j = 1, 2, \dots, W$
- 3 platform assignment: only one platform can be assigned to a selected well

$$\sum_{i=1}^P a_{ij} = w_j, \quad j = 1, 2, \dots, W \quad \Leftrightarrow \quad \mathbf{1}^T A = w$$

- 4 only selected platform can be assigned:

$$\sum_{j=1}^W a_{ij} \leq p_i N_{\text{well},i}, \quad i = 1, 2, \dots, P \quad \Leftrightarrow \quad A \mathbf{1} \preceq N_{\text{well}}$$

- 5 OGIP constraint:

$$\sum_{j=1}^W a_{ij} g_j \geq \text{OGIP}_{\text{cut-off}} \cdot p_i, \quad i = 1, 2, \dots, P \quad \Leftrightarrow \quad A g \succeq p$$

- 6 physical constraint: $A \preceq C$ (can only be assigned if covered by C)

Objective

we maximize: hydrocarbon value - total distance to platform

$$\sum_{j=1}^W g_j w_j - \lambda \sum_{j=1}^W \sum_{i=1}^P d_{ij} a_{ij}$$

the objective in vector form

$$g^T w - \lambda \mathbf{1}^T (D \odot A) \mathbf{1}$$

- $\lambda > 0$ is a trade-off constant between two objectives
- the objective is linear in w, A (variables)

the optimization problem is a pure linear IP (integer programming)

Results: without and with $A \preceq C$

Solver Status: optimal
Optimal hydrocarbon value: 596.792
Optimal distance: 20.179
Optimal Objective Value with lambda: 556.43

----Coverage matrix ----

```
[[1 1 0 0 1 0]
 [0 0 1 1 1 0]
 [0 1 1 0 0 0]
 [1 0 0 0 1 0]
 [0 0 0 0 1 1]
 [1 0 0 0 0 0]
 [0 0 0 0 0 1]]
```

--- Selection Vectors ---

Selected Platforms (p): [1 1 0 0 1 0 0]
Selected platform 1-based index: [1 2 5]
Selected Wells (w): [1 1 1 1 1 1]

--- Assignment Matrix A (P x W) ---

```
[[1 0 0 0 1 0]
 [0 0 0 1 0 1]
 [0 0 0 0 0 0]
 [0 0 0 0 0 0]
 [0 1 1 0 0 0]
 [0 0 0 0 0 0]
 [0 0 0 0 0 0]]
```

--- Sanity Checks ---

Platform 1 assigned gas = 153.1 (Must be \geq 100.0)
Platform 2 assigned gas = 175.5 (Must be \geq 100.0)
Platform 5 assigned gas = 268.3 (Must be \geq 100.0)

Solver Status: optimal
Optimal hydrocarbon value: 596.792
Optimal distance: 36.508
Optimal Objective Value with lambda: 523.78

----Coverage matrix ----

```
[[1 1 0 0 1 0]
 [0 0 1 1 1 0]
 [0 1 1 0 0 0]
 [1 0 0 0 1 0]
 [0 0 0 0 1 1]
 [1 0 0 0 0 0]
 [0 0 0 0 0 1]]
```

--- Selection Vectors ---

Selected Platforms (p): [1 1 0 0 1 0 0]
Selected platform index (1-based index): [1 2 5]
Selected Wells (w): [1 1 1 1 1 1]

--- Assignment Matrix A (P x W) ---

```
[[1 1 0 0 0 0]
 [0 0 1 1 0 0]
 [0 0 0 0 0 0]
 [0 0 0 0 0 0]
 [0 0 0 0 1 1]
 [0 0 0 0 0 0]
 [0 0 0 0 0 0]]
```

--- Sanity Checks ---

Platform 1 assigned gas = 232.5 (Must be \geq 100.0)
Platform 2 assigned gas = 233.1 (Must be \geq 100.0)
Platform 5 assigned gas = 131.2 (Must be \geq 100.0)

Result

without versus with $A \preceq C$

without $A \preceq C$

- the optimal hydrocarbon are the same (as all wells are selected)
- the distance is smaller (better)
- the optimal value with λ -trade-off is higher (better)
- **catch!** but the assignment matrix is not realizable!
 - well 6 is assigned to platform 2
 - but well 6 can only be covered by platform 5 and 7 (check from C)

