Discrete Optimization

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Non-Linear Optimization

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Framework

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- A general introduction to discrete optimization
- Discrete Optimization in Radiation Therapy
- Discrete Optimization in Medical Imaging
- Bipartite Matching

Definition of discrete optimization

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- **Discrete optimization** is a branch of optimization in applied mathematics and computer science, as opposed to continuous optimization, the variables used in the mathematical program (or some of them) are restricted to assume only **discrete values**, such as the integers
- Two notable branches of discrete optimization are:
  - combinatorial optimization, which refers to problems on graphs, matroids and other discrete structures
  - integer programming

Definition of discrete optimization

- **combinatorial optimization** is a topic that consists of finding an optimal object from a finite set of objects
- An **integer programming** problem is a mathematical optimization in which some or all of the variables are restricted to be integers

Some examples in discrete optimization

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- Integer linear programming
- Set cover problem
- Knapsack problem
- Graph theory
  - Minimum spanning tree
  - Vertex cover problem
  - Traveling salesman problem (Hamiltonian circuit)
  - Shortest path problem
- Scheduling problem
- Maximum flow problem

Integer linear programming (NP-hard)

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- An ILP in canonical form is expressed as:

$$
\begin{array}{ll}
\text{maximize} & c^T x \\
\text{subject to} & Ax \le b \\
 & x \ge 0 \\
 & \text{and } \; x \text{ integer}
\end{array}
$$

Integer linear programming (NP-hard)

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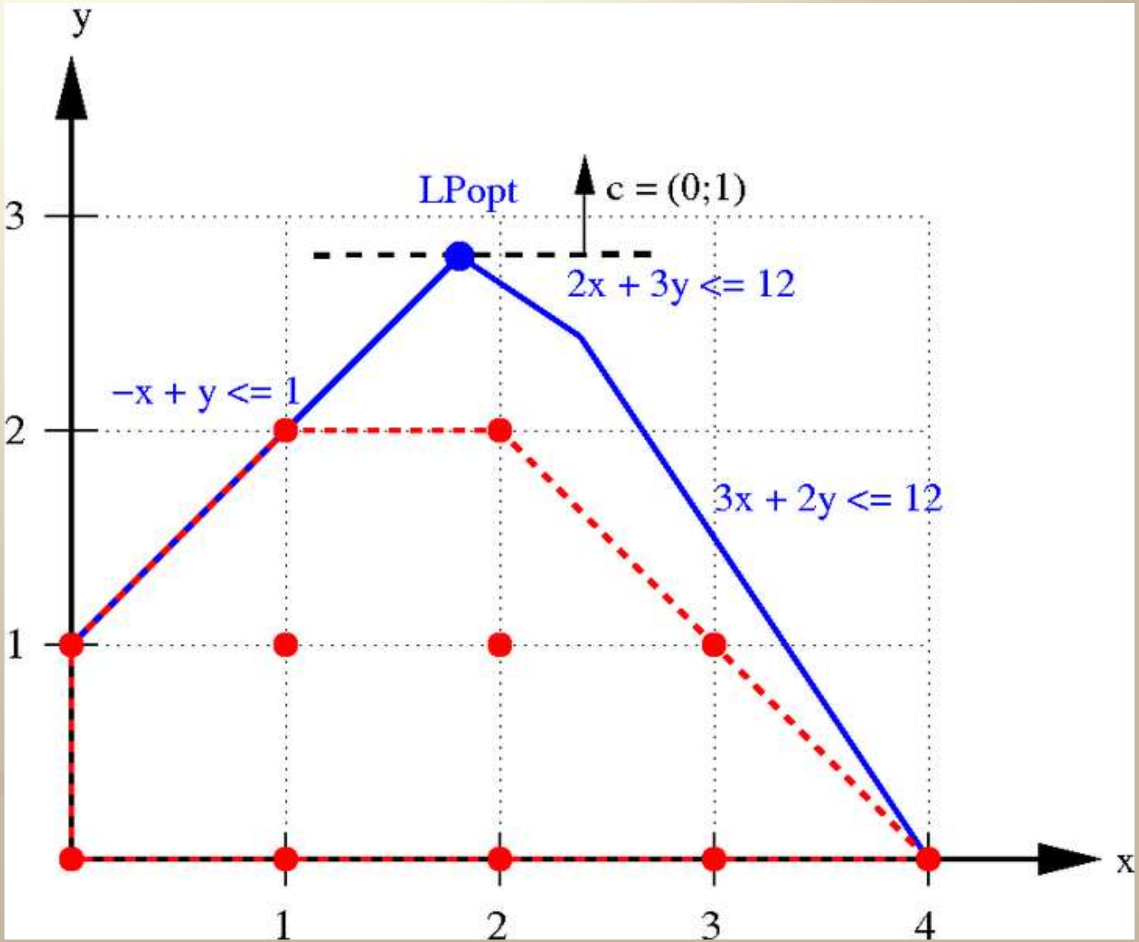
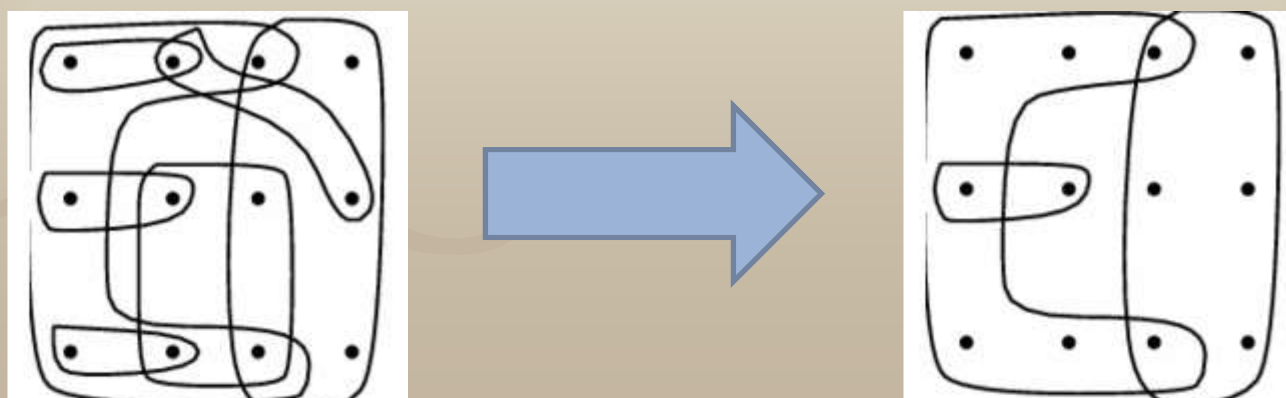
- An example:

