Comparing the Theory and Practice of Spectral Algorithms to Combinatorial Flow Algorithms for Expander Ratio, Normalized Cut, Clustering and Conductance

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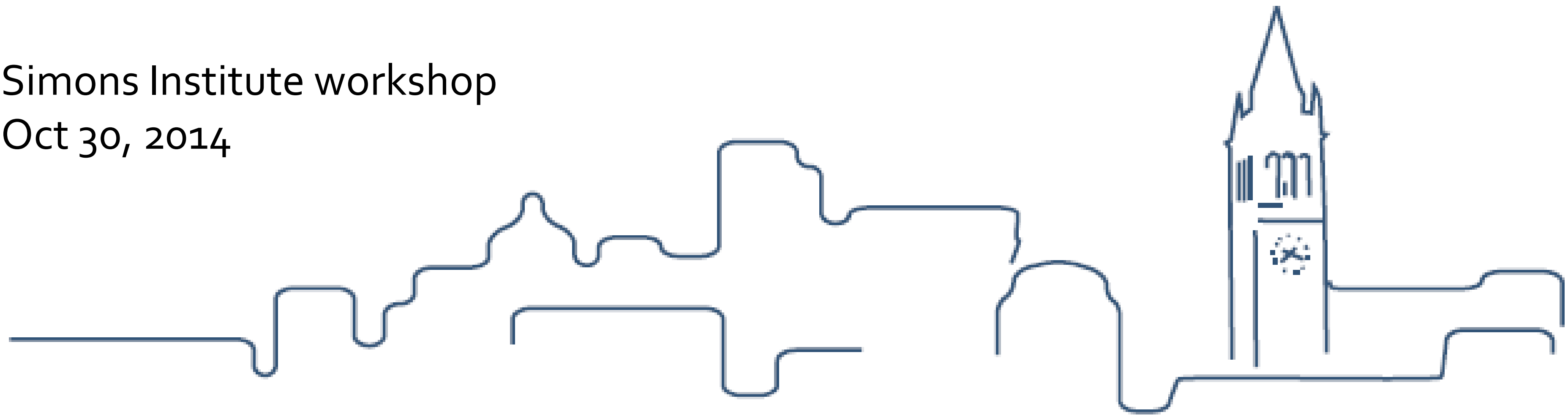


Notations and Preliminaries

- An undirected graph G=(V,E) $n = |V|$ $m = |E|$
- Edges' weights $w_{ij} \quad \forall [i,j] \in E$
- Nodes' weights $q_i \quad \forall i \in V$
- Capacity of a Cut $C(A,B) = \sum_{i \in A, j \in B} w_{ij}$
- Weighted degree $d_i = \sum_{j | [i,j] \in E} w_{ij}$
- Degree Volume $d(A) = \sum_{i \in A} d_i = 2C(A,A) + C(A,\bar{A})$
- Node Volume $q(A) = \sum_{i \in A} q_i$

The graph expander problem

- The graph expander problem:
  Expander graphs are used to generate good error correcting codes, and in cryptography.

$$\min_{|S|\le\frac{n}{2}} \frac{C(S,\bar{S})}{|S|} = \min_{S\subset V} \frac{C(S,\bar{S})}{\min\{|S|,|\bar{S}|\}}$$

The Cheeger problem

- The Cheeger problem, normalized cut:
  for effective segmentation of images.

$$\min_{d(S)\le\frac{d(V)}{2}} \frac{C(S,\bar{S})}{d(S)} = \min_{S\subset V} \frac{C(S,\bar{S})}{\min\{d(S),d(\bar{S})\}}$$

Also called Conductance, when the underlying graph is directed and used to assess the convergence rate of Markov chain processes.

A generalization: quantity normalized cut

- The q-normalized cut of a graph:
  Useful in clustering where q_i is a "characteristic" (e.g. texture) of node i

$$\min_{q(S)\leq\frac{q(V)}{2}} \frac{C(S,\bar{S})}{q(S)} = \min_{S\subset V} \frac{C(S,\bar{S})}{\min\{q(S),q(\bar{S})\}}$$

Formulations summary

- The graph expander problem

$$\min_{|S|\le\frac{n}{2}} \frac{C(S,\bar{S})}{|S|}$$

- The Cheeger problem, Normalized cut, Conductance

$$h_G = \min_{d(S)\le\frac{d(V)}{2}} \frac{C(S,\bar{S})}{d(S)}$$

- The q-normalized cut of a graph

$$\min_{q(S)\le\frac{q(V)}{2}} \frac{C(S,\bar{S})}{q(S)}$$

An intuitive clustering criterion

Find a cluster that combines two objectives:
One, is to have large similarity within the cluster, and
to have small similarity between the cluster its complement.