Discussion

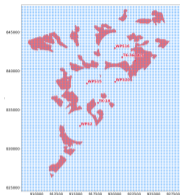
without $A \preceq C$, it might encounter a loophole that we assign A to maximize gas and minimize distance but forget to realize the reality check that $a_{ij} = 1$ only if $c_{ij} = 1$ too

the constraint 2 catch: $\sum_{i=1}^P C_{ij} p_i \geq w_j$

- if we select well j , we must build at least one platform $p_i = 1$ that is mathematically capable of covering it $c_{ij} = 1$
- it dictates which platform are built (p), but it says nothing about how A is filled out

Well combination optimization

setting:



Well	G1	G2	G3	G4	G5	G6	G7	G8	G9	G10	G11	G12	G13	G14	G15
W1	1	1	1	1											
W2			1	1	1	1									
W3						1	1	1	1						
W4										1	1	1			
W5											1	1	1	1	
W6												1	1	1	1

- given information about n_w wells and 2D n_g grids via a coverage matrix C
- $c_{ij} = 1$ if the well i is laid out on grid j
- each grid j has different value
- some grids may be covered by more than one well

goal: select K wells that maximize the total value while avoiding the number of overlapped grids

Well combination: Formulation 1

variables:

- $x \in \{0, 1\}^{n_g}$: $x_i = 1$ if grid i is selected
- $y \in \{0, 1\}^{n_w}$: $y_i = 1$ if well i is selected

parameters:

- $w \in \mathbf{R}^{n_g}$: the value coefficient of each grid
- $C \in \{0, 1\}^{n_w \times n_g}$: the coverage matrix
- $K \in \mathbf{Z}_+$: target number of selected wells

objective: maximize $w^T x$

constraint:

- 1 number of selected wells: $\mathbf{1}^T y = K$
- 2 well and grid coverage: $\sum_{i=1}^{n_w} c_{ij} y_i \geq x_j, \quad j = 1, 2, \dots, n_g$

the problem is pure IP where n_g can be in order of million (x)

Well combination: Formulation 2 (BQP)

motivation: avoid using grid variable (higher dimension)

- from the value vector $w \in \mathbf{R}^{n_g}$ and C , we can compute the value of each well, described by $s \in \mathbf{R}^{n_w}$
- from C , we can construct the overlap matrix $O \in \mathbf{Z}^{n_w \times n_w}$ where O_{ij} is the number of overlapped grids between well i and j
- when y is given, we can count the number of total overlapped grids occurred in the selected well; let's denote it by

$$h(y) = \sum_{ij} O_{ij} y_i y_j = y^T O y$$

formulation: weighted objective between the total value and number of overlaps

$$\begin{aligned} & \text{maximize}_y && s^T y - \lambda y^T O y \\ & \text{subject to} && \mathbf{1}^T y = K \end{aligned}$$

the problem becomes **binary quadratic program (BQP)** in $y \in \{0, 1\}^{n_w}$

Well combination: Formulation 3

the quadratic function $y^T O y$ can be linearized using **McCormick Envelopes**

- introduce $z_{ij} = y_i y_j$ (aim $z_{ij} = 1$ only when $y_i = y_j = 1$)
- force z_{ij} to be binary without using product form

$$z_{ij} \leq y_i, \quad z_{ij} \leq y_j, \quad z_{ij} \geq y_i + y_j - 1, \quad z_{ij} \geq 0$$

- as the objective is to minimize $y^T O y$, it naturally drives z_{ij} to zero
- the third inequality tends to force $z_{ij} = 1$ *only* when $y_i = y_j = 1$

Well combination: Formulation 3

the problem becomes linear IP

$$\begin{aligned} & \text{maximize}_{y,z} && s^T y - \lambda \sum_{ij} O_{ij} z_{ij} \\ & \text{subject to} && \mathbf{1}^T y = K \\ & && z_{ij} \leq y_i, \quad z_{ij} \leq y_j, \\ & && z_{ij} \geq y_i + y_j - 1, \quad z_{ij} \geq 0 \end{aligned}$$

with variables $y \in \{0, 1\}^{n_w}$ and $Z \in \{0, 1\}^{n_w \times n_w}$

while the problem is linearized, n_w^2 variables are added (from Z)

