Computational Optimization Methods

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University of Missouri, Columbia
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Overview of Syllabus

Objective

The course covers typical computational optimization methods widely used in many computing domains, such as bioinformatics, data mining and machine learning. The theoretical foundation of each optimization method is rigorously studied, followed by typical real-world applications in one or more domains.

Instructor, Office Hours, Course Web

- **Instructor:**

Prof. Jianlin Cheng (http://www.cs.missouri.edu/~chengji), Deb Bhattacharya (on August 21)

- **Office Hours**

Wed & Fri, 2:00 – 3:00

- **Course Website**

http://www.cs.missouri.edu/~chengji/com/

Topics

1. Markov chain Monte Carlo methods (MCMC) and their applications in sequence motif search

2. Simulated annealing and their applications in structure and network modeling

3. Dynamic programming and its applications in graph theory and sequence alignment

4. Quadratic programming and its applications in kernel methods

5. Maximum likelihood & maximum a posterior and their applications in text mining

6. Gradient descent and hill climbing and their applications in reinforcement learning and structure modeling

Topics (Continued)

6. Gradient descent and hill climbing and their applications in reinforcement learning and structure modeling

7. Contrastive divergence optimization and its applications in deep learning network

8. Expectation and Maximization optimization theory and its application in text clustering

9. Lagrange theory of constraint-based optimization and its applications in decision theory

10. Message passing and its applications to probabilistic graphical models (Bayesian networks and Markov random fields)

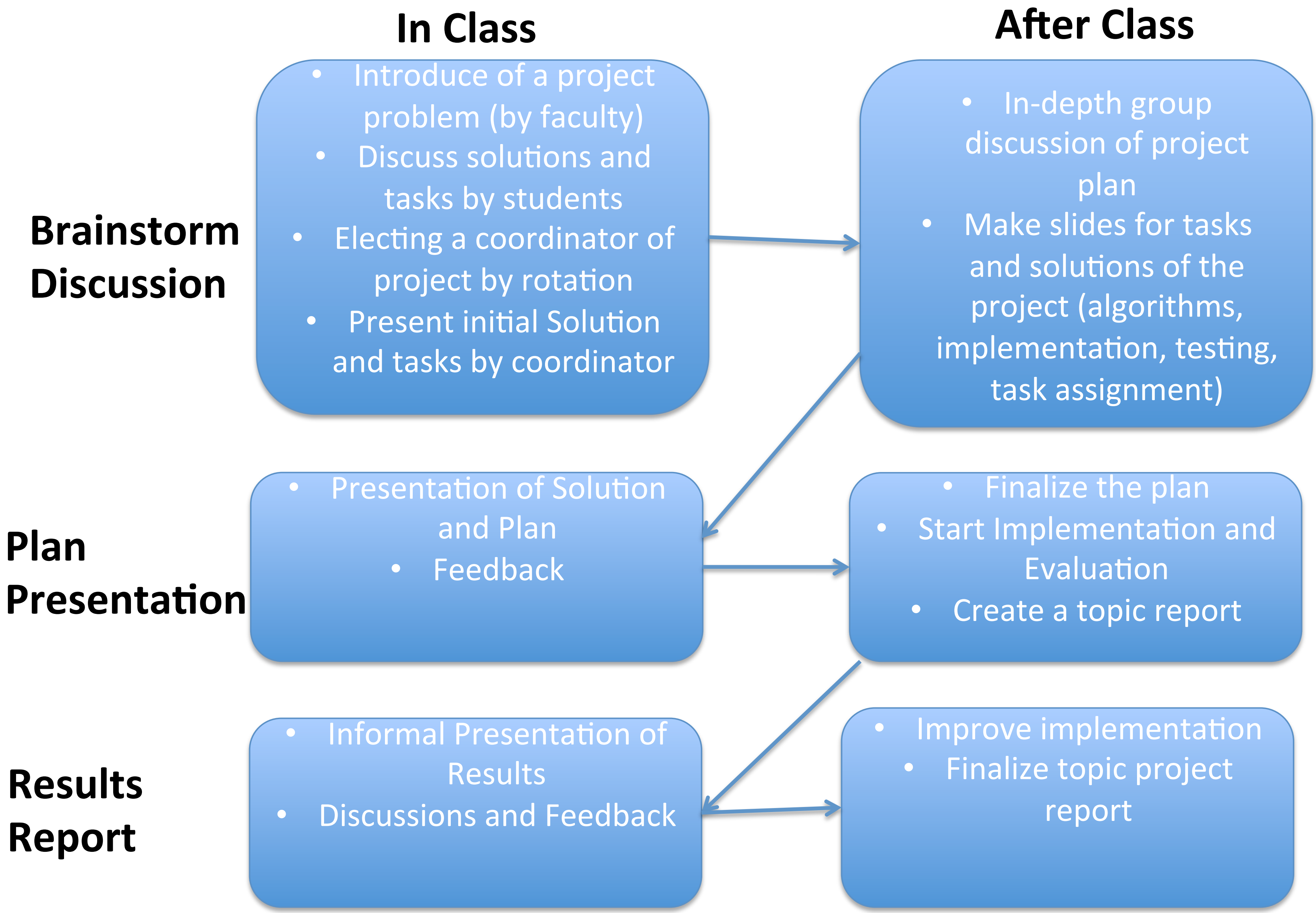
Assignments