The combination of the two objectives can be expressed as:

$$\min_{S \subset V} \frac{C(S,\bar{S})}{C(S,S)} \quad \text{or}$$

$$\min_{S \subset V} C(S,\bar{S}) - \lambda C(S,S) \quad \text{or}$$

We call this problem **normalized-cut-prime,** or **NC’**.

$$\min_{S \subset V} C_1(S,\bar{S}) - \lambda C_2(S,S)$$

Normalized Cut and NC'

- Shi and Malik 2001:

  Normalized cut: NP-hard

$$\min_{S \subset V} \frac{C(S,\bar{S})}{d(S)} + \frac{C(S,\bar{S})}{d(\bar{S})}$$

- Sharon et al. 2007 called this problem normalized cut:

  Normalized cut': NP-hard?

$$\min_{S \subset V} \frac{C(S,\bar{S})}{C(S,S)}$$

How do NC and NC' compare [H10]

- Shi & Malik

$$\min_{S\subset V} \frac{C(S,\bar{S})}{d(S)} + \frac{C(S,\bar{S})}{d(\bar{S})}$$

- Sharon et. al

$$\min_{S\subset V} \frac{C(S,\bar{S})}{C(S,S)} = \frac{C(S,\bar{S})}{1/2[d(S)-C(S,\bar{S})]} =$$

$$= \frac{1}{\frac{d(S)}{2C(S,\bar{S})}-1} \Rightarrow \max_{S\subset V} \frac{d(S)}{2C(S,\bar{S})} \Rightarrow \min_{S\subset V} \frac{C(S,\bar{S})}{d(S)}$$

Matrix Representation

$$W = \begin{bmatrix} 0 & & & \\ & \ddots & w_{ji} & \\ & w_{ij} & \ddots & \\ & & & 0 \end{bmatrix}$$

$$Q = \begin{bmatrix} q_1 & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \vdots \\ \vdots & 0 & q_i & 0 \\ 0 & \cdots & 0 & q_n \end{bmatrix}$$

$$D = \begin{bmatrix} \sum_{\{i=1|[i,j]\in E\}} w_{ij} & 0 & \cdots & 0 \\ 0 & \ddots & 0 & \vdots \\ \vdots & 0 & \sum_{\{i|[i,j]\in E\}} w_{ij} & 0 \\ 0 & \cdots & 0 & \sum_{\{i=n|[i,j]\in E\}} w_{ij} \end{bmatrix}$$

The Laplacian Matrix $\mathcal{L} = D - W$

Two-terms forms of the problems:

Expander
s-normalized

$$\min_{\substack{\emptyset \neq S \subset V \\ S \neq V}} \frac{C(S,\bar{S})}{|S|} + \frac{C(S,\bar{S})}{|\bar{S}|}$$

Cheeger constant
Normalized Cut

$$\min_{\substack{\emptyset \neq S \subset V \\ S \neq V}} \frac{C(S,\bar{S})}{d(S)} + \frac{C(S,\bar{S})}{d(\bar{S})}$$

Half-q-normalized
q-normalized

$$\min_{\substack{\emptyset \neq S \subset V \\ S \neq V}} \frac{C(S,\bar{S})}{q(S)} + \frac{C(S,\bar{S})}{q(\bar{S})}$$

Single and two-term forms are within a factor of 2:

Expander $\leftrightarrow$ S-normalized

$$\frac{1}{2}(S-normalized) \le Expander \le (S-normalized)$$

Cheeger $\leftrightarrow$ Normalized Cut

$$\frac{1}{2}(NC) \le Cheeger \le (NC)$$

Half-q-normalized $\leftrightarrow$ q-normalized

$$\frac{1}{2}(q-normalized) \le half-q-normalized \le (q-normalized)$$

Two terms expressions and the Rayleigh ratio (Lemma 3.1, [H13])

Lemma 1

$$\min_{\emptyset \neq S \subset V} \frac{C(S,\bar{S})}{q(S)} + \frac{C(S,\bar{S})}{q(\bar{S})} = \min_{\substack{y^T Q\vec{1}=0 \\ y_i \in \{-b,1\}}} \frac{y^T \overbrace{(D-W)}^{\mathcal{L}} y}{y^T Q y}$$

A special case of this was shown by Shi and Malik, for q(S)=d(S).