$$\max\ y$$
$$-x + y \leq 1$$
$$3x + 2y \leq 12$$
$$2x + 3y \leq 12$$
$$x, y \geq 0, integer$$



Set cover problems (NP-hard)

- Given a set of elements {1,2, … , n} (called the universe) and a set S of m sets whose union equals the universe, the set cover problem is to identify the smallest subset of the union of which contains all elements in the universe.



Knapsack problems (NP-hard)

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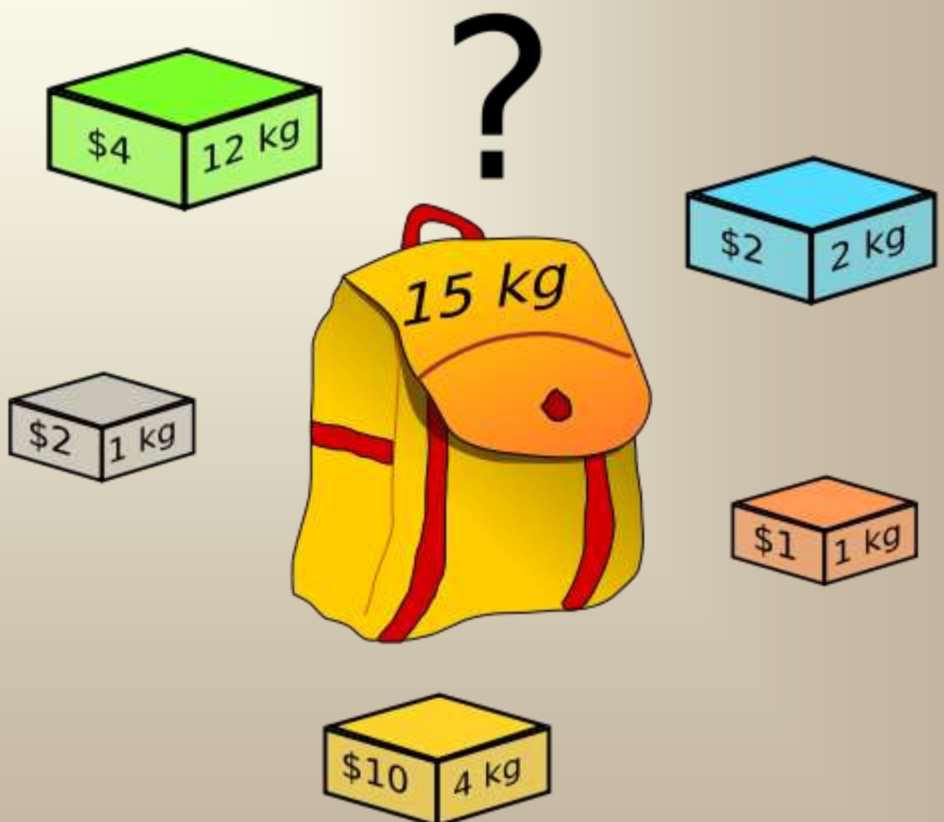
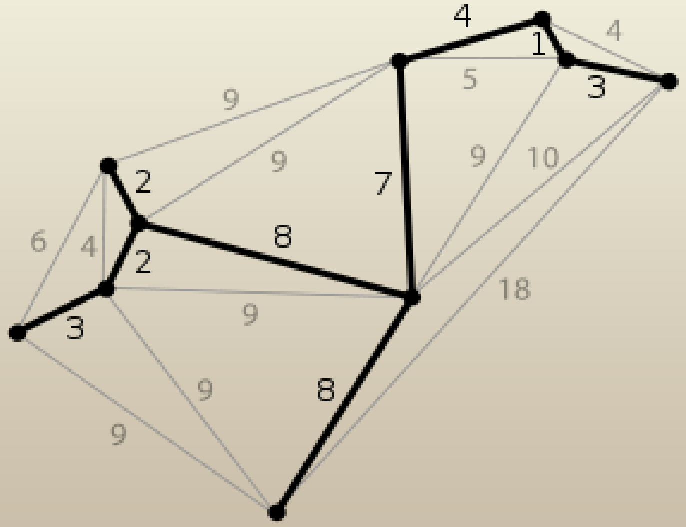
- Given a set of items, each with a weight and a value, determine the number of each item to include in a collection so that the total weight is less than or equal to a given limit and the total value is as large as possible.
- Backtracking Algorithm