- **Reading Assignments**: There is possibly one reading assignment for each topic. Students are required to read one paper regarding each topic and write a half-page overview of the method and application described in the paper.
- **Group Projects**: There is possibly one group project for each topic. Under the instructor's guidance, students work in a group to design and implement one optimization method for each topic and apply it to solve one computing problem. Each group may five to six students.

Problem Solving Based Teaching and Learning

Two Phases for Each Topic

- **Phase I – Theory**: a lecture (problem, algorithms, data structures) by instructor, reviewing a paper by students, 1/4 – 1/3 class time
- **Phase II – Practice**: Under the direction of the faculty, students will apply the techniques learned in the first phase to develop and apply a computational optimization method of each topic by working on a group software development project.


In Class
After Class
Brainstorm Discussion
Introduce of a project problem (by faculty)
Discuss solutions and tasks by students
Electing a coordinator of project by rotation
Present initial Solution and tasks by coordinator
In-depth group discussion of project plan
Make slides for tasks and solutions of the project (algorithms, implementation, testing, task assignment)
Plan Presentation
Presentation of Solution and Plan
Feedback
Finalize the plan
Start Implementation and Evaluation
Create a topic report
Results Report
Informal Presentation of Results
Discussions and Feedback
Improve implementation
Finalize topic project report

Final Presentation and Report

- Cover all the topics
- All members give a final presentation together
- A final report assembling all the results and methods of all the topics together

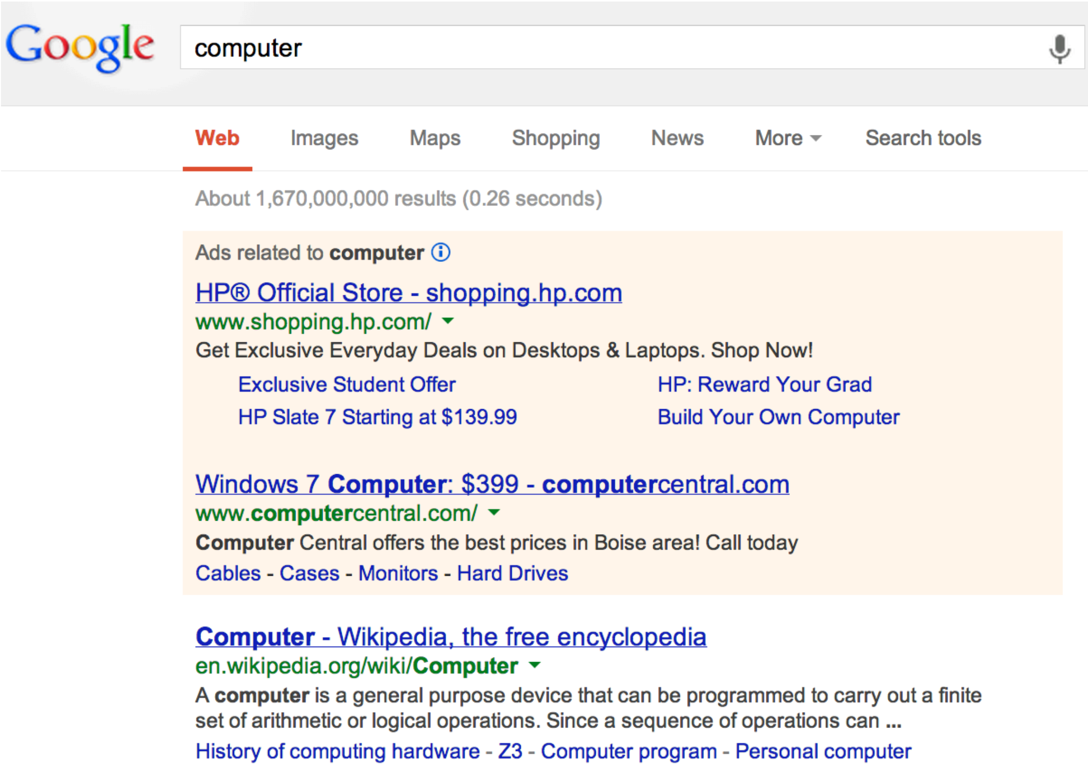
Introduction to Computational Optimization

Examples of Real World Optimization Problems - 1

- Find directions
- Given a map of Europe, find the shortest driving path from Paris to Rome.

