## Mathematical Optimization in Machine Learning/Decision-Making

CUHKSZ, APRIL 6, 2023

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Stanford University and CUHKSZ (Sabbatical Leave)

#### Linear Programming and LP Giants won Nobel Prize...

$$\max \sum \pi_j x_j$$

s.t. 
$$\sum_{j} a_{j} x_{j} \leq b,$$

$$0 \leq x_{j} \leq 1 \quad \forall j = 1, ..., n$$



#### ChatGPT求解优化问题?

优化问题根据变量、约束和目标函数的特性,可以分为不同种类,如线性规划、非线性规划和整数规划等

小规模整数优化问题,可以通过穷举法求解 大规模整数规划问题一般由专业的整数规划软件求解(Gurobi, COPT)

#### 一个简单的整数线性规划问题

假设有一个最多能承重5kg的背包和5个重量不同的物品,每个物品都具有一定的价值。将哪些物品装入背包,可以使得背包内的物品总价值最大? 物品的重量和价值如下表所示:

物品	1	2	3	4	5
重量 (kg)	2	1	2.5	3.5	1.5
▶价值 (元)	18	10	20	28	15

此问题的最优解是将物品2、物品3和物品5装入背包,总价值为45元。



#### ChatGPT求解优化问题?

#### 将上述背包问题向ChatGPT提问:



假设有5件物品和一个最多能承重5kg的背包。第1件物品的重量是2kg,其价值为18元;第2件物品的重量是1kg,其价值为10元;第3件物品的重量是2.5kg,其价值为20元;第4件物品的重量是3.5kg,其价值为28元;第5件物品的重量是1.5kg,其价值为15元。请问将哪些物品装入背包里,物品的价值总和最大?请使用整数规划求解该问题。



这是一个经典的背包问题,可以使用整数规划方法求解。

我们可以定义0/1变量\$x\_i\$,表示是否将第\$i\$件物品放入背包中。同时,我们还需要定义一个非负整数变量\$z\$,表示物品的总价值。

然后,我们可以将问题转化为以下的线性规划问题:

最大化 \$z=18x 1+10x 2+20x 3+28x 4+15x 5\$

满足约束条件:

\$2x 1+x 2+2.5x 3+3.5x 4+1.5x 5 \leq 5\$

 $x i \in \{0,1\}, i=1,2,3,4,5$ 

由于\$x\_i\$是整数变量,这是一个整数规划问题。可以使用整数规划求解器求解。

求解结果表明,将第1件、第3件、第5件物品装入背包中,可以使得物品的总价值最大,为\$18+20+15=53\$元。



ChatGPT 在不调用求解器的前提下,能否求解大规模优化问题?



在不调用求解器的前提下,对于大规模的优化问题,通常也比较难直接求解得到最优解,因为现实中的大多数优化问题都非常复杂,存在着多个目标、多个约束、非线性、离散等多种问题,很容易遇到组合爆炸的问题。

#### 向ChatGPT提问:

ChatGPT 会尝试性给出解答, 但是不能保证答案的正确性。

ChatGPT会建议调用求解器求解优化问题。

ChatGPT 并不是万能的,它是一个语言处理模型,回答复杂的计算问题还需要调用专业的软件

上述问答产生于2023年3月12日

#### Today's Sharing

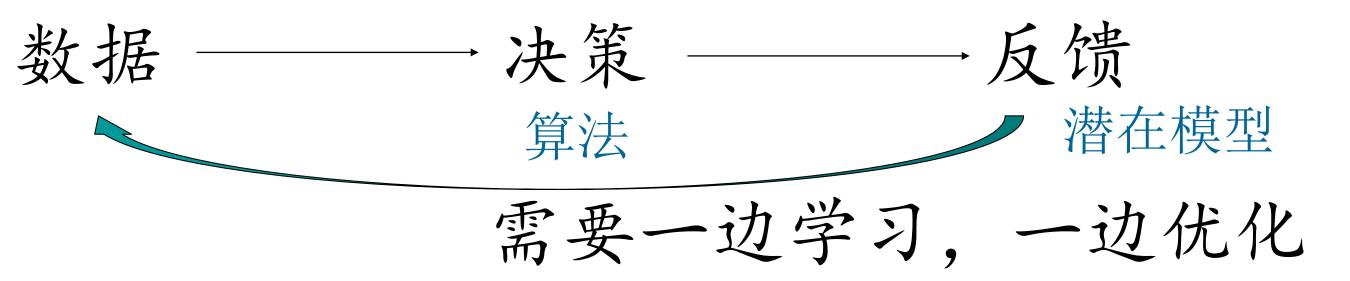
- 1. Online Linear Programming Algorithms and Applications
- 2. Accelerated Second-Order Methods for Nonlinear Optimization and Applications
- 3. Mixed Integer Linear Programming Solver and Applications
- 4. Equitable Covering & Partition Divide and Conquer and Applications
- 5. Beyond Math: Love Sport and Have a Belief

#### Topic 1. Online Linear Programming

- 1、在线学习理论与算法研究 (Agrawal et al. 2010, 14, Li&Y 2022)
- What is OLP?
  - □传统机器学习问题:有大量(训练)数据,找到最佳模型 (例子:回归模型、树模型)
    - 已有数据

最佳模型

□ 在线学习:数据的生成和学习是同时发生的,由决策影响 (例如多臂老虎机问题)



#### Online Auction Example

- There is a fixed selling period or number of buyers; and there is a fixed inventory of goods
- Customers come and require a bundle of goods and make a bid
- Decision: To sell or not to sell to each individual customer on the fly?
- Objective: Maximize the revenue.

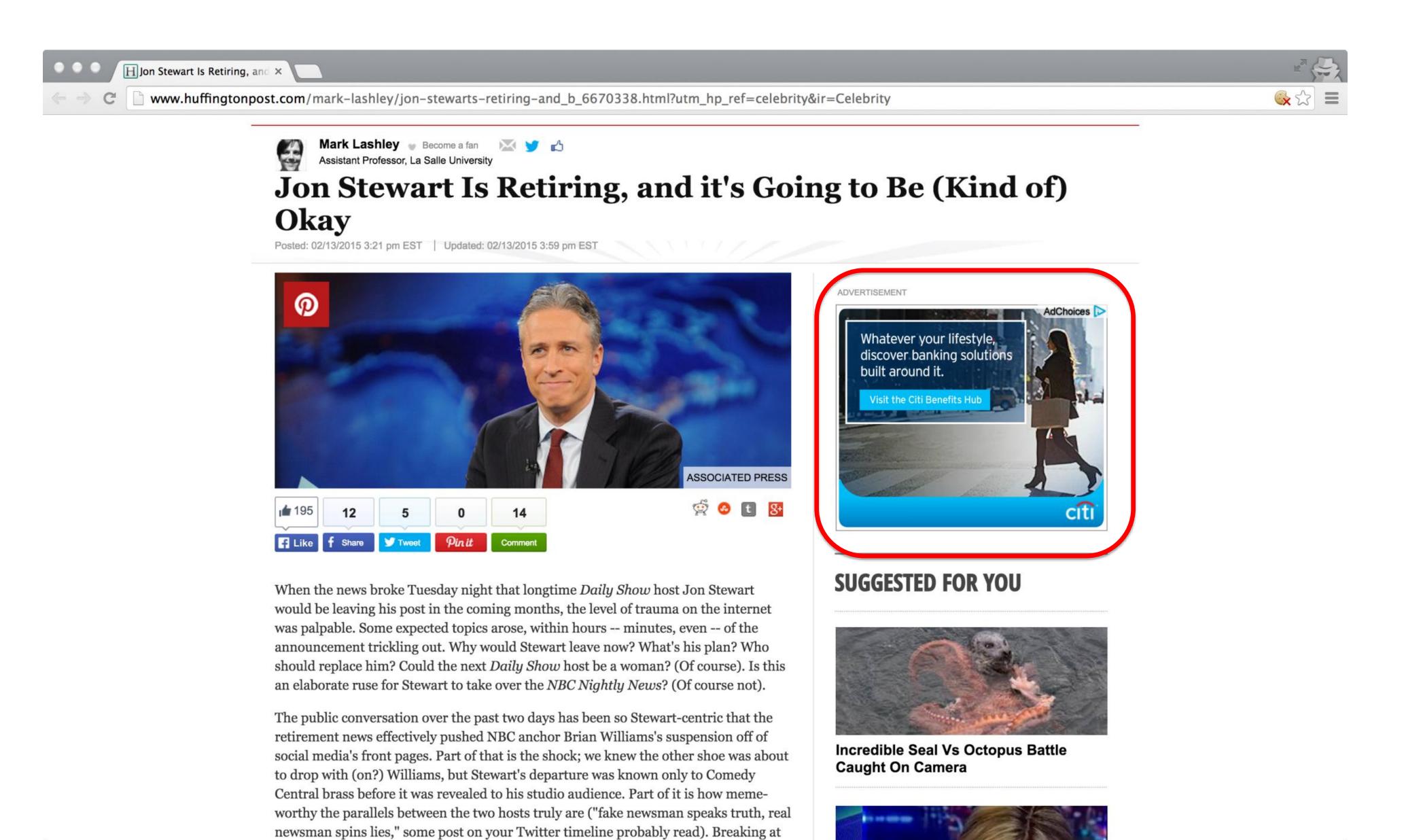
Bid#	\$100	\$30	•••	 •••	Inventory
Decision	<b>x1</b>	<b>x2</b>			
Pants	1	0		 	100
Shoes	1	0			50
T-Shirts	0	1			500
Jackets	0	0			200
Hats	1	1		 	1000

#### Price Mechanism for Online Auction

- Learn and compute itemized optimal prices
- Use the prices to price each bid
- Accept if it is a over bid, and reject otherwise

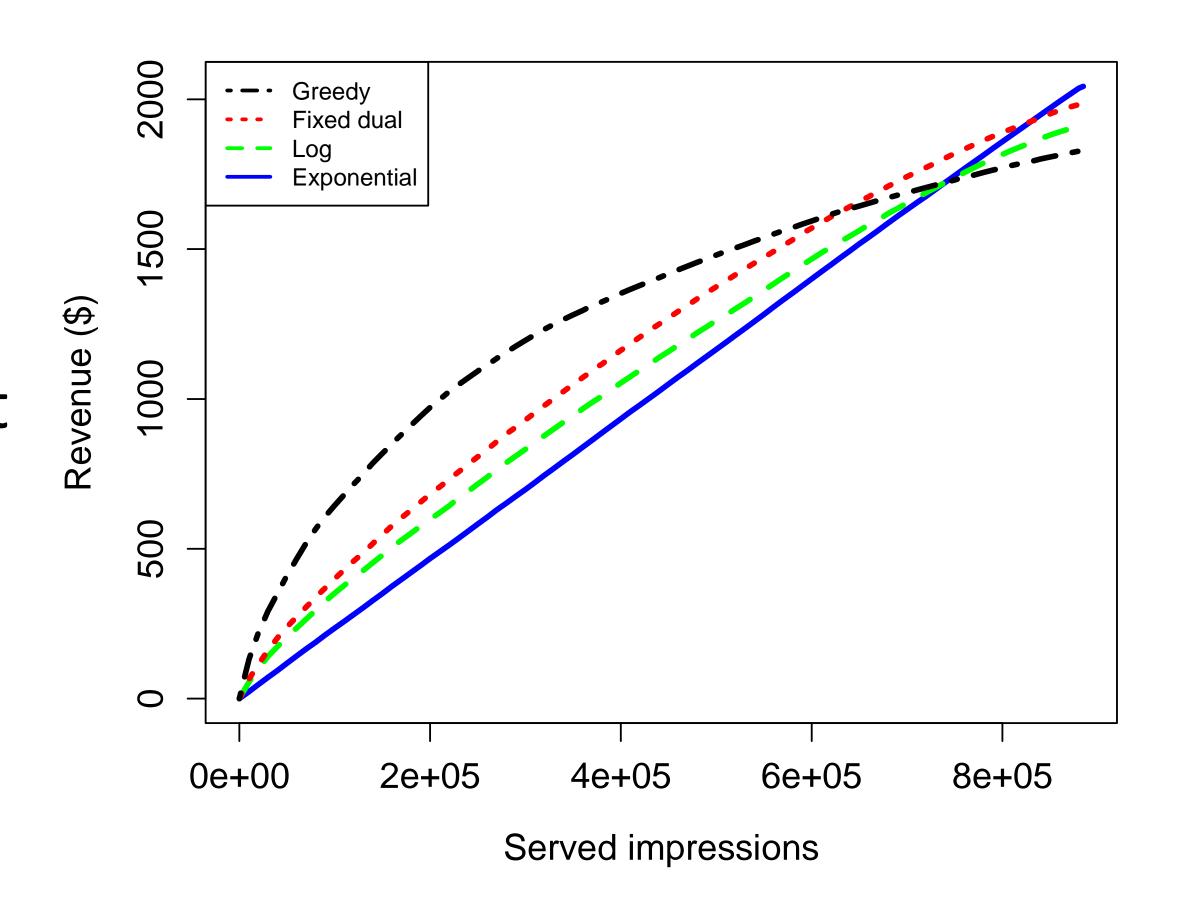
Bid #	\$100	\$30	 	 Inventory	Price?
Decision	<b>x1</b>	<b>x2</b>			
Pants	1	0	 	 100	45
Shoes	1	0		50	45
T-Shirts	0	1		500	10
Jackets	0	0		200	55
Hats	1	1	 	 1000	15