Minimum spanning tree($O(n^2)$)

- A **minimum spanning tree** (**MST**) is then a spanning tree with weight less than or equal to the weight of every other spanning tree.



- Kruskal's algorithm (greedy Alg.)

Traveling salesman problem (NP-hard)

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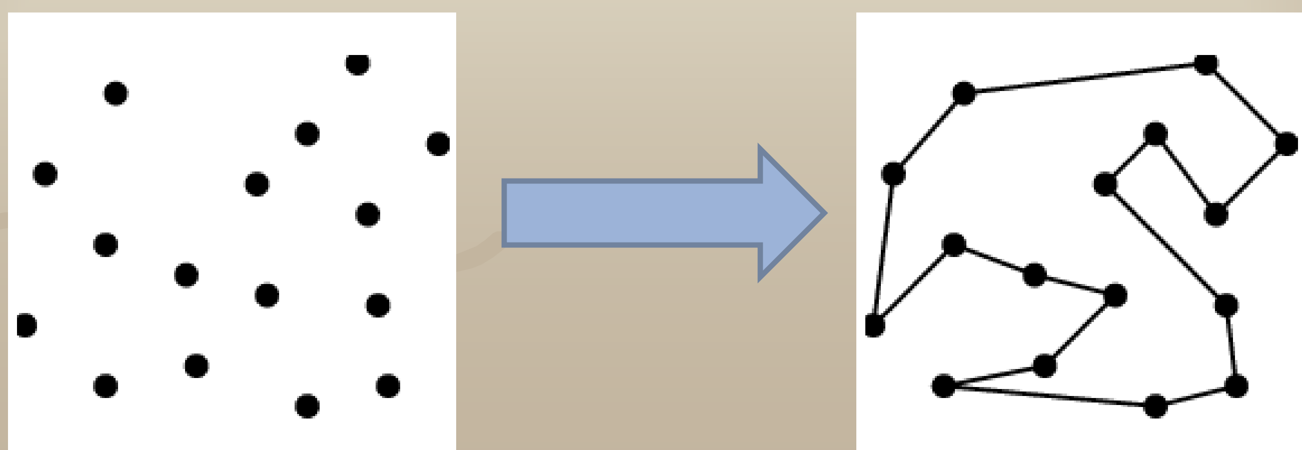
- The **travelling salesman problem (TSP)** asks the following question: given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?



Shortest path problem

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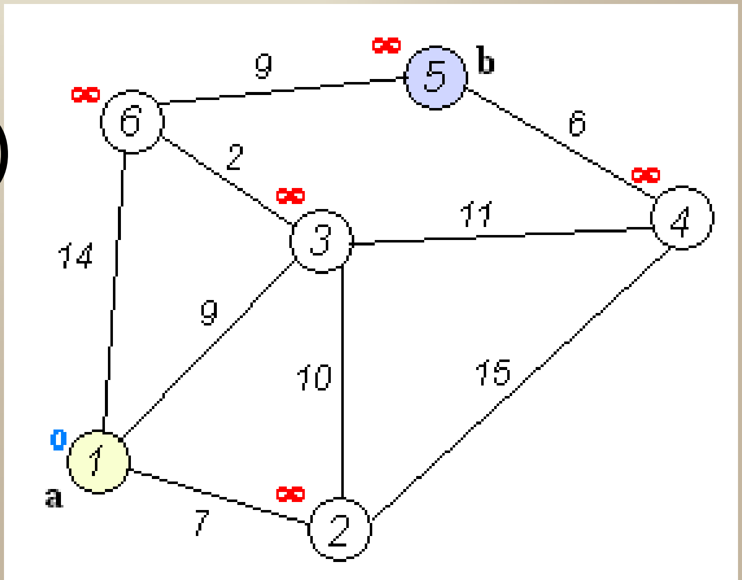
- The shortest path problem is the problem of finding a path between two vertices (or nodes) in a graph such that the sum of the weights of its constituent edges is minimized
- Dijkstra's algorithm($O(n^2)$)
- Floyd's algorithm($O(n^3)$)