The combinatorial versus the spectral continuous relaxations

$$(RRP) \quad \min \frac{y^T \mathcal{L} y}{y^T Q y}$$

~~$Y^T Q \vec{1} = 0$~~

~~$y_i \in \{-b, 1\}$~~

Combinatorial relaxation of Raleigh ratio Problem

The spectral method

An optimal solution is achieved for $\mathcal{L}y = \lambda Q y$

Where λ is the smallest non-zero eigenvalue (Fiedler Eigenvalue). We solve for the eigenvector z:

$$\left(Q^{-1/2}\mathcal{L}Q^{-1/2}\right)z = \lambda z$$

and set $y = Q^{-1/2}z$ which solves the continuous relaxation.

Solving the combinatorial relaxation

$$y_i = \begin{cases} 1 & i \in S \\ -b & otherwise \end{cases}$$

The combinatorial relaxation Rayleigh problem

Lemma 2:

$$\alpha(b) = \min_{y\in\{-b,1\}} \frac{y^T(D-W)y}{y^TQy} = \min_{\emptyset\neq S\subset V} \frac{(1+b)^2 C(S,\bar{S})}{q(S)+b^2 q(\bar{S})}$$

For all b,

Two - term $\geq \alpha$(b)

Single - term $\geq \dfrac{\alpha(\mathrm{b})}{2}$

$$(S-normalized),(NC),(q-normalized)\geq \alpha(b)$$

$$Expander, Cheeger, \text{half - q - normalized} \geq \frac{\alpha(b)}{2}$$

Recall Lemma 1:

$$\min_{\substack{y^TQ\vec{1}=0,\\ y\in\{-b,1\}}} \frac{y^T(D-W)y}{y^TQy} = \min_{\emptyset\neq S\subset V} \frac{C(S,\bar{S})}{q(S)} + \frac{C(S,\bar{S})}{q(\bar{S})}$$

Solving the combinatorial Rayleigh problem optimally

- The problem is a ratio problem

General technique for ratio Problems: **The λ-question**

$$\min_{x \in F} \frac{f(x)}{g(x)} < \lambda\ ?$$

can be solved if one can solve the following λ-question:

$$f(x) - \lambda g(x) < 0\ ?$$

*This λ is unrelated to an eigenvector –just a parameter

Solving the λ-question

- The λ-question of whether the value of RRP is less than λ is equivalent to determining whether:

$$\min_{y_i \in \{-b.1\}} y^T(D-W)y - \lambda y^T Q y < 0\,?$$

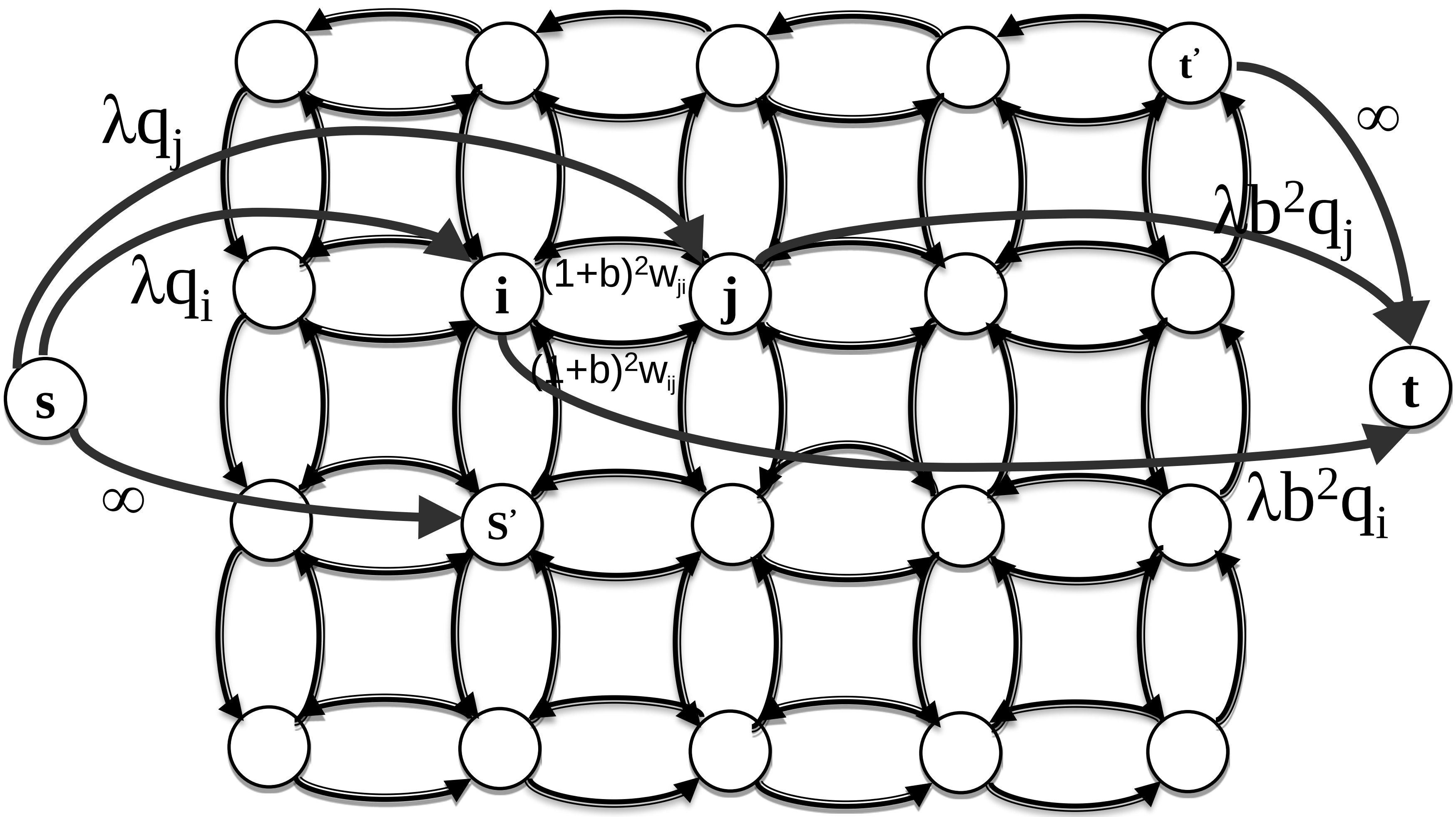
$$\Downarrow \text{OR (from Lemma 1)} \Downarrow$$