#### App. I: Online Matching for Display Advertising



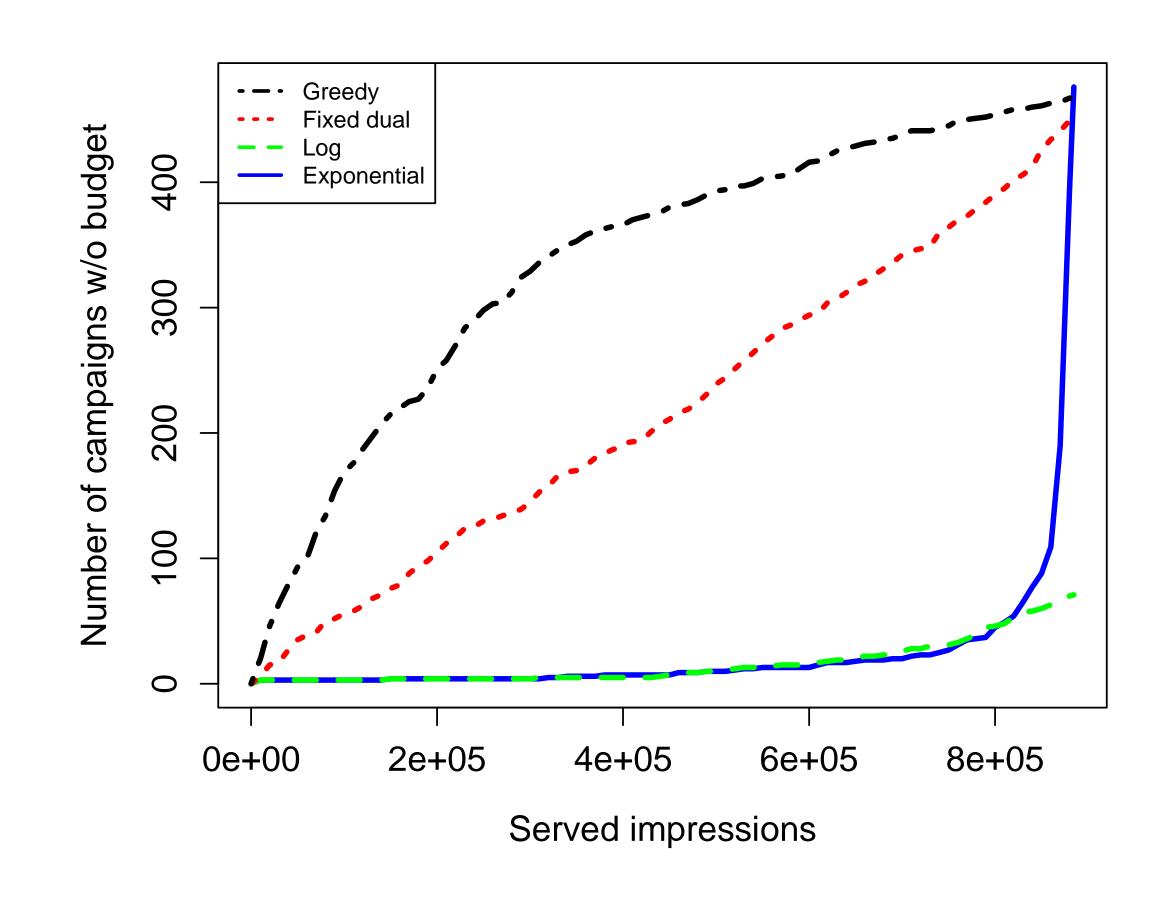
#### Revenues generated by different methods

 Total Revenue for impressions in T2 by Greedy and OLP with different allocation risk functions

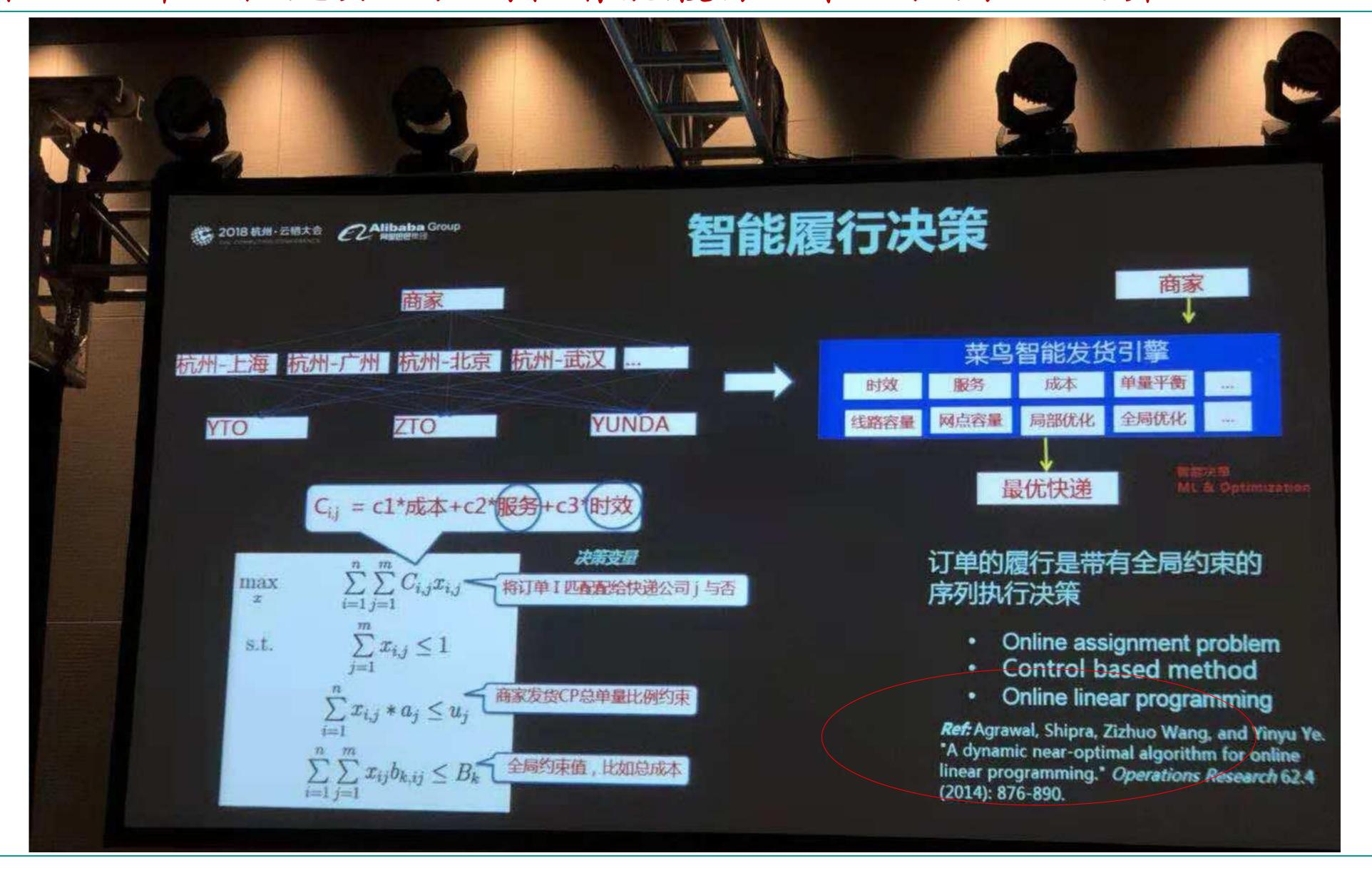


#### # of Out-of-Budget Advertisers

- Greedy exhausts budget of many advertisers early.
- Log penalty keeps advertisers in budget but it is very conservative.
- Exponential penalty Keeps advertisers in budget until almost the end of the timeframe.



#### 阿里巴巴在2019年云栖大会上提到在智能履行决策上使用OLP的算法



### 阿里巴巴团队在2020年CIKM会议论文Online Electronic Coupon Allocation based on Real-Time User Intent Detection上提到他们设计的发红包的机制也使用了OLP的方法[2]

#### Spending Money Wisely: Online Electronic Coupon Allocation based on Real-Time User Intent Detection

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$$\max \sum_{i=1}^{M} \sum_{j=1}^{N} v_{ij} x_{ij}$$

$$s.t. \sum_{i=1}^{M} \sum_{j=1}^{N} c_{j} x_{ij} \leq B,$$

$$\sum_{j}^{N} x_{ij} \leq 1, \quad \forall i$$

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

$$(5)$$

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#### 3.3 MCKP-Allocation

We adopt the primal-dual framework proposed by [2] to solve the problem defined in Equation 5. Let  $\alpha$  and  $\beta_j$  be the associated dual variables respectively. After obtaining the dual variables, we can solve the problem in an online fashion. Precisely, according to the principle of the primal-dual framework, we have the following allocation rule:

$$x_{ij} = \begin{cases} 1, & \text{where } j = \arg\max_{i} (v_{ij} - \alpha c_j) \\ 0, & \text{otherwise} \end{cases}$$
 (9)

# **App. II**: The Online Algorithm can be Extended to Bandits with Knapsack (BwK) Applications

- For the previous problem, the decision maker first wait and observe the customer order/arm and then decide whether to accept/play it or not.
- An alternative setting is that the decision maker first decides which order/arm (s)he may accept/play, and then receive a random resource consumption vector  $\mathbf{a}_j$  and yield a random reward  $\pi_j$  of the pulled arm.
- Known as the Bandits with Knapsacks, and it is a tradeoff exploration v.s. exploitation
- First algorithm to achieve the  $O(\log T)$  regret bound [Li, Sun & Y 2021 ICML]

(https://proceedings.mlr.press/v139/li21s.html)





#### Topic 2. Accelerated Second-Order Methods for Unconstrained Optimization and Applications

$$\min f(x), x \in X \text{ in } \mathbb{R}^n$$

• where *f* is nonconvex and twice-differentiable,

$$g_k = \nabla f(x_k), H_k = \nabla^2 f(x_k)$$

• Goal: find  $x_k$  such that:

```
\|g_k\| \le \epsilon (primary, first-order condition)
\lambda_{min}(H_k) \ge -\sqrt{\epsilon} (secondary, second-order condition)
```