Maximum flow problem (NP-hard)

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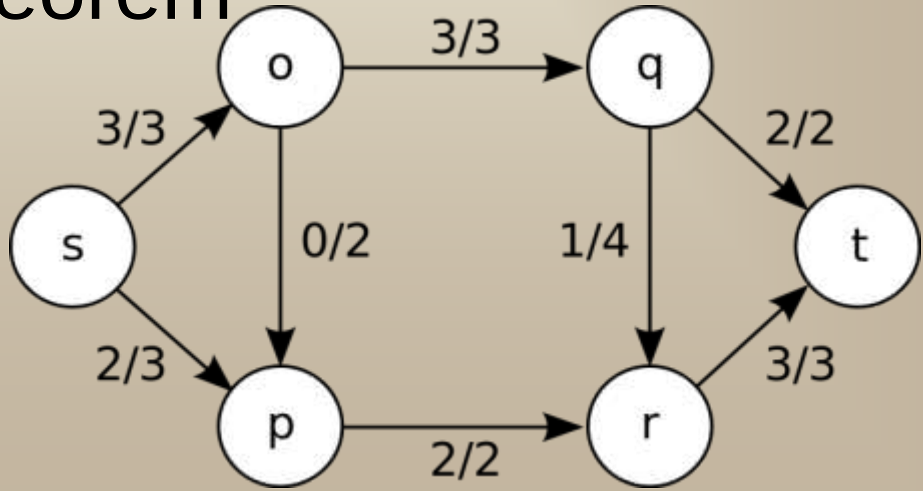
- **Maximum flow problem** is to find a feasible flow through a single-source, single-sink flow network that is maximum
- Max-flow min-cut theorem



Uses of Discrete Optimization

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- Resource managment
- Supply Chain
- Off-shore oil drilling infrastructure planning
- Medical
  - Computational molecular biology
  - Pharmaceutical testing schedules
  - Radiation Treatment Planning
  - Medical Imaging

Radiation Treatment for Cancer

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- Types
  - Photons (x-rays and γ-rays)
  - Protons
- Delivery
  - External beam
  - Intensity Modulated Radiation Treatment (IMRT)
  - Gamma Knife
  - Brachytherapy (seeds)

Goals of Radiation Therapy

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- 50% isodose line coverage of the target volume
- Minimize the non-target volume covered by external beams
- Minimize dose to near-by sensitive structures
- Minimize the number of shots → maximize the number of treated patients
- Simplicity

Optimization

- Calculate Dose (Gy) to each voxel (i,j,k) in the target volume and surrounding volume

$$
\begin{aligned}
Dose(i,j,k) &\leq U_{\mathcal{R}} + M * Exceed(i,j,k) \quad \forall (i,j,k) \in \mathcal{R} \\
\sum_{(i,j,k)\in\mathcal{R}} Exceed(i,j,k) &\leq \beta_{\mathcal{R}} * card(\mathcal{R}).
\end{aligned}
$$

U_R – Threshold dose

M – contant

R – target region

β_R – percent over-dose allowed (tolerance)

