Optimization methods Lecture 10: Intro to combinatorial optimization problems and its convex relaxations

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Brief reminder of the previous lecture

► Newton method

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- Newton method
- Quasi-Newton methods

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- Quasi-Newton methods
- Limited memory quasi-Newton methods

Gradient-free methods

Why do they need?

- ► Target vector is discrete
- Gradient is difficult to compute

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Examples

- Problems from the decision making and selection of element from the finite set
- ▶ Hyper-parameter selection in the machine learning models

Simulated annealing

- Main steps
 - Initialization of the initial vector and parameters
 - Every iteration follows the rule

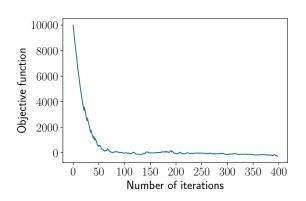
$$\mathbb{P}(\mathbf{x}_k \to \mathbf{x}^*) = \begin{cases} 1 & f(\mathbf{x}^*) < f(\mathbf{x}_k) \\ \exp\left(-\frac{f(\mathbf{x}^*) - f(\mathbf{x}_k)}{T/k}\right) & f(\mathbf{x}^*) > f(\mathbf{x}_k) \end{cases}$$

Denominator tuning is heuristic

Example

Partition problem with adjacency matrix ${f W}$

$$\min \mathbf{x}^{ op} \mathbf{W} \mathbf{x}$$
 s.t. $x_i \in \{-1, 1\}$



$$\alpha_k = 1/k$$

Other gradient-free methods

- Genetic algorithms
- Particle swarm optimization approach
- Many others, more details in the webinar

From LP to SDP

LP in standard form

$$\min_{\mathbf{x}} \langle \mathbf{c}, \mathbf{x} \rangle$$
s.t. $\mathbf{A}\mathbf{x} = \mathbf{b}$

$$\mathbf{x} \ge 0$$

- Replace vectors by matrices
- $ightharpoonup \mathbb{R}^n_+ o \mathbf{S}^n_+$
- ► Inner product between vectors → inner product between matrices

SDP

Standard form

$$\min_{\mathbf{X}} \operatorname{trace}(\mathbf{CX})$$
s.t. $\operatorname{trace}(\mathbf{A}_{i}\mathbf{X}) = b_{i}$
 $\mathbf{X} \succeq 0,$

where $\mathbf{C} \in \mathbf{S}^n$ and $\mathbf{A}_i \in \mathbf{S}^n$

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Dual form

$$\min_{\mathbf{x}} \mathbf{c}^{\top} \mathbf{x}$$
s.t. $\mathbf{A}\mathbf{x} = \mathbf{b}$

$$\mathbf{G} + \sum_{i=1}^{n} x_i \mathbf{F}_i \leq 0,$$

where $\mathbf{G} \in \mathbf{S}^n$ and $\mathbf{F}_i \in \mathbf{S}^n$.

► Initial non-convex QP problem

$$\begin{aligned} & \min \mathbf{x}^{\top} \mathbf{A} \mathbf{x} + \mathbf{b}^{\top} \mathbf{x} \\ \text{s.t. } & \mathbf{x}^{\top} \mathbf{A}_i \mathbf{x} + \mathbf{b}_i^{\top} \mathbf{x} \leq 0 \end{aligned}$$

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Equivalent transformation

$$\min \operatorname{trace}(\mathbf{A}\mathbf{X}) + \mathbf{b}^{\top}\mathbf{x}$$

s.t.
$$\operatorname{trace}(\mathbf{A}_{i}\mathbf{X}) + \mathbf{b}_{i}^{\top}\mathbf{x} \leq 0$$
$$\mathbf{X} = \mathbf{x}\mathbf{x}^{\top}$$

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Relax non-convex rank constraint

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► The last constraint is equivalent to $\begin{bmatrix} \mathbf{X} & \mathbf{x} \\ \mathbf{x}^\top & 1 \end{bmatrix} \succeq 0$

MAXCUT

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Formal problem statement

$$\max_{\mathbf{x}} \frac{1}{4} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (1 - x_i x_j)$$
 s.t. $x_i \in \{+1, -1\}$

Denote by c^* the optimal value of the objective function

 $\blacktriangleright \ \mathsf{Introduce} \ \mathsf{matrix} \ \mathbf{X} = \mathbf{x} \mathbf{x}^\top$

- Introduce matrix $\mathbf{X} = \mathbf{x}\mathbf{x}^{\top}$
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- ▶ Rank constraint is replaced with $\mathbf{X} \in \mathbf{S}^n_+$
- lacktriangle Optimal value of the objective function is denoted by p^*
- lacktriangle Since the feasible set is expanded, then $p^* \geq c^*$

How to reconstruct the solution?

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Q: how to recover the cut?