- First-order methods typically need  $O(n^2 \epsilon^{-2})$  operations
- Second-order methods typically need  $O(n^3 \epsilon^{-1.5})$  operations
- New? Yes, HSODM and DRSOM: a single-loop method with  $O(n^2 \epsilon^{-1.75})$  operations (https://arxiv.org/abs/2211.08212)

#### App. III: HSODM for Policy Optimization in Reinforcement

Learning policy optimization of linearized objective in reinforcement learning

$$egin{aligned} & \max_{ heta \in \mathbb{R}^d} L( heta) := L(\pi_ heta), \ heta_{k+1} &= heta_k + lpha_k \cdot M_k 
abla \eta( heta_k), \end{aligned}$$

- $M_k$  is usually a preconditioning matrix.
- The Natural Policy Gradient (NPG) method (Kakade, 2001) uses the Fisher information matrix where  $M_{\rm k}$  is the inverse of

$$F_k( heta) = \mathbb{E}_{
ho_{ heta_k},\pi_{ heta_k}}ig[
abla \log \pi_{ heta_k}(s,a)
abla \log \pi_{ heta_k}(s,a)^Tig]$$

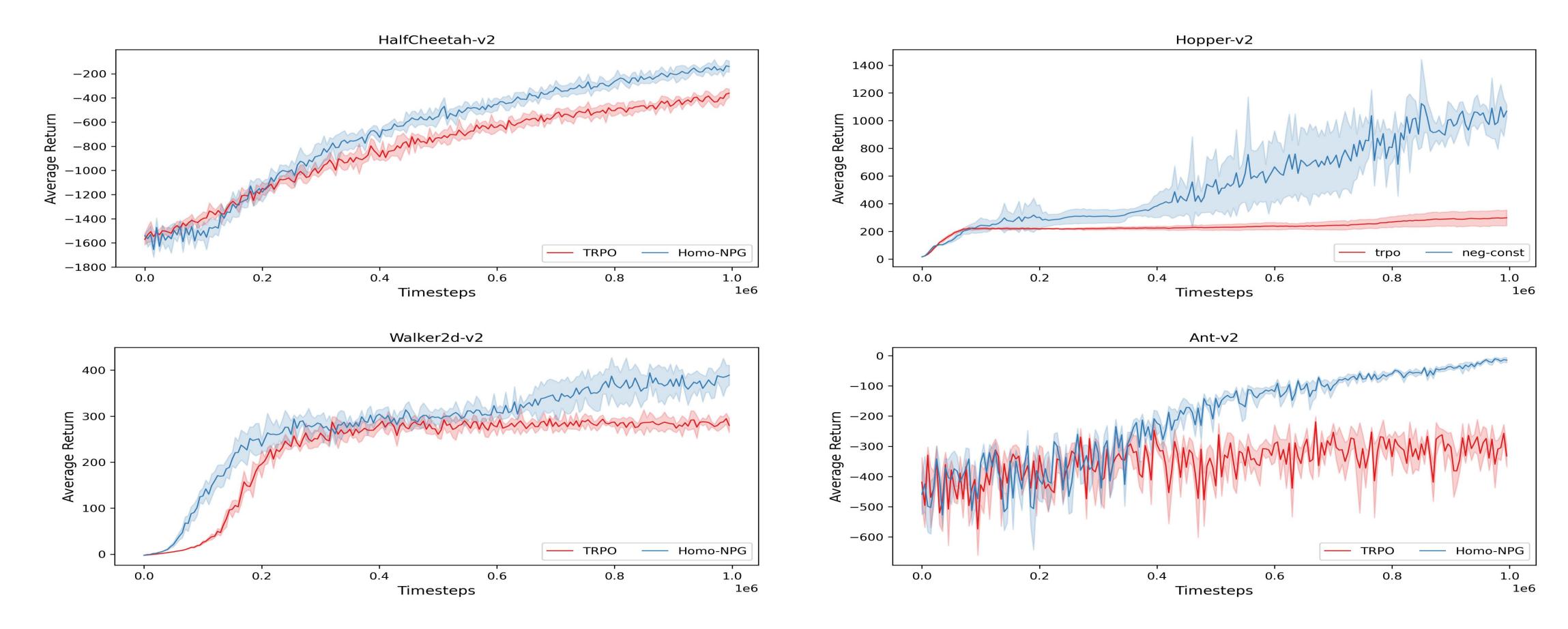
• Based on KL divergence, TRPO (Schulman et al. 2015) uses KL divergence in the constraint:

$$egin{aligned} \max_{ heta} & 
abla L_{ heta_k}( heta_k)^T ( heta - heta_k) \ & ext{s.t.} \ \mathbb{E}_{s \sim 
ho_{ heta_k}}[D_{KL}(\pi_{ heta_k}(\cdot \mid s); \pi_{ heta}(\cdot \mid s))] \leq \delta. \end{aligned}$$

Homogeneous NPG: Apply HSODM!

#### Preliminary Results: HSODM for Policy Optimization in RL

A comparison of Homogeneous NPG and Trust-region Policy Optimization (Schultz, 2015)



- HSODM provides significant improvements over TRPO
- Ongoing: second-order information of L?
- Further reduce the computation cost per step

#### Dimension Reduced Second-Order Method (DRSOM)

- Motivation from Multi-Directional FOM and Subspace Method, such as CG and ADAM, DRSOM applies the trust-region method in low dimensional subspace.
- This results in a low-dimensional quadratic sub-minimization problem:
- Typically, DRSOM adopts two directions  $d = -\alpha^1 \nabla f(x_k) + \alpha^2 d_k$ where  $g_k = \nabla f(x_k)$ ,  $H_k = \nabla^2 f(x^k)$ ,  $d_k = x_k - x_{k-1}$
- Then we solve a 2-d quadratic minimization problem:

$$\min \ m_k^{\alpha}(\alpha) \coloneqq f(x_k) + (c_k)^T \alpha + \frac{1}{2} \alpha^T Q_k \alpha$$

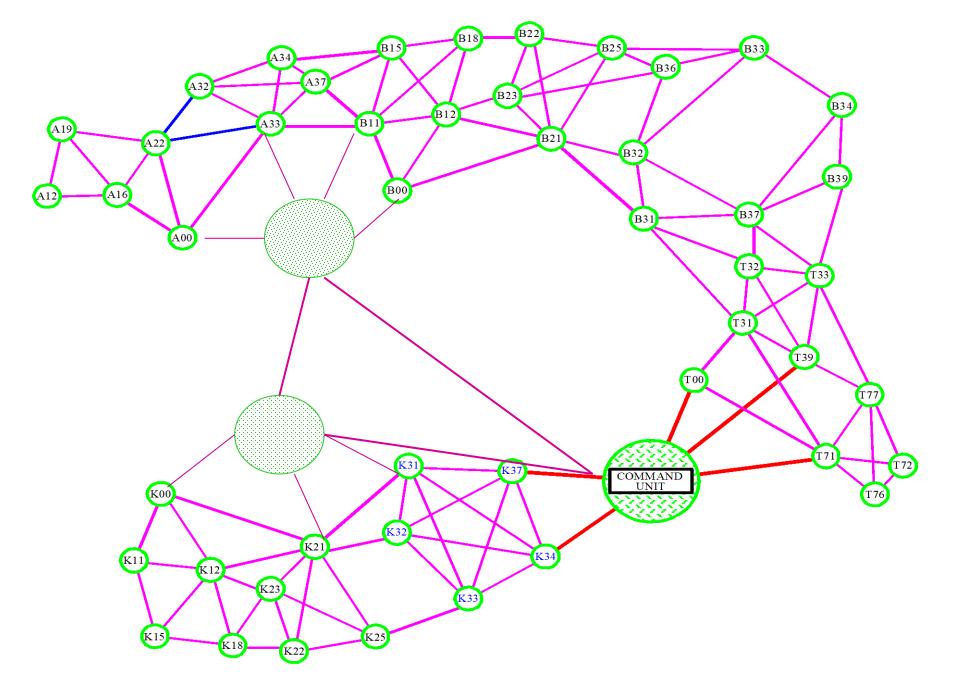
$$||\alpha||_{G_k} \le \Delta_k$$

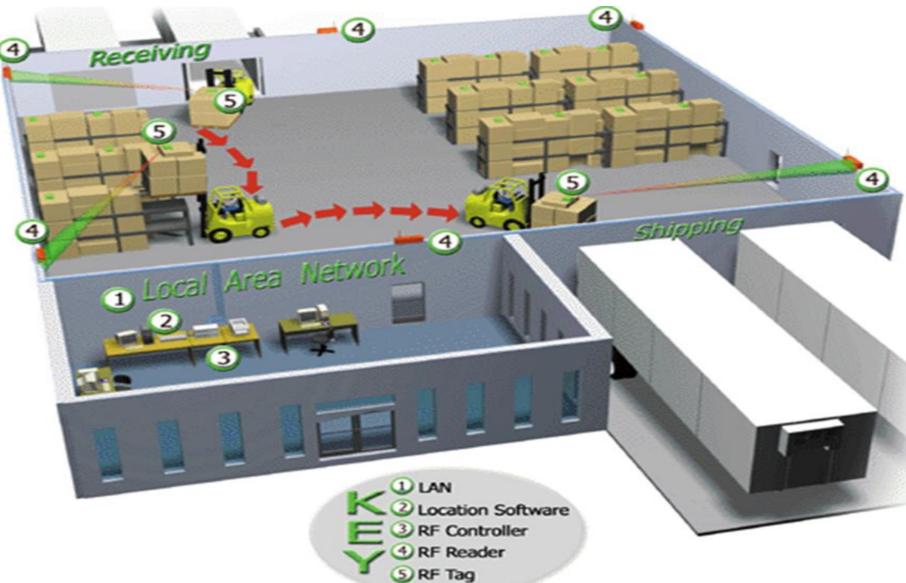
$$G_k = \begin{bmatrix} g_k^T g_k & -g_k^T d_k \\ -g_k^T d_k & d_k^T d_k \end{bmatrix}, Q_k = \begin{bmatrix} g_k^T H_k g_k & -g_k^T H_k d_k \\ -g_k^T H_k d_k & d_k^T H_k d_k \end{bmatrix}, c_k = \begin{bmatrix} -||g_k||^2 \\ g_k^T d_k \end{bmatrix}$$

#### App. IV: Sensor Network Location (SNL)

- Localization
  - -Given partial pairwise measured distance values
  - -Given some anchors' positions
  - -Find locations of all other sensors that fit the measured distance values

    This is also called graph realization on a fixed dimension Euclidean space









#### Mathematical Formulation of Sensor Network Location (SNL)

Consider Sensor Network Location (SNL)

$$N_x = \{(i,j) : ||x_i - x_j|| = d_{ij} \le r_d\}, N_a = \{(i,k) : ||x_i - a_k|| = d_{ik} \le r_d\}$$

where  $r_d$  is a fixed parameter known as the radio range. The SNL problem considers the following QCQP feasibility problem,