Linearized Rayleigh ratio problem (RRP)

$$\left\{\min_{s \subset V} (1+b)^2 C(S,\bar{S}) - \lambda\left[q(S) + b^2 q(\bar{S})\right]\right\} < 0\,?$$

The graph G_{st} for testing the λ-question

(looks arbitrary, but not to worry - it works, as shown next)



It works because the problem can be formulated as "monotone integer program"

Theorem

The source set of a minimum cut in the graph G_{ST} is an optimal solution to the linearized (RRP) (here $T = \bar{S}$)

Proof

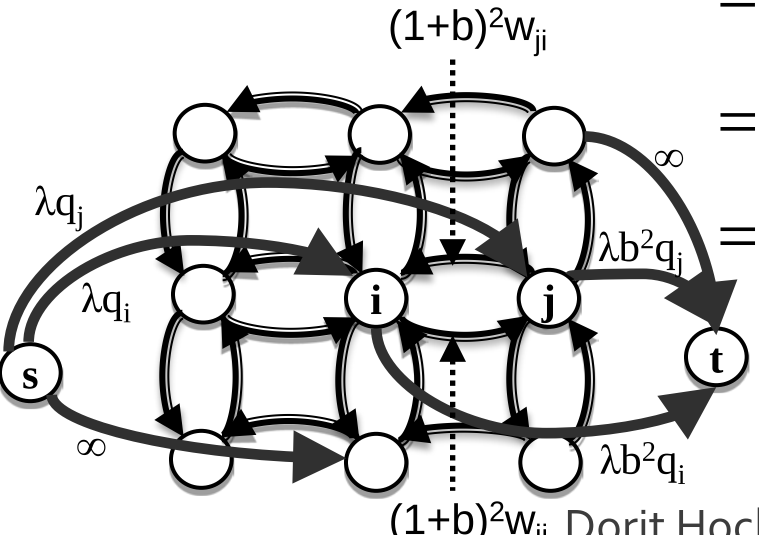
$$C(S \cup \{s\}, T \cup \{t\}) = \lambda q(T) + \lambda b^2 q(S) + C(S,T) =$$