Exceed – binary variable

Mixed Integer Programming to solve

Gamma Knife Radio-surgery

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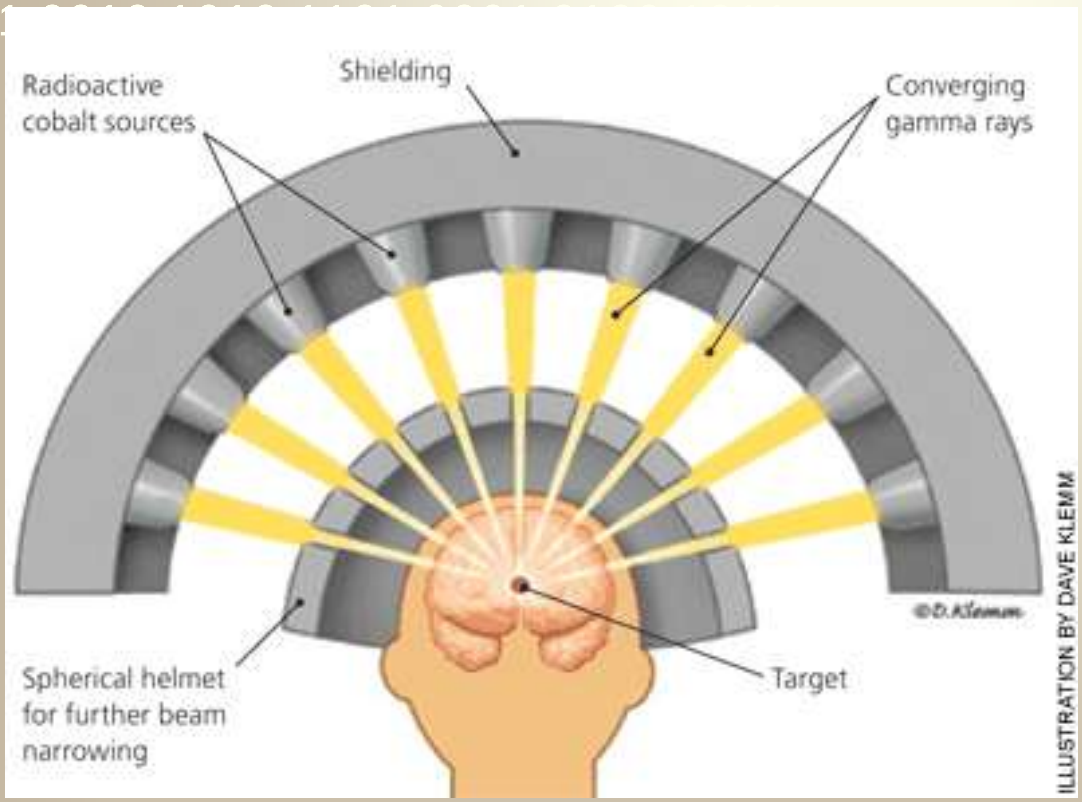

Co-60 source emits gamma rays by radioactive decay

Allows for much fewer fractions of radiation

Main application to brian tumors

Delivered in several “shots” – time and weight are controlled

Gamma Knife Optimization

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- Two steps to optimization
  - Continuous variables optimized using quassi-Newton method
    - position and weight of shots
  - Discrete variables optimized using simulated annealing
    - number of shots and collimator size

Gamma Knife Optimization

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- Mixed Integer Programming
  - Very large solution space

$$
\begin{aligned}
\min \quad & \sum_{(i,j,k)\in\mathcal{N}} Dose(i,j,k) \\
\text{subject to} \quad & Dose(i,j,k) = \sum_{(s,w)\in\mathcal{S}\times\mathcal{W}} t_{s,w} D_w(x_s, y_s, z_s, i, j, k) \\
& \Theta \le Dose(i,j,k) \le 1, \quad \forall (i,j,k) \in \mathcal{T} \\
& n = \sum_{(s,w)\in\{1,\ldots,n\}\times\mathcal{W}} H_\alpha(t_{s,w}) \\
& t_{s,w} \ge 0.
\end{aligned}
$$

IMRT

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IMRT

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- Mixed Integer Programming
  - Optimize beam angles, wedge orientations, beam intensities
  - Long run time to solve

$$
\begin{array}{llll}
\min\limits_{w} & \multicolumn{3}{l}{\lambda_t \|D_{\mathcal{T}} - \theta e_{\mathcal{T}}\|_\infty + \lambda_s \dfrac{\|(D_{\mathcal{S}} - \phi e_{\mathcal{S}})_+\|_1}{\operatorname{card}(\mathcal{S})} + \lambda_n \dfrac{\|D_{\mathcal{N}}\|_1}{\operatorname{card}(\mathcal{N})}} \\
\text{s.t.} & D_\Omega = & \displaystyle\sum_{A \in \mathcal{A}, F \in \mathcal{F}} w_{A,F} \mathcal{D}_{A,F,\Omega}, & \Omega \in \mathcal{T} \cup \mathcal{S} \cup \mathcal{N}, \\
& \frac{u}{\rho_A}\psi_A \geq & w_{A,0} + \tau_1 \displaystyle\sum_{F \in \mathcal{F} \setminus 0} w_{A,F} & \\
& K \geq & \sum_{A \in \mathcal{A}} \psi_A, & \\
& w_{A,F} \geq & 0, & \forall A \in \mathcal{A}, \\
& \psi_A \in & \{0,1\}, & \forall A \in \mathcal{A}.
\end{array}
$$

Brachytherapy Optimization

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$$Dose(i,j,k) = \sum_{(r,s,t)\in\mathcal{T}} D_{r,s,t}(i,j,k) * Seed(r,s,t).$$

$$\min \quad \alpha * \sum_{(i,j,k)\in\mathcal{T}} Underdose(i,j,k) + \beta * \sum_{(i,j,k)\in OAR} Overdose(i,j,k) + \gamma * \sum_{(i,j)\in template} Needle(i,j)$$