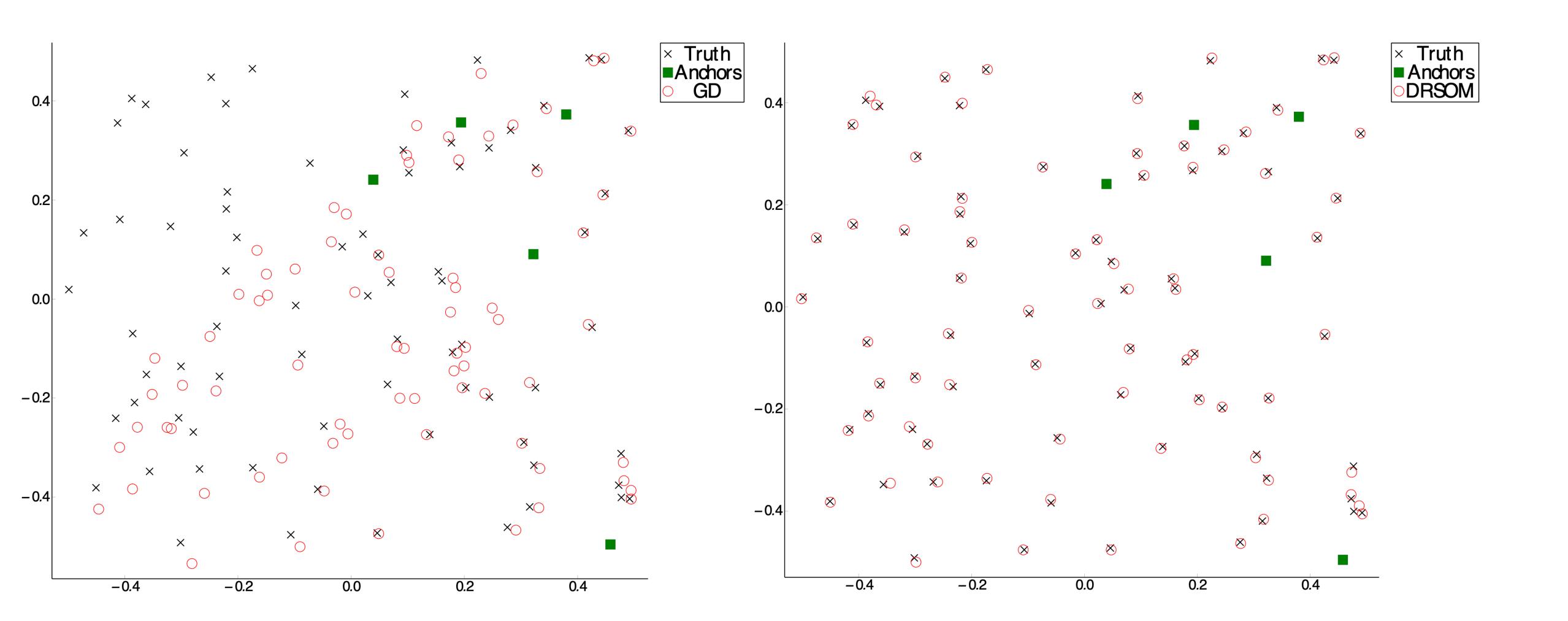
$$||x_i - x_j||^2 = d_{ij}^2, \forall (i, j) \in N_x$$
  
 $||x_i - a_k||^2 = \bar{d}_{ik}^2, \forall (i, k) \in N_a$ 

• Alternatively, one can solve SNL by the nonconvex nonlinear least square (NLS) problem

$$\min_{X} \sum_{(i < j, j) \in N_x} (\|x_i - x_j\|^2 - d_{ij}^2)^2 + \sum_{(k, j) \in N_a} (\|a_k - x_j\|^2 - \bar{d}_{kj}^2)^2.$$

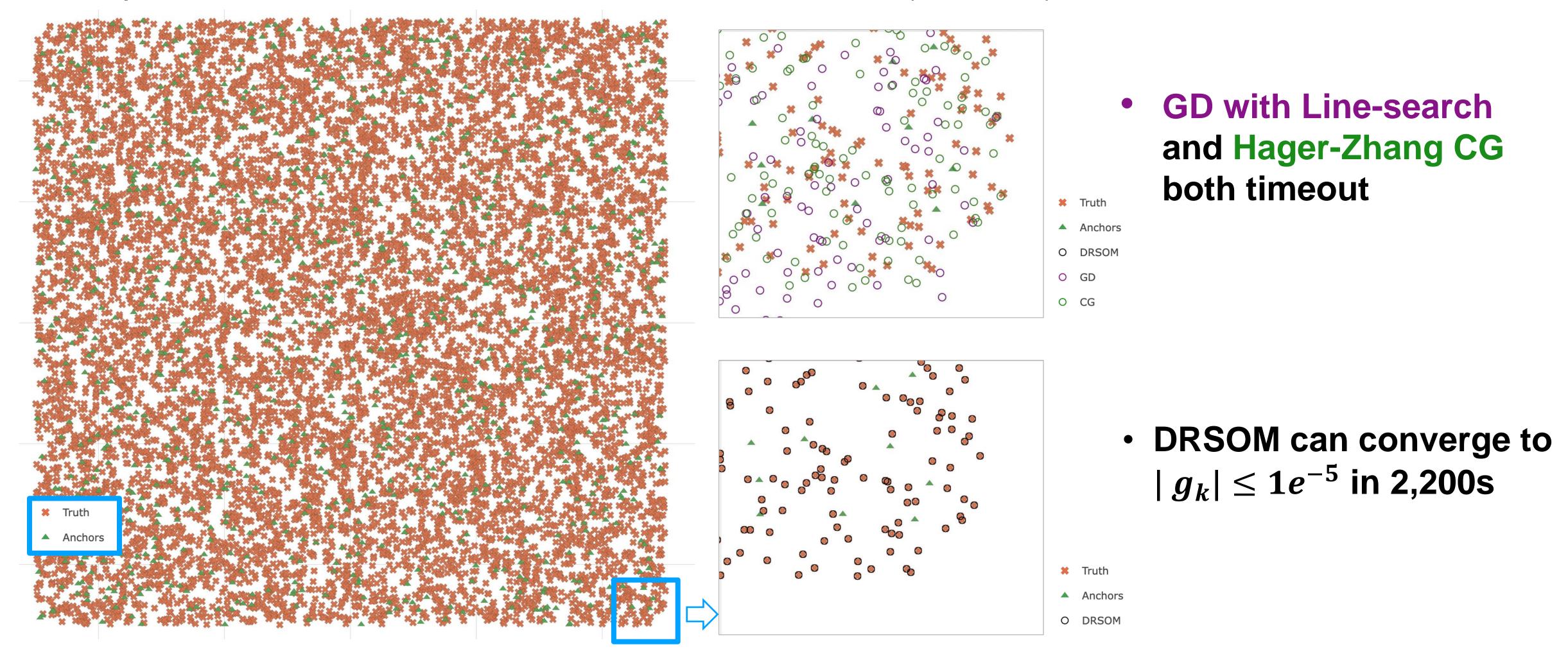
#### Sensor Network Location (SNL)

DRSOM vs the First-Order-Gradient-Descent Method



#### Sensor Network Location, Large-Scale Instances

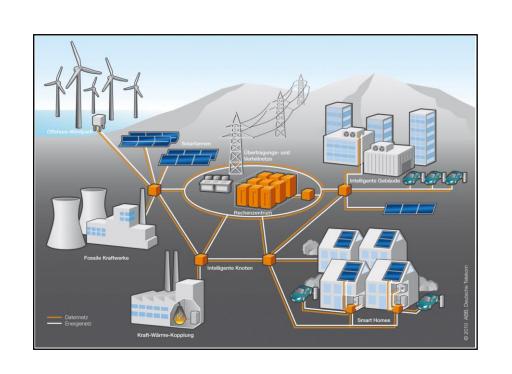
Graphical results with 10,000 nodes and 1000 anchors (no noise) within 3,000 seconds

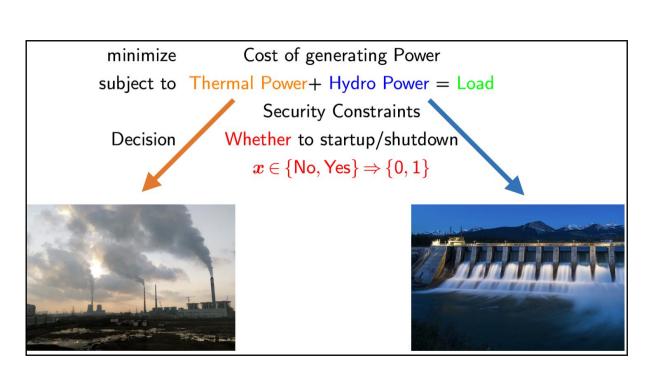


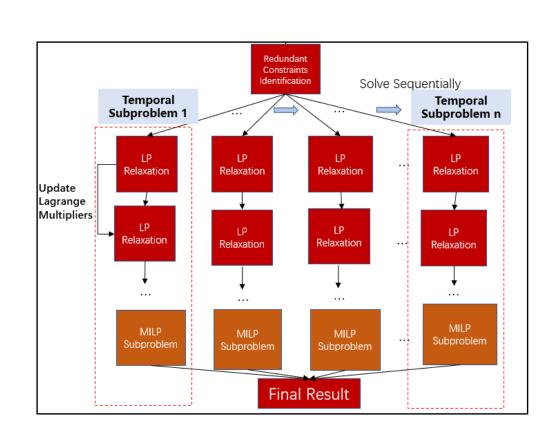
Sensor Network Online Tracking, 2D and 3D

#### Topic 3: Mixed Integer Linear Programming Solver

### **Application V: Unit Commitment and Power Grid Optimization COPT, Cardinal Operations** 2022







#### **Unit Commitment Problem**

- Electricity is generated from units (various generators)
- Transmitted safely and stably through power grids
- Consumed at minimum (reasonable) price

Optimization has its role to play

minimize Cost of electricity
subject to Safety and Stability
Adaptivity to various units









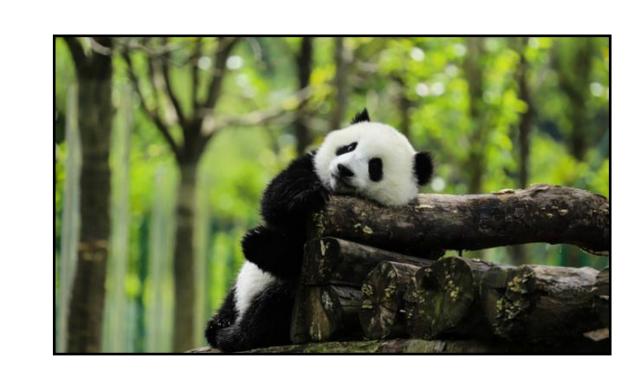




Unit commitment problem dispatches the units safely and stably at minimum cost

#### Case Study: Sichuan Thermal-Hydro Hybrid Model

- A UC problem from real-life background (Sichuan Province)
- With 20 thermal and 230 hydro units
- Hydro units involve no decision (binary variables)

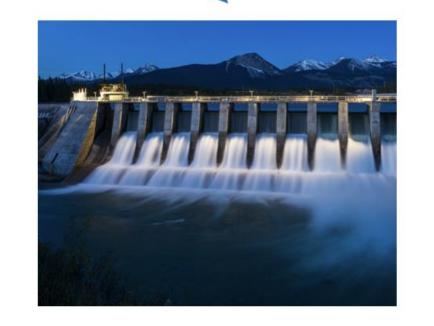


#### Hardness

- Costs are piecewise in generated power
- All the units are coupled by the Load balancing constraint
- A much larger and harder MILP model, but

minimize Cost of electricity
subject to Thermal Power+ Hydro Power = Load
Other Constraints
Decision Unit Operation Decision

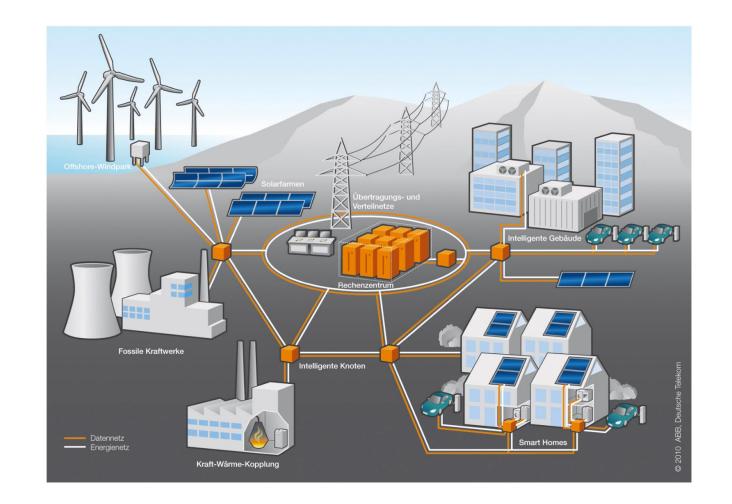




Better Modeling + Algorithm Makes it Easier!