Goemans-Williamson's algorithm

- 1. Generate random vector \mathbf{v} in the unit sphere
- 2. $S = \{i \mid \langle \mathbf{v}, \mathbf{u}_i \rangle \geq 0\}$, where \mathbf{u}_i form matrix $\mathbf{U} : \mathbf{X} = \mathbf{U}^{\top} \mathbf{U}$

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Accuracy estimate

Goemans-Williamson's algorithm in average gives the solution r^{*} of the original problem, which is not less than

$$c^* \ge r^* \ge 0.878p^*$$

Authors won the Fulkerson prize in 2000 for this algorithm

Proof

1. Since the method maps any vector \mathbf{u}_i to ± 1 randomly, we can compute the expectation value of the cut C

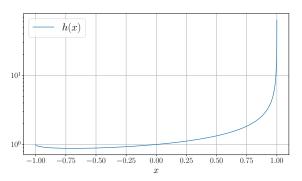
$$\mathbb{E}_{\mathbf{v}}(C) = \mathbb{E}_{\mathbf{v}} \frac{1}{2} \left(\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} [\operatorname{sign}(\mathbf{v}^{\top} \mathbf{u}_{i}) \neq \operatorname{sign}(\mathbf{v}^{\top} \mathbf{u}_{j})] \right)$$
$$= \frac{1}{2} \left(\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \mathbb{P}(\operatorname{sign}(\mathbf{v}^{\top} \mathbf{u}_{i}) \neq \operatorname{sign}(\mathbf{v}^{\top} \mathbf{u}_{j})) \right)$$

- 2. Probability of the different signs of $\mathbf{v}^{\top}\mathbf{u}_i$ and $\mathbf{v}^{\top}\mathbf{u}_j$ is equal to $\frac{\angle(\mathbf{u}_i, \mathbf{u}_j)}{\pi} = \frac{\arccos(\mathbf{u}_i^{\top}\mathbf{u}_j)}{\pi}$
- 3. As a result $\mathbb{E}_{\mathbf{v}}(C) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n w_{ij} \frac{\arccos(\mathbf{u}_i^\top \mathbf{u}_j)}{\pi}$

4. Now reduce this expression to the known one

$$\mathbb{E}_{\mathbf{v}}(C) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \frac{2 \arccos(\mathbf{u}_{i}^{\top} \mathbf{u}_{j})}{\pi (1 - \mathbf{u}_{i}^{\top} \mathbf{u}_{j})} \frac{1 - \mathbf{u}_{i}^{\top} \mathbf{u}_{j}}{2}$$

5. Find minimum of $h(x) = \frac{2\arccos(x)}{\pi(1-x)}$ for $x \in [-1,1)$



6. $h(x^*) \approx 0.8785 = \alpha_{GW}$

7. Then

$$\mathbb{E}_{\mathbf{v}}(C) \ge \alpha_{GW} \frac{1}{4} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (1 - \mathbf{u}_{i}^{\top} \mathbf{u}_{j}) = \alpha_{GW} p^{*} \ge \alpha_{GW} c^{*}$$

8. Since Goemans-Williamson's method gives some cut, then

$$c^* \ge \mathbb{E}_{\mathbf{v}}(C) \ge \alpha_{GW} p^* \ge \alpha_{GW} c^*$$

9. Finally

$$c^* \le p^* \le \frac{1}{\alpha_{GW}} c^* \approx 1.1382 c^*$$

Another interpretation of MAXCUT problem

$$\max_{x_{i}=\pm 1} \frac{1}{4} \sum_{i,j=1}^{n} w_{ij} (1 - x_{i}x_{j}) = \max_{x_{i}=\pm 1} \frac{1}{4} \sum_{i,j=1}^{n} w_{ij} \left(\frac{x_{i}^{2} + x_{j}^{2}}{2} - x_{i}x_{j} \right)$$

$$= \max_{x_{i}=\pm 1} \frac{1}{4} \left(-\sum_{i,j=1}^{n} w_{ij}x_{i}x_{j} + \frac{1}{2} \sum_{i=1}^{n} \left[\sum_{j=1}^{n} w_{ij} \right] x_{i}^{2} + \frac{1}{2} \sum_{j=1}^{n} \left[\sum_{i=1}^{n} w_{ij} \right] x_{j}^{2} \right)$$

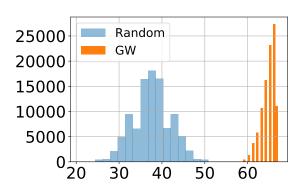
$$= \max_{x_{i}=\pm 1} \frac{1}{4} \left(-\sum_{i,j=1}^{n} w_{ij}x_{i}x_{j} + \frac{1}{2} \sum_{i=1}^{n} \deg(i)x_{i}^{2} + \frac{1}{2} \sum_{j=1}^{n} \deg(j)x_{j}^{2} \right)$$

$$= \max_{x_{i}=\pm 1} \frac{1}{4} \left(\sum_{i=1}^{n} \deg(i)x_{i}^{2} - \sum_{i,j=1}^{n} w_{ij}x_{i}x_{j} \right) = \max_{x_{i}=\pm 1} \frac{1}{4} \mathbf{x}^{\top} \mathbf{L} \mathbf{x},$$

where \mathbf{L} is a graph Laplacian, $\mathbf{L} = \mathbf{D} - \mathbf{W}$, where \mathbf{D} is a diagonal matrix, where the vertices degrees in the diagonal.

Comparison with random sampling

$$\max_{x_i = \pm 1} \frac{1}{4} \mathbf{x}^\top \mathbf{L} \mathbf{x}$$



Can this bound be improved?

- It is known that the method to compute the approximation with accuracy $\frac{16}{17}$ of the optimal value is already an NP-hard problem!
- ▶ Open problem: how to compute the better approximation with the algorithm of subexponential complexity

Summary

- Gradient-free methods
- ► SDP
- ► Convex relaxation of non-convex problems
- ► Goemans-Williamson's algorithm