- Subject to constraints related to limiting needles to place the seed, limited dose to sensitive organs
- Mixed integer programming and branch-and-bound methods

Discrete Optimization in Medical Imaging

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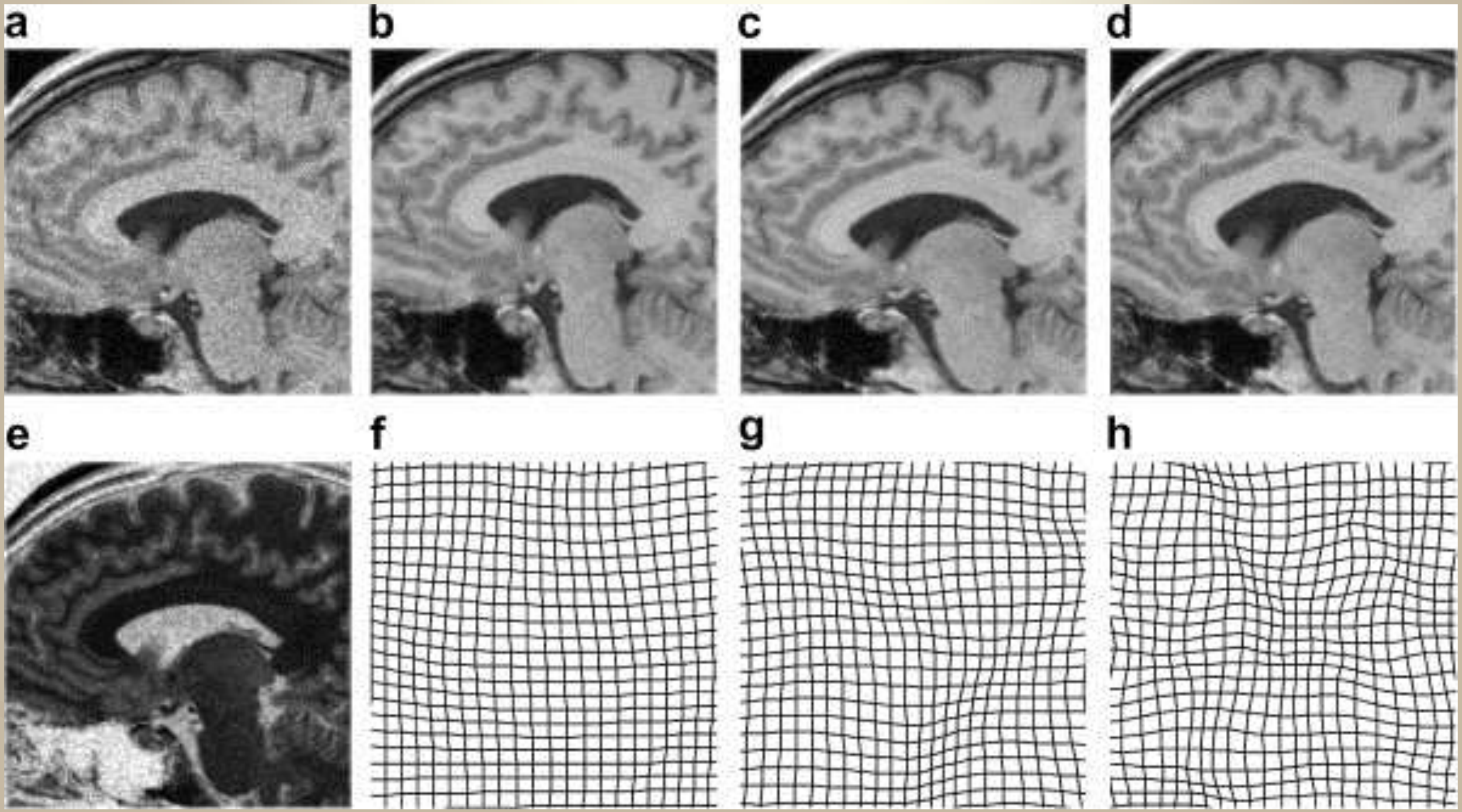

Glocker B, Komodakis N, Tziritas G, et al. Dense image registration through MRFs and efficient linear programming. *Medical Image Analysis* 2008;12:731-741

Basics of Image Registration

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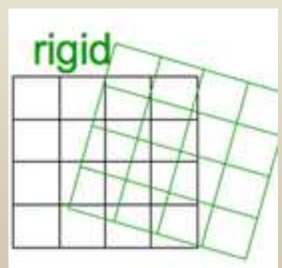
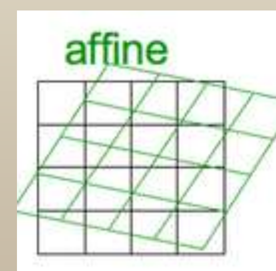
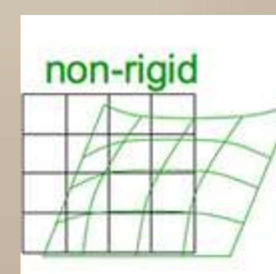
- Images must be registered in order to compare multiple subjects in a group
- From the most simple to the most complex:
  - Rigid
  - Affine
  - Non-rigid
    - Varying DOF







Why does medical imaging need optimization?