#### Successively Implemented in a Much Larger Region

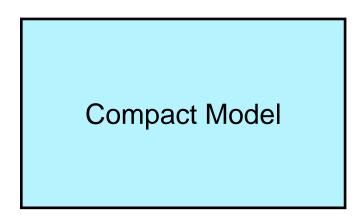
- A much larger UC problem with security constraint
- With much more (millions of) constraints and variables
- More than 1000 units of Thermal, Hydro and New energy
- Consider interaction between regions and time periods

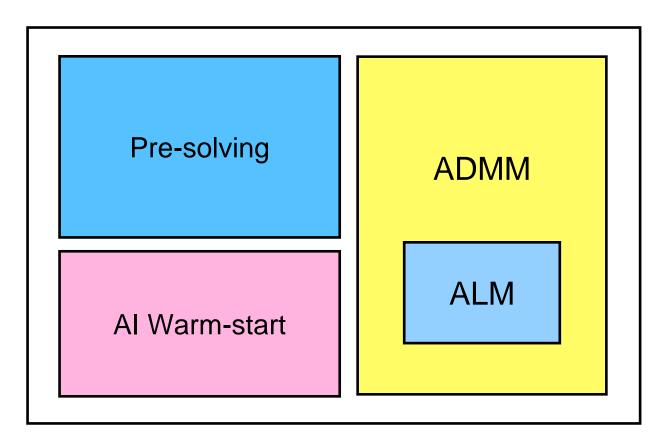


Huge size + Various business logic + Complicated coupling constraints

- Intractable without exploring structure
- Accurate and succinct model helps
- Domain specific algorithms matter a lot
- ML/Al has a big role to play

Model, Algorithm and ML/Al together make it tractable





App. VI: Beijing Public Transport Intelligent Urban Bus Operations Management with Mixed Fleet Types and Charging Schedule



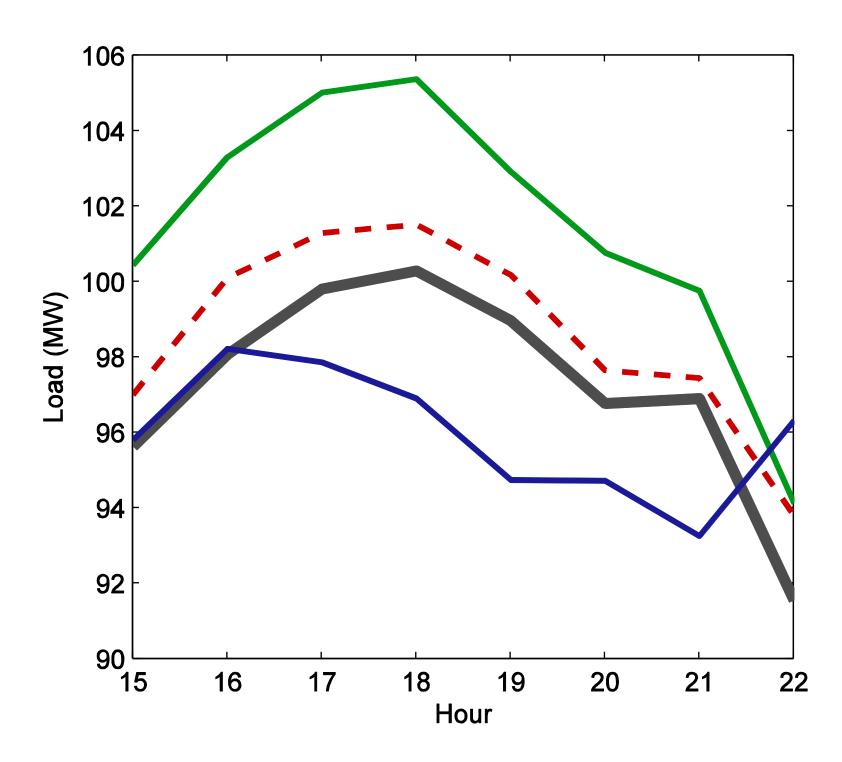


**Kickoff 2022.8** 





#### Peak Reduction due to Smart Charging and Discharging



	Standard	Low PGE	Linear Progr.
Total Fleet (\$)	97,678	83,695	65,349
Mean Cost / Mile	0.068	0.044	0.0054
Increase in Peak	5.1%	1.4%	-0.25%

### Background: Decision Intelligence in the case of Beijing Public Transport





最大化工作效率 最小化总体运营成本

新能源车购车选型、车线匹配、能源布局、保养计划

运筹优化、求解器、机器学习等智能决策技术

#### 北京市"十四五规划"目标

#### 加快构建"综合、绿色、智能、安全"的立体 化现代化城市交通系统

- 到2025年,中心城区绿色出行比例提高至 76.5%
- 全面推进智慧城市建设,重点发展智慧交通
- 围绕轨道交通优化地面公交线网,减少长距离、长时间运行线路,提高车辆利用率

加快建立科学、高效的 "城市智能运行决策管理体系"

- 高水平推动城市交通的数字转型和智慧升级,形成城市交通整体解决方案
- 加快建设公共交通网络化智能调度体系, 让公交出行越来越可靠, 时间有保证

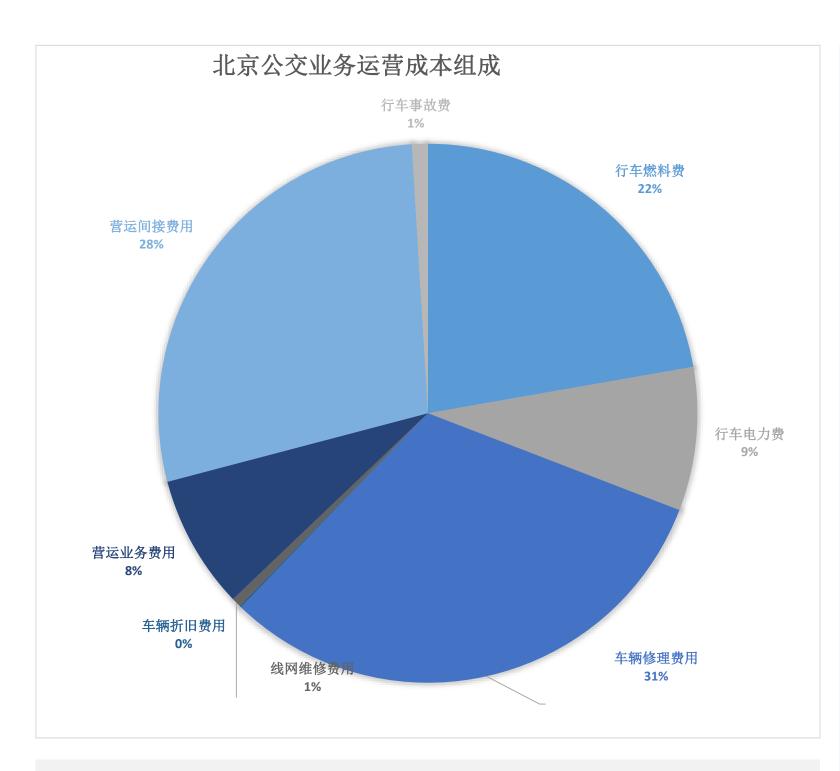
More efficient and intelligent decision-making to achieve 14th Five-Year Plan goals

Beijing Public Transport Line
7 is selected as the Key Pilot
Unit of the intelligent
transformation of Beijing
Public Transport

### Intelligent Transformation Empowered by Cardinal Operations







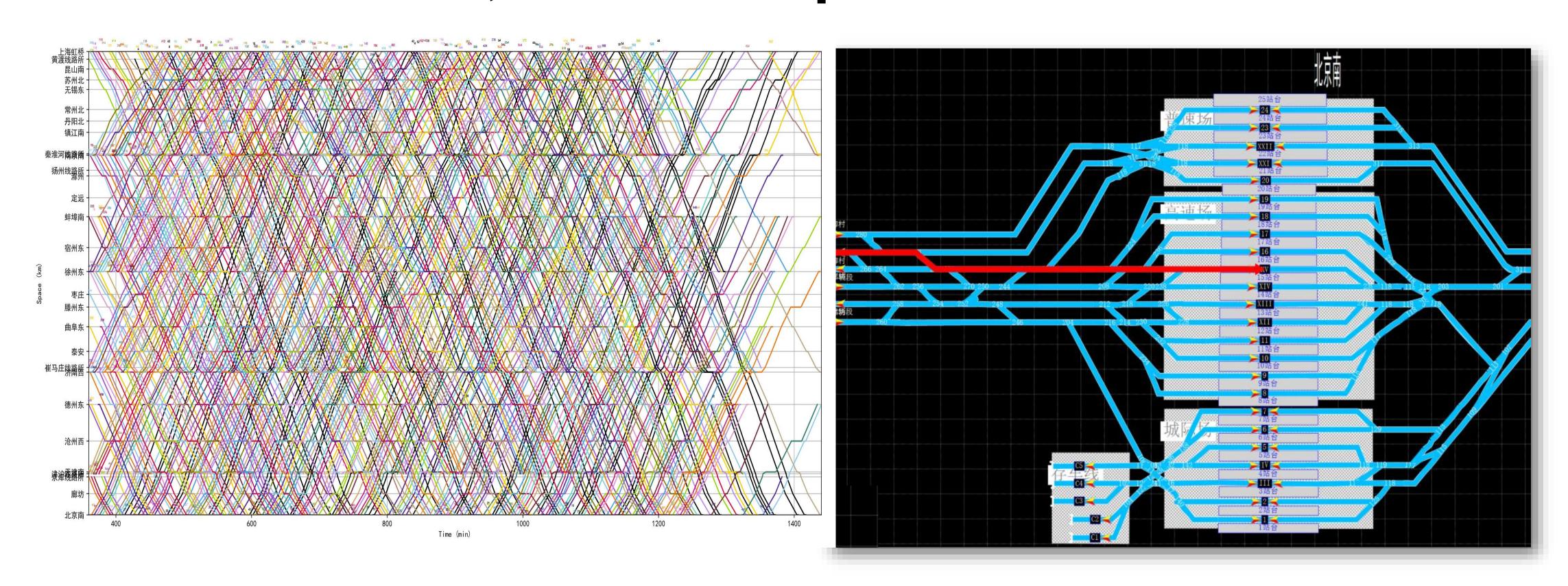
Beijing Public Transport's total operational costs reached 6.65 billion Yuan in 2020, of which fuels, electricity, maintenance, repair and other indirect costs accounted for over 90%.

Preliminary analysis shows various potential use cases for optimization in cost reduction.