Well combination: Formulation 4

motivation: avoid using grid variable by re-arranging the objective in terms of y

- we can compute how many wells cover a grid j : $\sum_{i=1}^{n_w} C_{ij}y_i$ (ranges in $0, 1, \dots$)
- the status of a grid j is chosen is capped by minimum operation

$$\min \left(\sum_{i=1}^{n_w} C_{ij}y_i, 1 \right) \quad (\text{which is nonlinear in } y \text{ and its value is either } 0 \text{ or } 1)$$

the problem becomes nonlinear IP

$$\begin{aligned} & \text{maximize}_y && \sum_{j=1}^{n_g} w_j \min \left(\sum_{i=1}^{n_w} C_{ij}y_i, 1 \right) \\ & \text{subject to} && \mathbf{1}^T y = K \end{aligned}$$

with variables $y \in \{0, 1\}^{n_w}$

Well combination: Formulation 4

CP-SAT solver has conditional implication that can handle how to evaluate the objective function more effectively without introducing more variables

Well / Grid	G1	G2	G3	G4	G5	G6	G7	G8	G9	G10
W1	■	■								
W2		■	■	■						
W3				■	■	■				
W4						■	■	■		
W5								■	■	■
Grid value	59	74	64	59	48	68	49	90	97	45
Selected well (0-based Indices): [1 4]										
Active z (selected profiles with their covering wells):										
[(0, 1), (1,), (1, 2), (3, 4), (4,)]										

introduce compressed profiles (dict):

- profile of covering wells
- combined grid value

Compressed grid profiles

Grids 1 has the profile: (1,) (Only Well 1)

Grids 2 has the profile: (1,2) (Well 1 and Well 2)

Grids 3 has the profile: (2,) (Only Well 2)

Grids 4 has the profile: (2,3) (Well 2 and Well 3)

...

Grids 9 and 10 have the profile: (5,) (Well 5) --> add w9+w10

when C has a staircase structure:

the grids in C naturally group into two distinct types of structural columns:

- 1 exclusive zones: grids covered by exactly one well (e.g., only well 1, only well 2).
- 2 overlap zones: grids covered by exactly two consecutive wells

let's calculate exactly how many unique keys will end up in the compressed profiles dictionary for $n_w = 100$:

- single-well keys: every well has an exclusive zone; this creates profiles like (0,), (1,), (2,), ..., (99,).

Total = 100 profiles

- consecutive overlap keys: every consecutive pair of wells shares a few overlap zone; this creates profiles like (0, 1), (1, 2), (2, 3), ..., (98, 99).

Total = 99 profiles

the dictionary z will contain at most 199 unique keys

it does not matter if n_g is 1 million, or 10 million (for this structure of C)

Profile activation variable

for each covering wells in the compressed profiles, create z_k

```
z_k = model.NewBoolVar(f'z_profile_{covering_wells}')
```

- if $z_k = 1$, it means this grid profile is successfully covered by our well selection, and we get to claim its value using conditional implication

```
model.Add(sum(y[i] for i in covering_wells) >= 1).OnlyEnforceIf(z_k)
```

(at least one well is selected)

- if $z_k = 0$, no wells in this profile can be selected

```
model.Add(sum(y[i] for i in covering_wells) == 0).OnlyEnforceIf(z_k.Not())
```

the objective function is $\sum_{k=1}^{\text{no. profiles}}$ combined weight $_k \cdot z_k$

variables are y (length of n_w) and z (length = number of compressed profiles)

Well combination: Formulation 4 results

10 grids and 5 wells

compress profiles and combined weight:

Well / Grid	G1	G2	G3	G4	G5	G6	G7	G8	G9	G10
W1	■	■								
W2		■	■	■						
W3				■	■	■				
W4						■	■	■		
W5								■	■	■
Grid value	59	74	64	59	48	68	49	90	97	45
Selected well (0-based Indices): [1 4]										
Active z (selected profiles with their covering wells):										
[(0, 1), (1,), (1, 2), (3, 4), (4,)]										

(0-based indices)

(0,) : 59

(0,1) : 74

(1,) : 64

(1,2) : 59

(2,) : 48

(2,3) : 68

(3,) : 49

(3,4) : 90

(4,) : 97+45

- well 2 and 5 are selected (index 1 and 4)
- these selected well are covered in the active profiles