$$= \lambda(1+b^2)q(V) - \lambda q(S) - \lambda b^2 q(T) + C(S,T) =$$

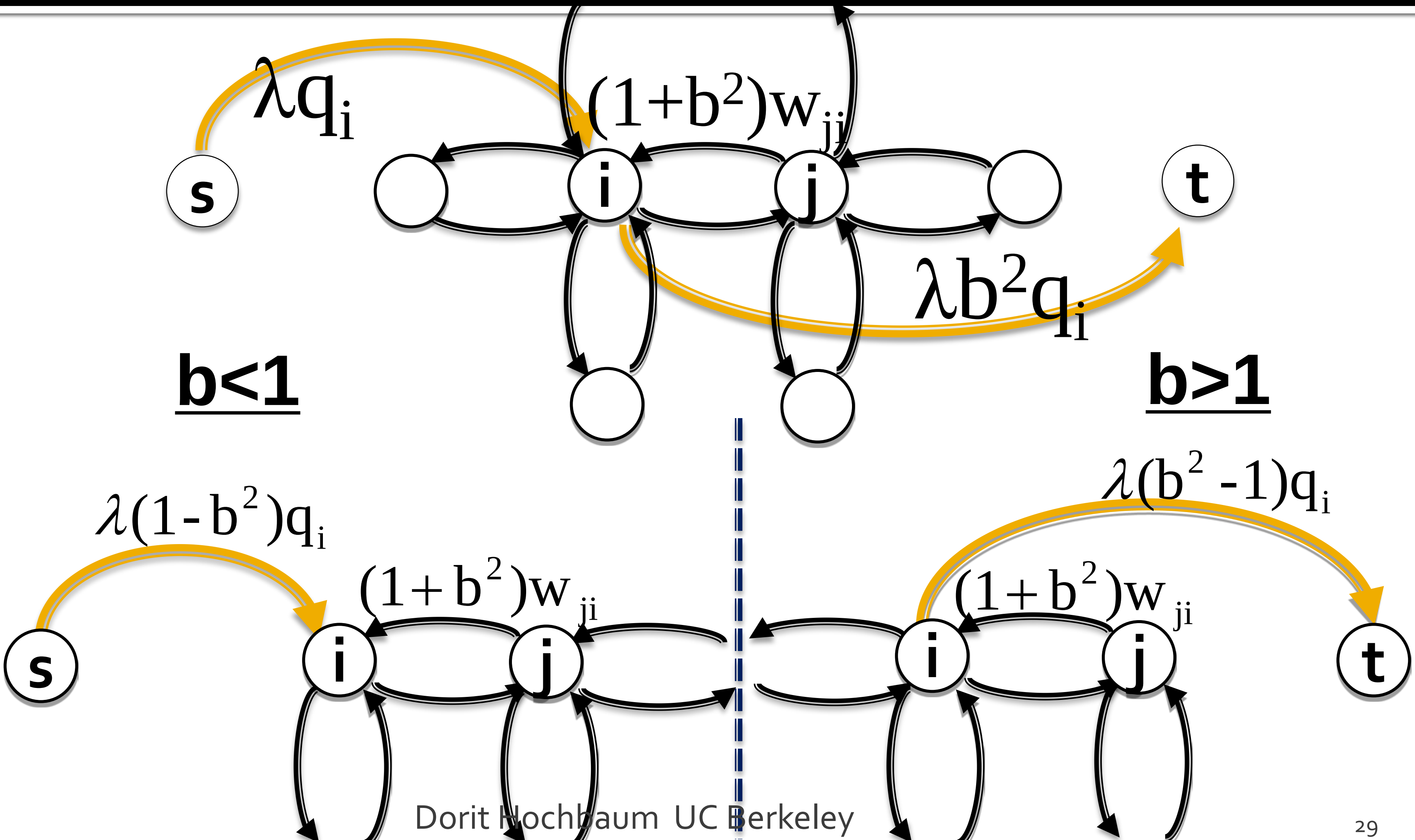
$$= \text{const} - \lambda q(S) - \lambda b^2 q(T) + C(S,T) =$$