### App. VII: Beijing-Shanghai High-speed Railway Scheduling Optimization

#### COPT, Cardinal Operations 2022



#### Background

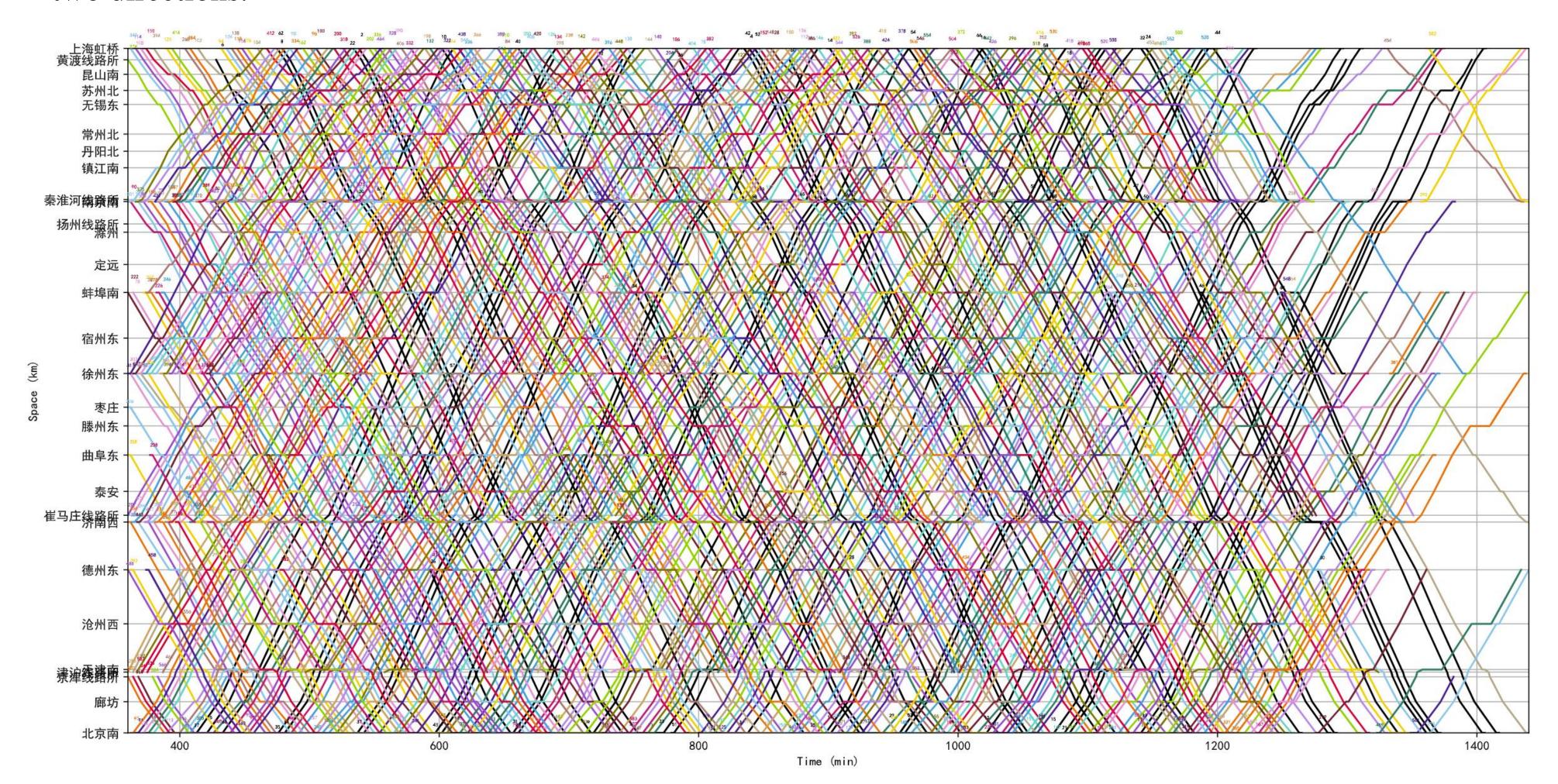
- China High-speed Railway has been committed to providing high-quality transportation services to passengers, and the formulation of train scheduling is a key link in the operation.
- At present, train scheduling is based on human experience, which becomes increasingly difficult to handle the growing network. Therefore, both industry and academia are seeking ways to automate train scheduling.
- The train scheduling problem can be divided into **Train Timetabling Problem (TTP)** and **Train Platforming Problem (TPP)**.

#### **Optimization Model:**

- Objective: maximize the number of trains placed in the train scheduling, thereby maximizing operating revenue;
- Constraints: describe the running behavior of trains and prevent train collisions;
- The project mainly solves TTP for Beijing-Shanghai High-speed Railway and TPP at Beijingnan Railway Station.
  - Beijing-Shanghai High-speed Railway is the busiest high-speed railway with the largest number of passengers in China. It is 1,318 km in total and passes 29 stations.
  - Beijingnan Railway Station is the largest railway station in Beijing, with the largest area and the largest number of trains.
  - Both problems are challenging scheduling tasks, which can be formulated as Mixed Integer Programming (MIP).

#### Numerical Results: TTP for Beijing-Shanghai & COPT

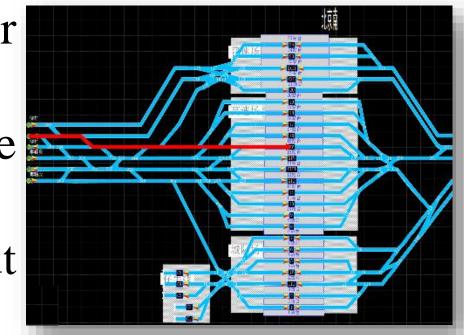
- We solve the TTP for Beijing-Shanghai high-speed railway using Cardinal Optimizer (COPT).
- COPT is the first fully independently developed mathematical programming solver in China with strong solving ability of MIP problem. It also has excellent performance in solving this problem.
- The result is presented in the following figure. We only need about 1000 seconds to schedule 584 train in two directions.



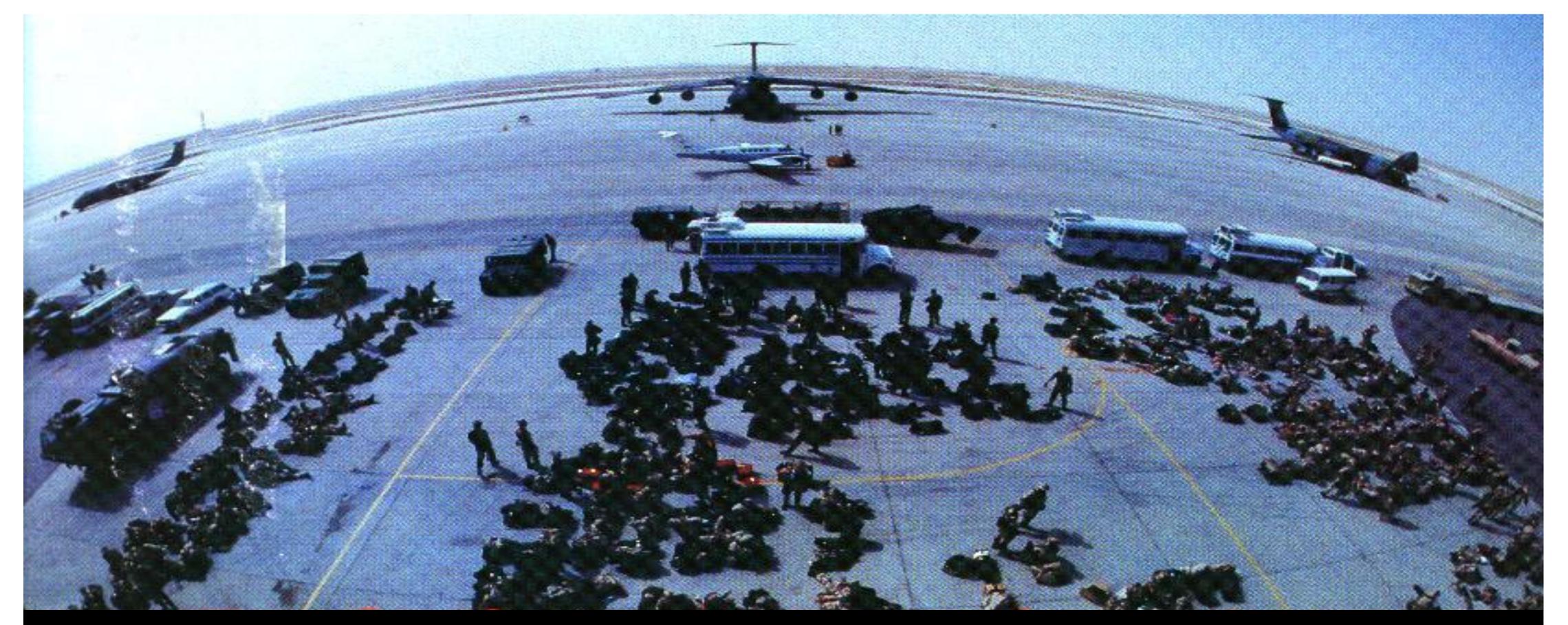
#### Numerical Results: TPP at Beijingnan Station



- We solve the TPP at Beijingnan Railway Station using Cardinal Optimizer (COPT).
- Considering the connection pairs and ensuring the feasibility, we solve the model within 2 hours, which is much less than manual scheduling.
- The result is presented in the following table, including time nodes about occupation at boundaries and tracks.

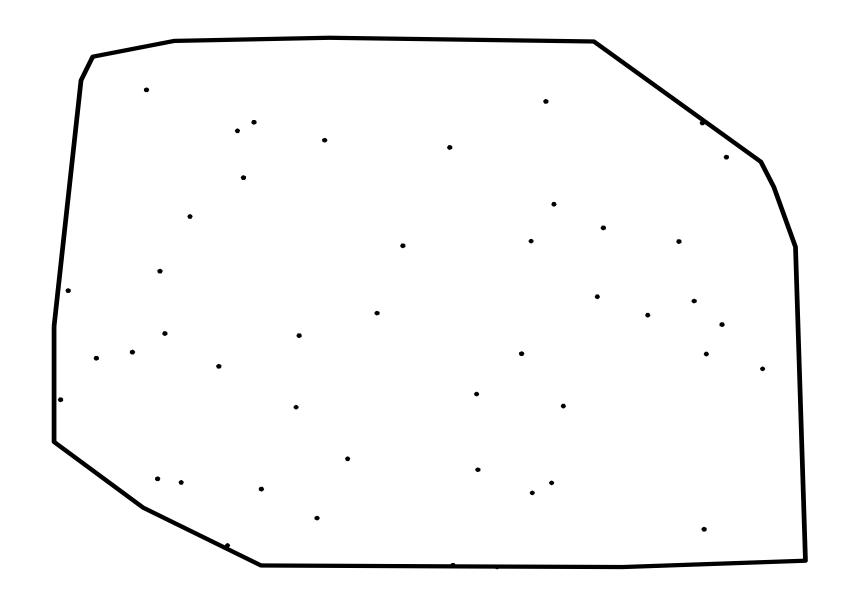


列车编号 前序车站	进入站界	进站路径	停靠站线	离开站界	出站路径	后序车站	进入站界时间	进入站线时间	离开站线时间	离开站界时间
361	站界:B10		站线:XIV	站界:B9	站线:10:XIV	廊坊		12:00:00	12:06:00	12:10:00
74 廊坊	站界:B8	站线:16:8	站线:8	站界:B7			11:57:00	12:02:00	12:17:00	
125	站界:B10		站线:11	站界:B9	站线:13:11	廊坊		12:06:00	12:13:00	12:17:00
114 廊坊	站界:B8	站线:7:17	站线:17	站界:B7			12:10:00	12:14:00	12:29:00	
251	站界:B10		站线:8	站界:B9	站线:16:8	廊坊		12:17:00	12:27:00	12:32:00
20 廊坊	站界:B8	站线:7:17	站线:17	站界:B7	站线:7:17		12:19:00	12:23:00	12:25:00	12:29:00
96 廊坊	站界:B8	站线:13:11	站线:11	站界:B7			12:25:00	12:29:00	12:44:00	
223	站界:B10		站线:17	站界:B9	站线:7:17	廊坊		12:29:00	12:44:00	12:48:00
8 廊坊	站界:B8	站线:8:16	站线:16	站界:B7			12:33:00	12:37:00	12:42:00	
23	站界:B10		站线:16	站界:B9	站线:8:16	廊坊		12:42:00	12:57:00	13:01:00
127	站界:B10		站线:11	站界:B9	站线:13:11	廊坊		12:44:00	12:49:00	12:53:00
572 廊坊	站界:B8	站线:5:19	站线:19	站界:B7			12:43:00	12:48:00	13:03:00	
124 廊坊	站界:B8	站线:6:18	站线:18	站界:B7			12:47:00	12:52:00	12:57:00	
102 廊坊	站界:B8	站线:15:9	站线:9	站界:B7			12:51:00	12:56:00	13:07:00	
225	站界:B10		站线:18	站界:B9	站线:6:18	廊坊		12:57:00	13:12:00	13:17:00
51	站界:B10		站线:17	站界:B9	站线:7:17	廊坊		12:59:00	13:01:00	13:05:00
116 廊坊	站界:B8	站线:13:11	站线:11	站界:B7			12:56:00	13:00:00	13:15:00	
169	站界:B10		站线:19	站界:B9	站线:5:19	廊坊		13:03:00	13:18:00	13:23:00
133	站界:B10		站线:9	站界:B9	站线:15:9	廊坊		13:07:00	13:22:00	13:27:00
161	站界:B10		站线:11	站界:B9	站线:13:11	廊坊		13:15:00	13:26:00	13:30:00
138 廊坊	站界:B8	站线:5:19	站线:19	站界:B7			13:13:00	13:18:00	13:33:00	
118 廊坊	站界:B8	站线:8:16	站线:16	站界:B7			13:27:00	13:31:00	13:36:00	
109	站界:B10		站线:19	站界:B9	站线:5:19	廊坊		13:33:00	13:41:00	13:46:00
100 廊坊	站界:B8	站线:8:16	站线:16	站界:B7			13:31:00	13:35:00	13:40:00	
229	站界:B10		站线:16	站界:B9	站线:8:16	廊坊		13:36:00	13:51:00	13:55:00
2 廊坊	站界:B8	站线:16:8	站线:8	站界:B7			13:34:00	13:39:00	13:47:00	
131	站界:B10		站线:16	站界:B9	站线:8:16	廊坊		13:40:00	13:55:00	13:59:00
3	站界:B10		站线:8	站界:B9	站线:16:8	廊坊		13:47:00	14:02:00	14:07:00
98 廊坊	站界:B8	站线:10:XIV	站线:XIV	站界:B7			13:43:00	13:47:00	14:02:00	
108 廊坊	站界:B8	站线:13:11	站线:11	站界:B7			13:47:00	13:51:00	14:06:00	