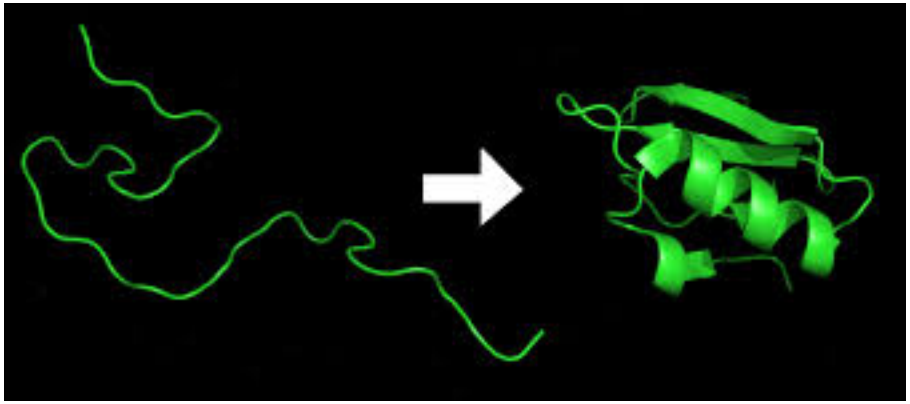
Examples of Real World Optimization Problems - 2

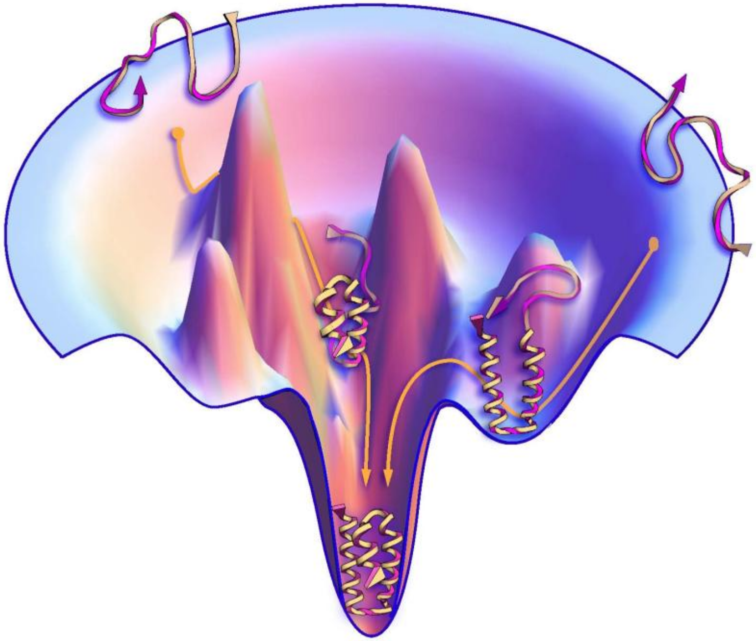
- Google Interview Question
- Given a list of ads and their probability being viewed by a user and the fees offered to show them, decide which ad to show by Google?