$$= \text{const} + C(S,T) - \lambda[q(S) + b^2 q(T)] =$$

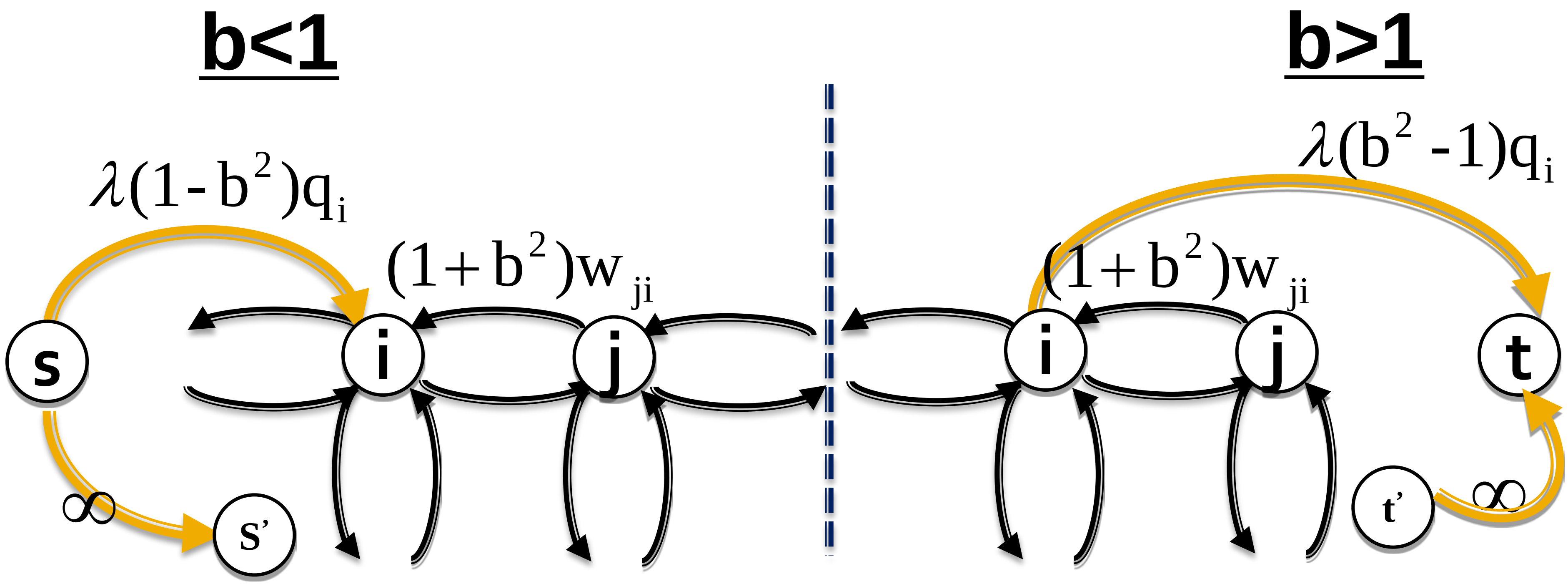
$$= \text{const} + (RRP)$$



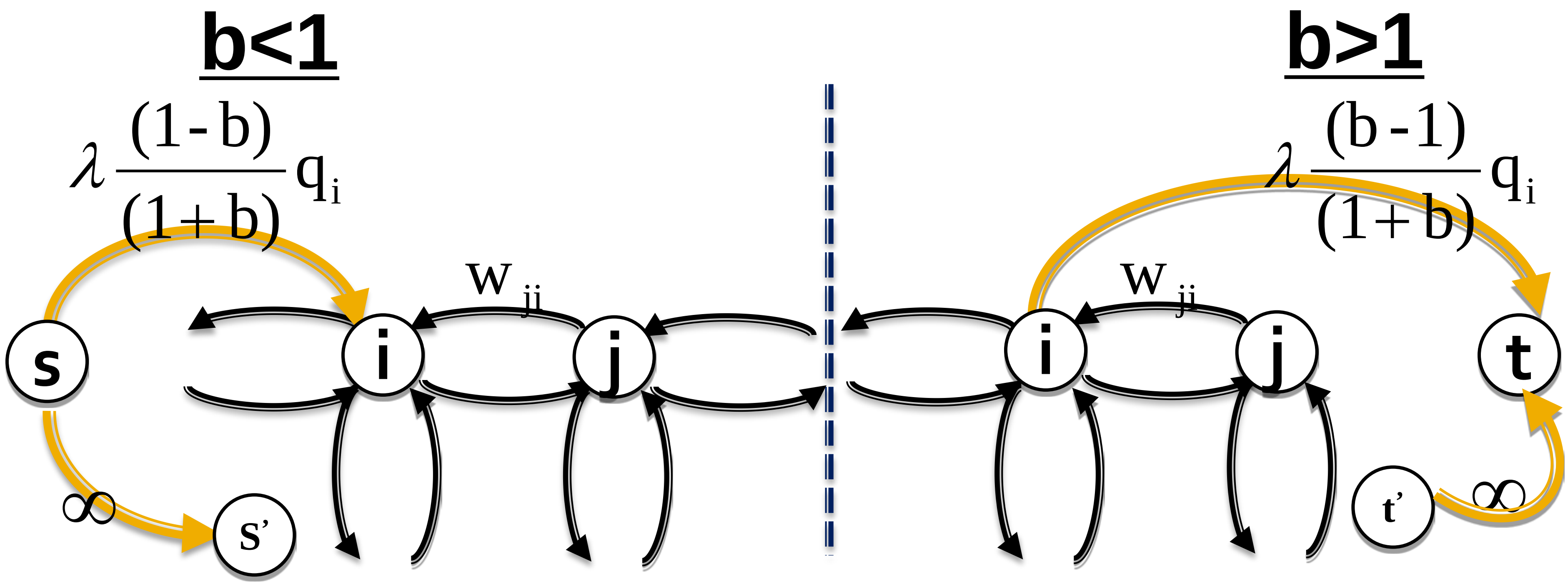
Simplifying the graph



Scaling arcs weights

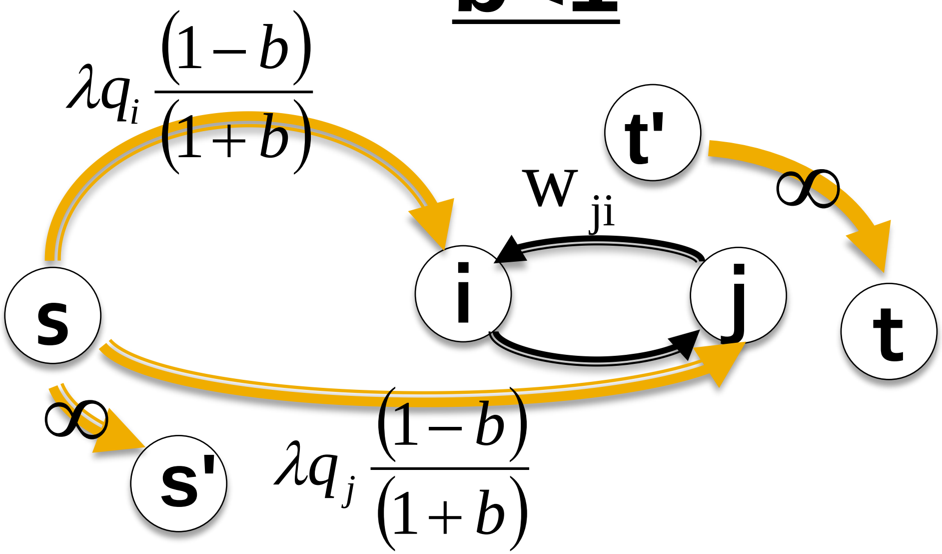


Scaling arcs weights

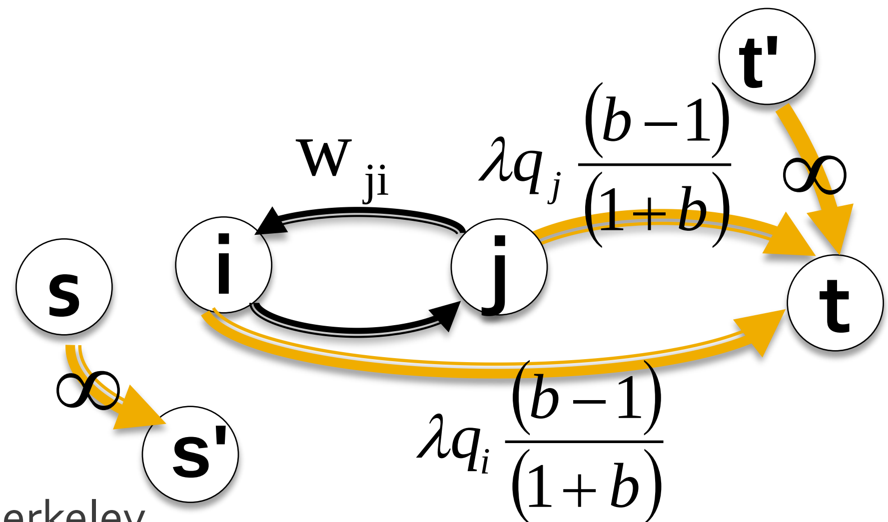


The Simplified equivalent graph

b<1



b>1



Solving the parametric min st cut

- The problem is a ***parametric*** cut problem: This is a graph setup when source adjacent arcs are monotone nondecreasing and sink adjacent are monotone nonincreasing (for b<1) with the parameter.
- A parametric cut problem can be solved in the complexity of a single minimum cut (plus finding the zero of n monotone functions) [GGT89], [H08].
- Here we let the parameter be β

$$\beta = \begin{cases} \lambda \dfrac{1-b}{1+b} & b < 1 \\ \lambda \dfrac{b-1}{1+b} & b \geq 1 \end{cases}$$

In G_{st}

- The cut problem in the graph G_{st}, as a function of β is parametric (the capacities are linear in the parameter on one side and independent of it on the other).
- In a parametric graph the sequence of source sets of cuts for increasing source-adjacent capacities is ***nested***.
- There are no more than n breakpoints for β.
- There are k≤n nested source sets of minimum cuts.

Solving for all values of b efficiently

- For

$$\beta = \begin{cases} \lambda \dfrac{1-b}{1+b} & b<1 \\ \lambda \dfrac{b-1}{1+b} & b \geq 1 \end{cases}$$

- Given the values of β at the breakpoints, we can generate, for each value of b, *all* the breakpoints.
- Consequently, by solving once the parametric problem for β we obtain simultaneously, *all the breakpoint solutions for all b*, in the complexity of a single minimum cut.
- To solve for the minimum ratio: For each b we find the last (largest value) breakpoint where the objective value <0.