Topic 4: Equitable Covering & Partition – Divide and Conquer (Carlsson et al. 2009)

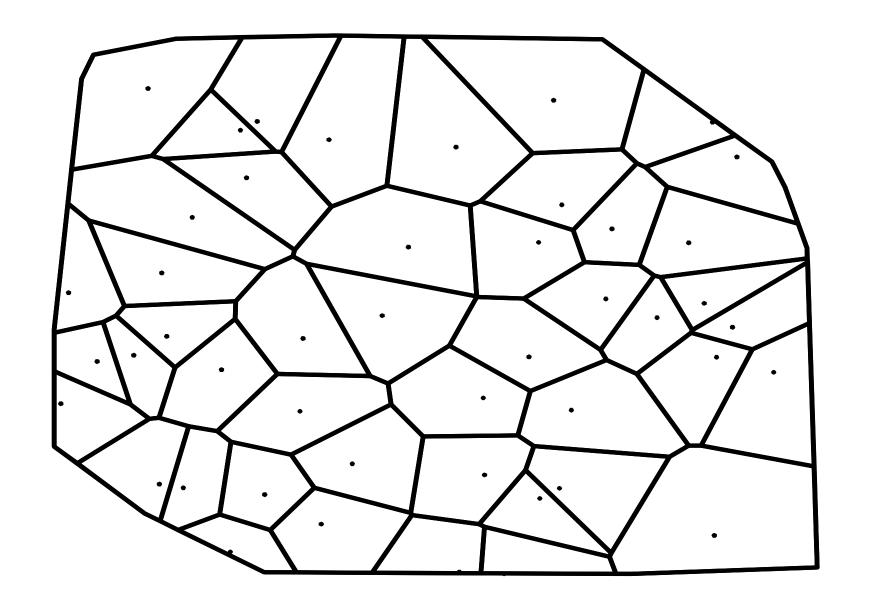
#### Problem Statement: Divide-Conquer



n points are scattered inside a convex polygon P (in 2D) with m vertices. Does there exist a partition of P into n sub-regions satisfying the following:

- Each sub-region is a convex polygon
- Each sub-region contains one point
- All sub-regions have equal area

#### Related ML Problem: Voronoi Diagram

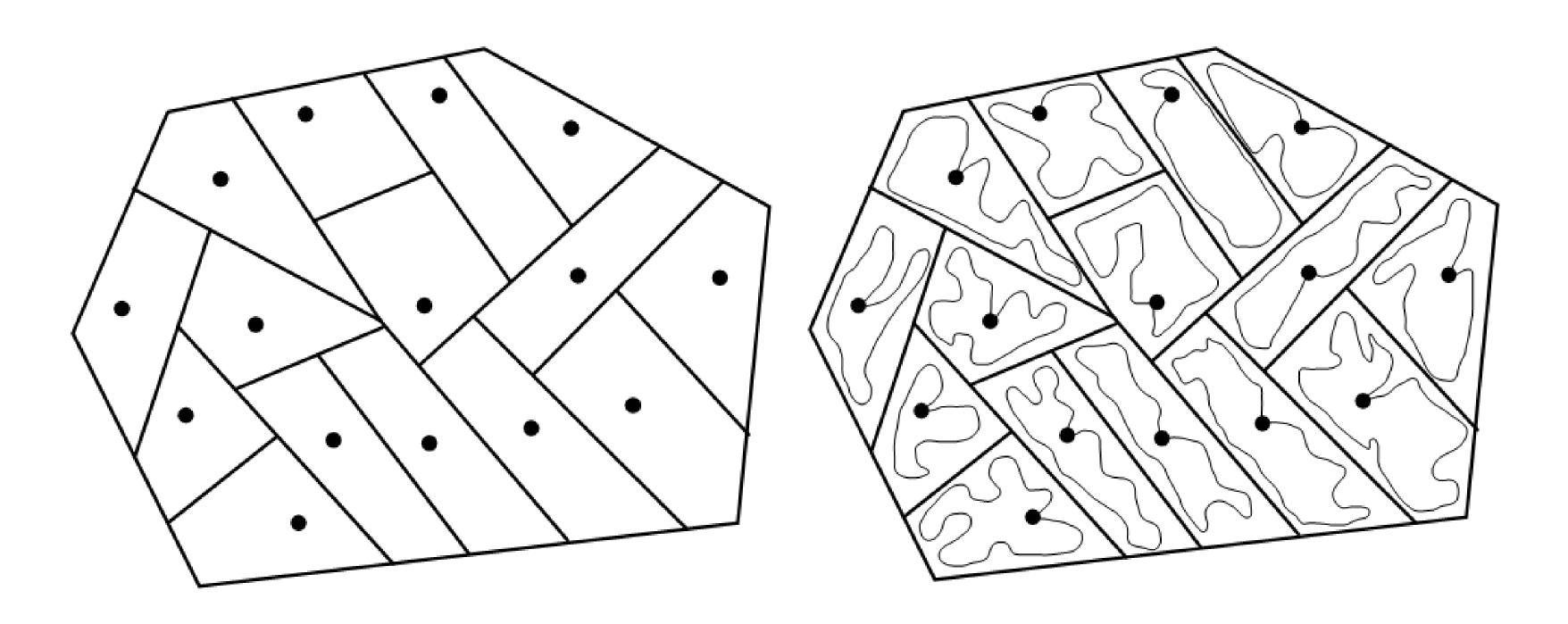


In the *Voronoi Diagram*, we satisfy the first two properties (each sub-region is convex and contains one point), but the sub-regions have different areas.



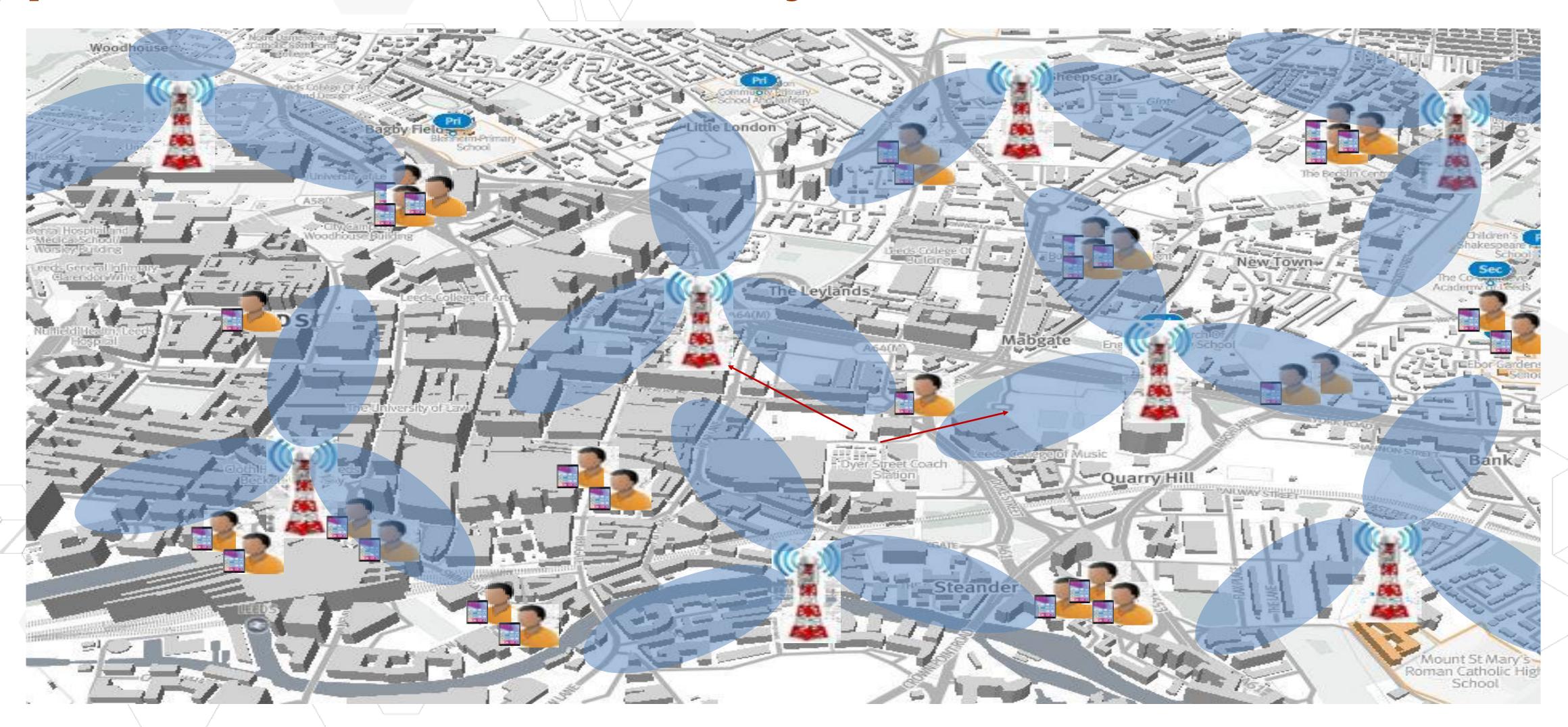
#### Our Result

Not only such an equitable partition always exists, but also we can find it exactly in running time  $O(Nn \log N)$ , where N = m + n.