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- Curse of Dimensionality
  - 1 million + voxels
- Curse of non-convexity
  - Ill-posed problem (more parameters than constraints)
- Curse of non-linearity
  - Not all registrations are affine
- Curse of modularity
  - Solutions for very specific problems

What have they already tried?

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- Powell's (conjugate direction) method
- Downhill Simplex
- Levenberg-Marquardt
  - Currently used by SPM8
- Newton-Raphson
- Stochastic search methods
- Gradient descent methods
- Quasi-exhaustive search methods

What’s going on now?

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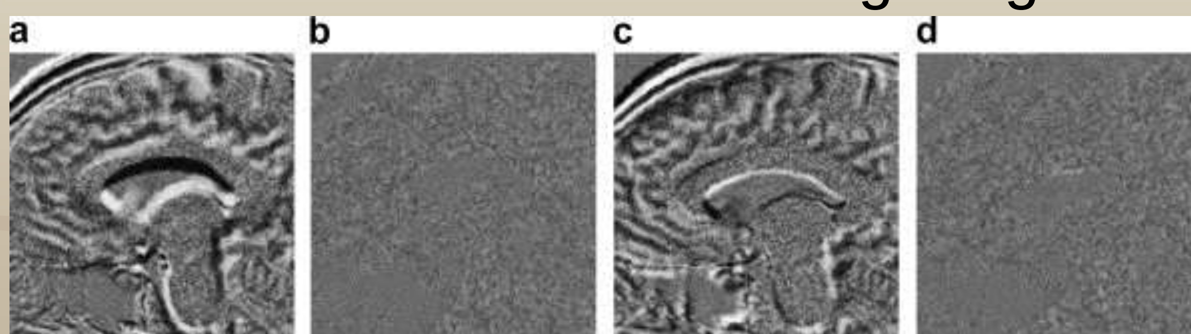
- Glocker et al. recently published a paper using discrete optimization techniques for image registration
  - Model registration as Markov Random Field
  - MRF is optimized using the primal-dual schema
  - Performs well on MRI brain image registration



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The Primal-Dual Schema

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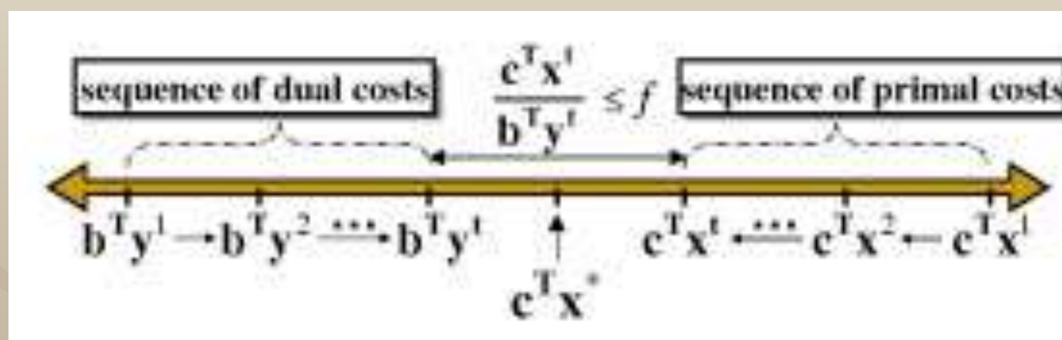
- Main goal: Minimize gap between the primal and dual costs
  - Primal problem is NP hard

$$\text{Primal}: \min \mathbf{c}^T\mathbf{x} \quad \text{s.t. } \mathbf{A}\mathbf{x} = \mathbf{b},\ \mathbf{x} \geqslant \mathbf{0}$$

$$\text{Dual}: \max \mathbf{b}^T\mathbf{y} \quad \text{s.t. } \mathbf{A}^T\mathbf{y} \leqslant \mathbf{c}$$



Estimating Biomarkers

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- Once the images are registered discrete optimization is also being used to find biomarkers related to the imaging data
- Biomarker = an indicator of a biological state
- Optimization helps with the curse of non-convexity
- Not much literature on this yet
  - Jobs?