Examples of Real World Optimization Problems - 3

- Protein Folding
- Find shape / conformation of a protein with lowest energy





Definition of Optimization Problems

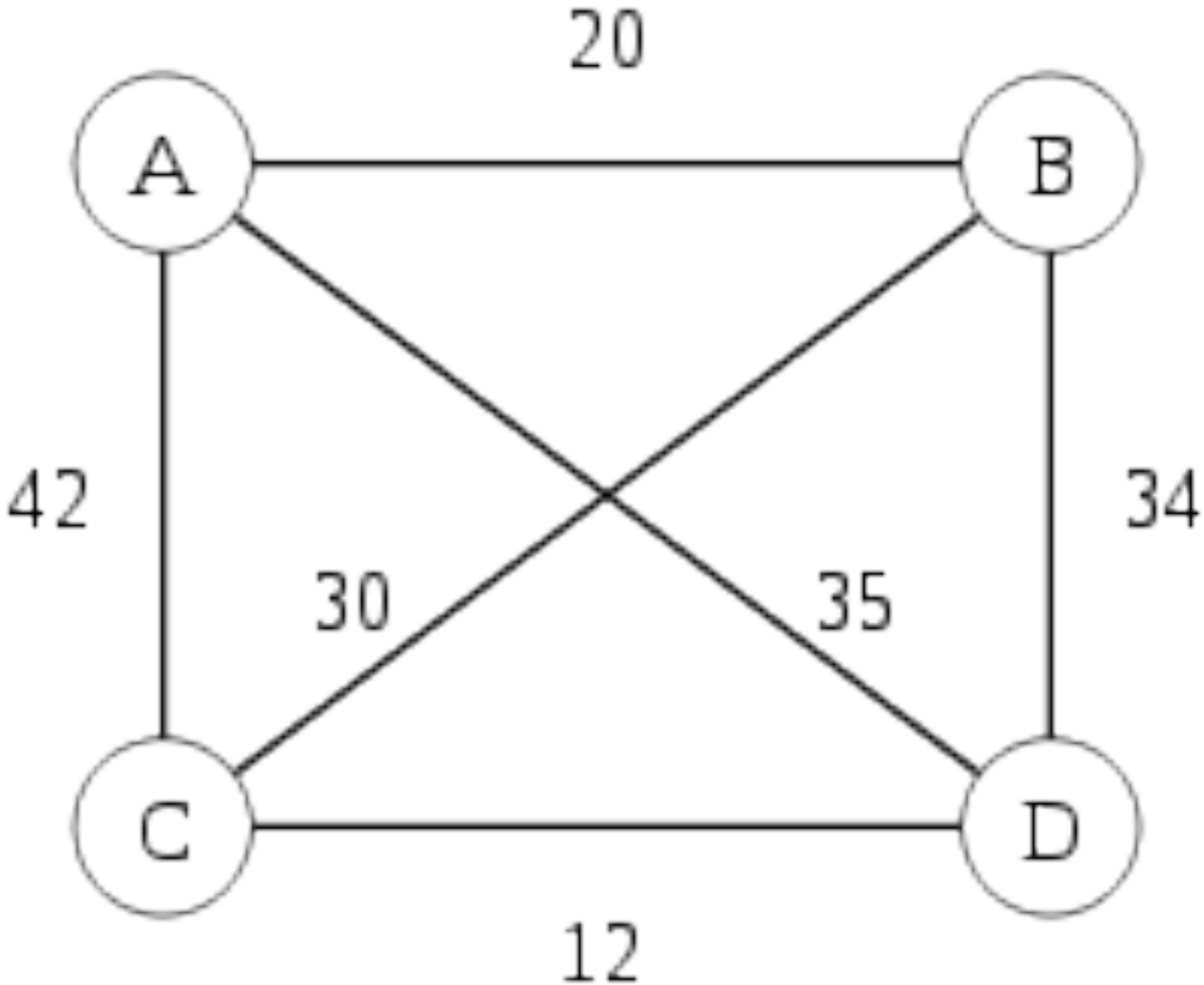
- An objective function defining a quantity to be optimized (maximize or minimize)
- A set of variables to be changed in order to optimize the objective function
- (Optionally) a set of constraints on the variables

Definition of An Integer Problem Problem

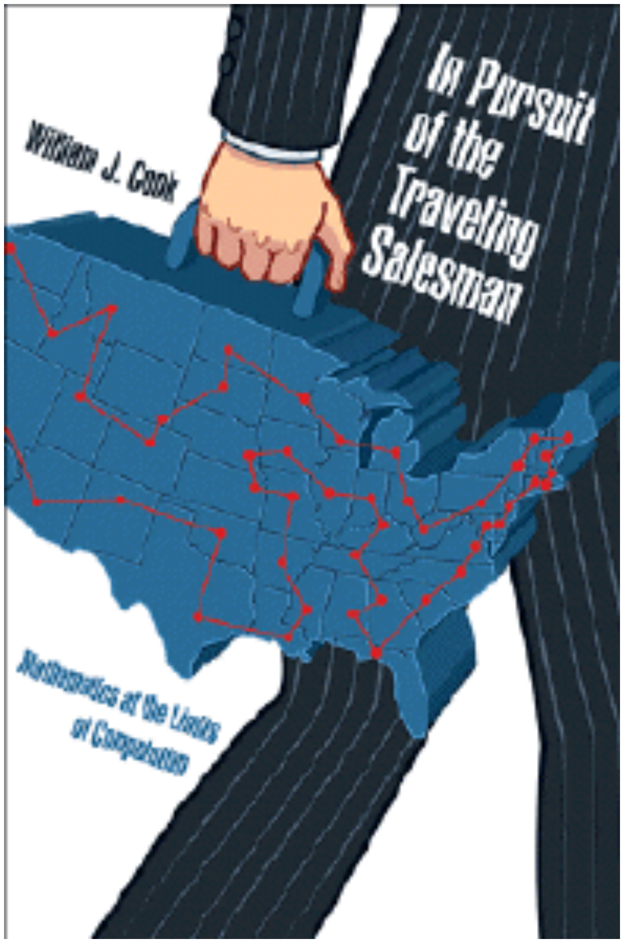
- An optimization problem in which some or all variables are restricted to be integers.
- Traveling salesman problem: Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?

William Rowan Hamilton

Graph Visualization of a Toy Example



Informal Definition



Objective:
Minimize the total distance of the tour over all the cities

Variables:
take a path between any two cities or not (0/1)

Constraints:
one city can be visited only once and all the selected paths form a round tour