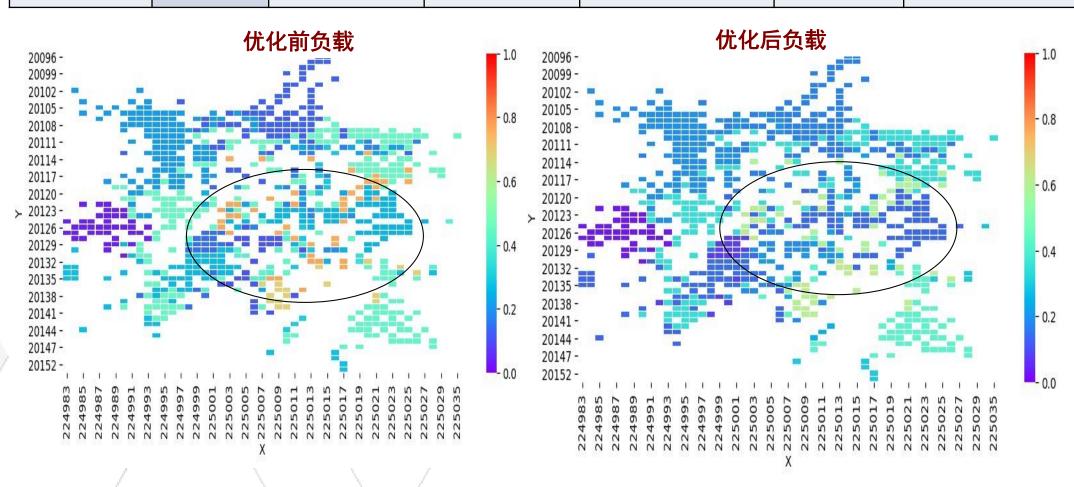
#### App. VIII: Wireless Tower – Dynamic Resource Allocation

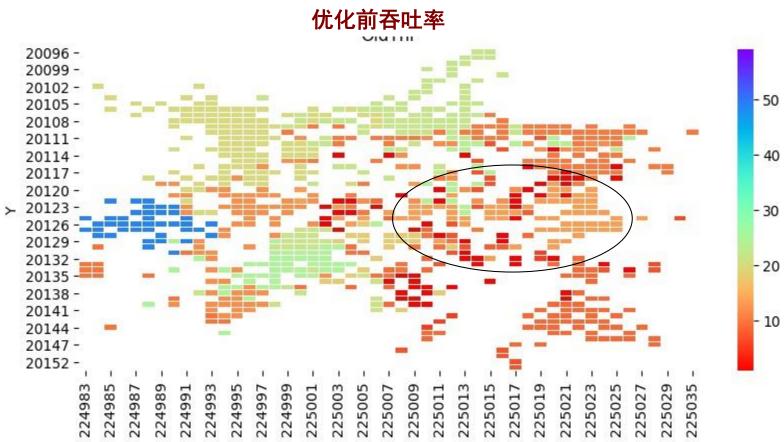


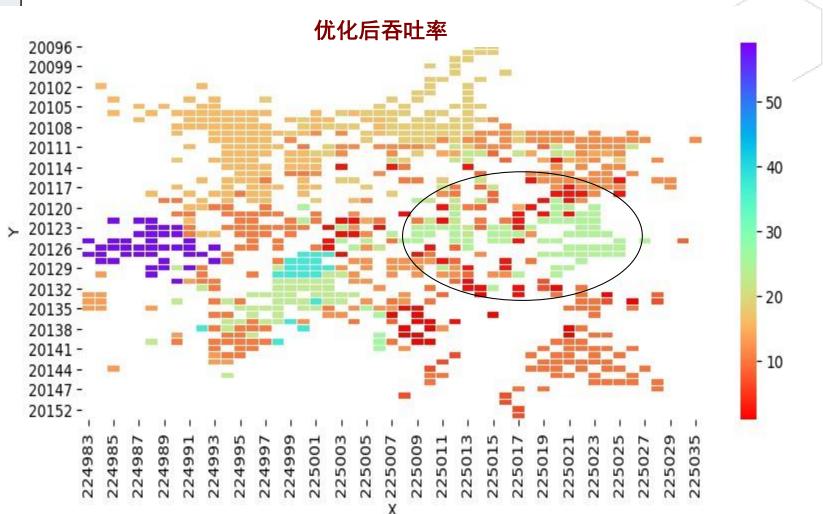
#### Preliminary Test Result—Effectiveness

#### 基于真实商用网络进行模型优化效果的测试验证验证统计结果:

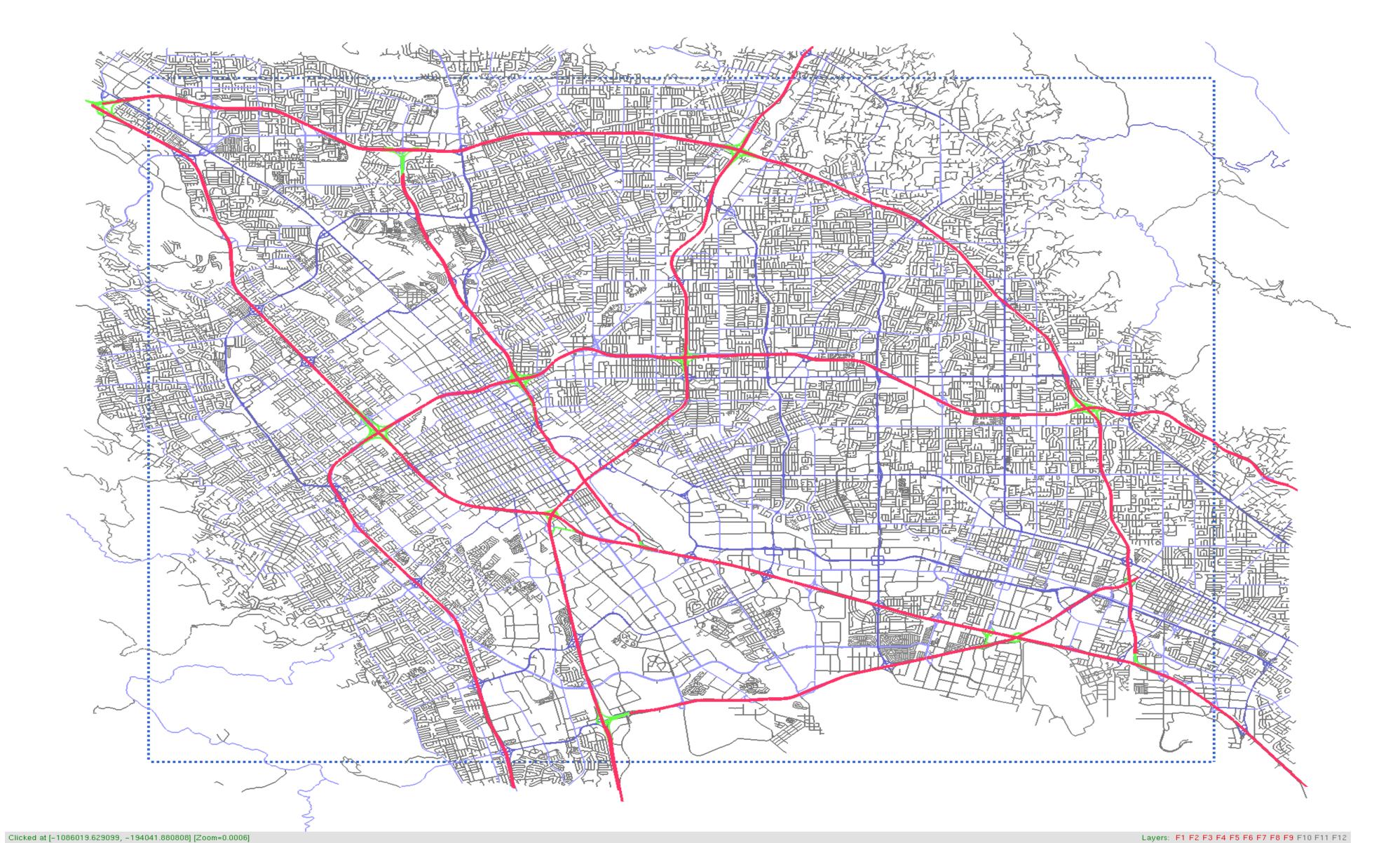
	小区数	时段	区域平均负 载	区域平均吞吐率 (Mb/S)	高负载小 区负载	高负载小区吞吐 率(Mb/S)
优化前		中午及晚共6	31%	5.3	68%	2.3
优化后	27	・ 小时 小时 晚7时话务高 峰	30%	6.12(提升15%)	66%	2.8(提升22%)
优化前	21		37%	3.9	77%	1.6
优化后			33%	5.2(提升33%)	68%	2.1(提升32%)







### App. IX: Street View Application Map-Making





#### Topic 5: Beyond Math - Love Sport and Have a Belief





#### Sport Changed my Life I



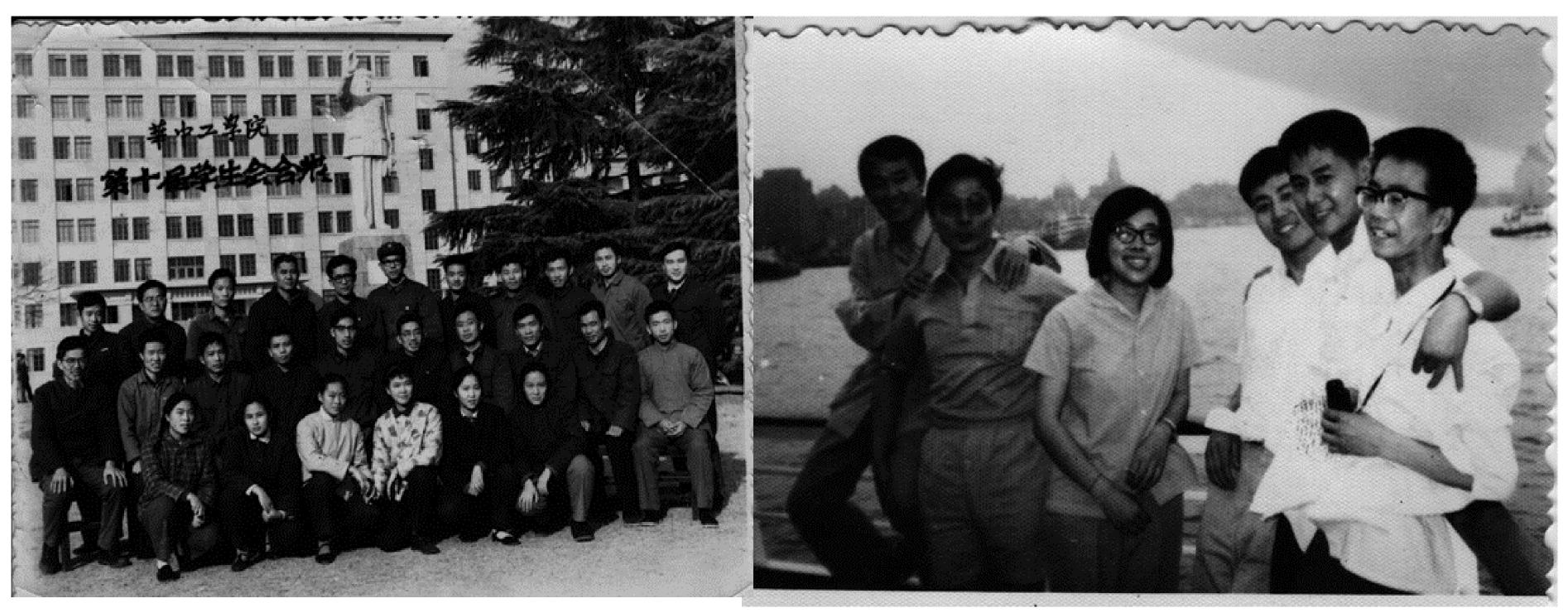




https://msande.stanford.edu/news/yinyu-ye-sports-led-me-rice-fields-stanford

# Sport Changed my Life II

Competitive spirit
Training hard
Team work
Take a loss
Play by rules





#### Beyond Academics

Be Grateful and Hopeful: no envy and nor self-doubt

Be Kind and Tolerant: love others and love yourself too

Have a Hobby: find something to relax

Have a Faith: find something to believe

#### Overall Takeaways

It is possible to maker online decisions for quantitative decision models with performance guarantees close to that of the offline decision-making with complete information

Second-Order Derivative information matters and better to integrate FOM and SOM for nonlinear optimization!

Mixed Integer LP solvers benefit real economy

Decomposition (Divide and Conquer) helps solving large-scale optimization problems

Life is bigger and richer than what you think – treasure and enjoy it at CUHKSZ

THANK YOU