Bipartite Matching

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- A graph $G = (V,E)$ consists of a set V of *vertices* and a set of E of pairs of vertices called *edges*.
  - An edge $e = (u,v)$
- A graph is bipartite if the vertex set V can be partitioned into two sets A and B such that no edge in E has both endpoints in the same set of the bipartition.
  - A matching is *perfect* if no vertex is exposed

Bipartite Matching

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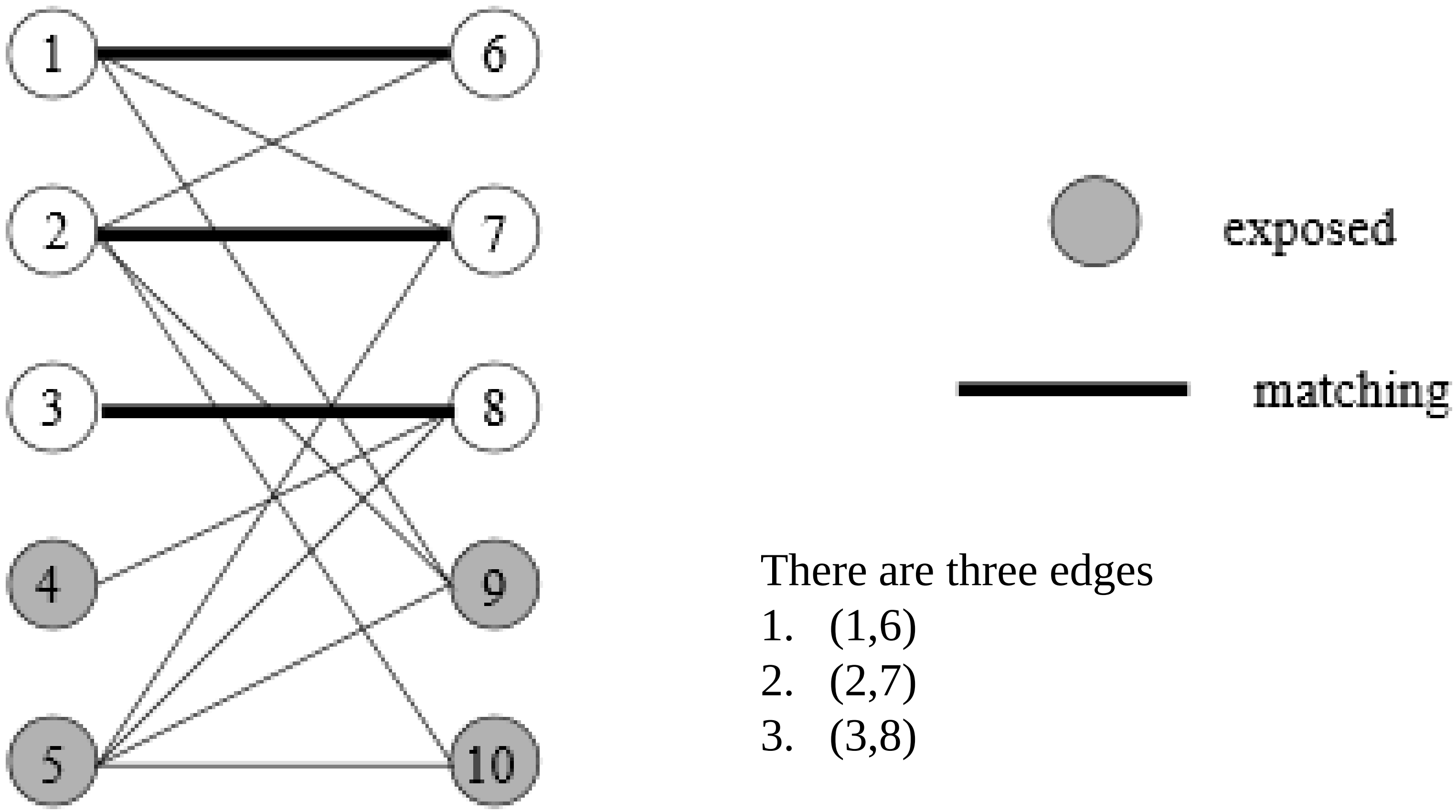

There are three edges

1. (1,6)
2. (2,7)
3. (3,8)

Bipartite Matching

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- Consider a rectangular matrix *A* of random numbers

```
A = rand(4,2)

A =

    0.4242    0.8010
    0.5079    0.0292
    0.0855    0.9289
    0.2625    0.7303
```

- Determine the matching

```
[val mi mj] = bipartite_matching(A);
```

  - mi = [2;3]
  - mj = [1;2]

Bipartite Matching

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- Rearrange the matrix based on the outputs of the previous problem

```
A1 = A(mi,mj)
```

```
A1 =

    0.5079    0.0292
    0.0855    0.9289
```

Bipartite Matching

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- Sum the diagonal of the new matrix

```
Ans = sum(diag(A1))

val


% The answer should verify that the maximum weighted matching is obtained
% when using the bipartite_matching command.
```

```
Ans =

    1.4367


val =

    1.4367
```

References

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