Recall problem NC'

$$\min_{S \subset V} \frac{C(S, \bar{S})}{C(S, S)}$$

It has the same solution as

$$\min_{S \subset V} \frac{C(S, \bar{S})}{d(S)} = \alpha(0)$$

Comparison between NC' and the spectral method

$$NC = 35 \cdot 10^{-4}$$

$$NC = 1.702 \cdot 10^{-4}$$

Original image **Eigenvector result** **NC' result**

Another comparison

$NC = 127 \cdot 10^{-4}$

$NC = 1.466 \cdot 10^{-4}$

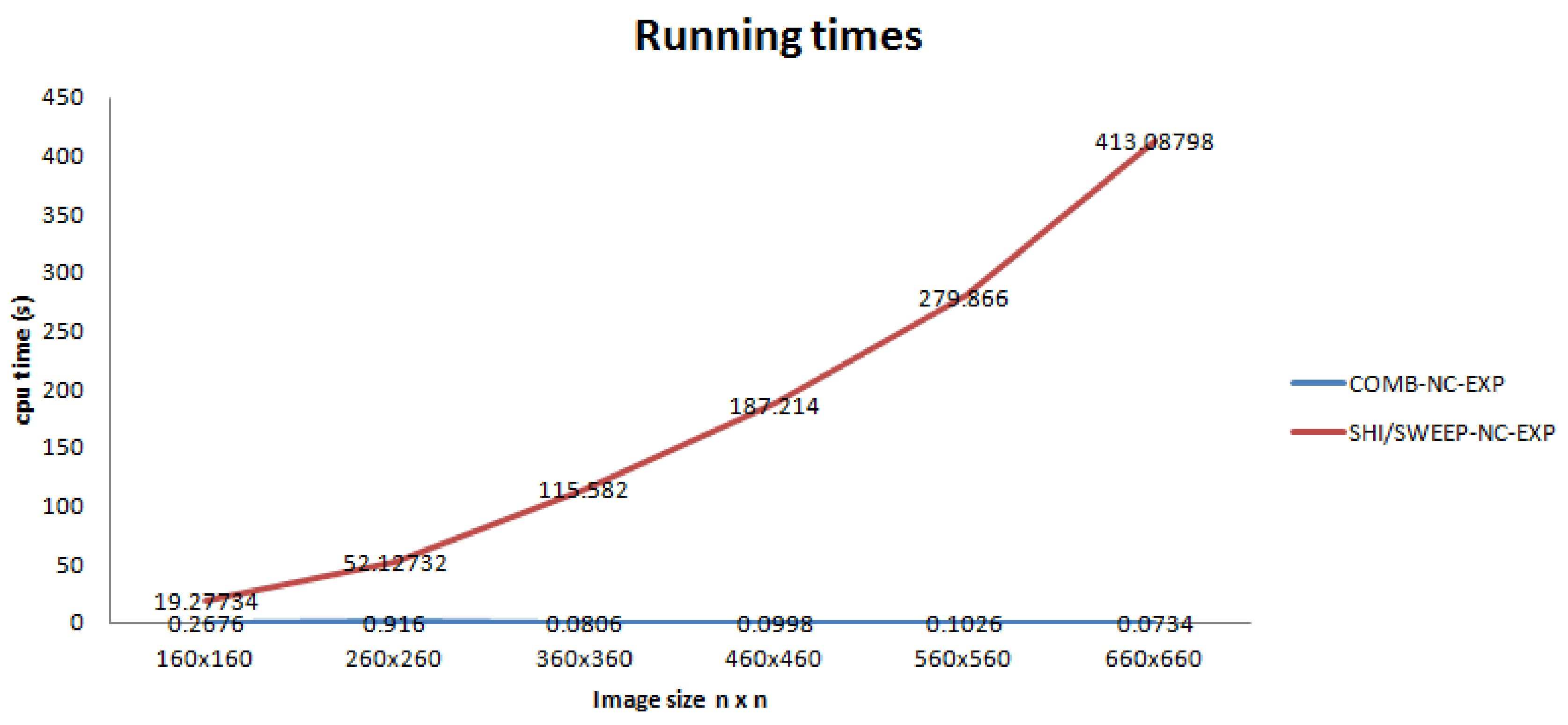
Original image **Eigenvector result** **NC' result**

Empirical testing for the general problems

- For normalized cut d_i is the sum of similarity weights.
- For q-normalized cut, there are, in addition to similarity weights defining the Laplacian, also node weights determined by entropy.
- Exponential similarity weights are applied.
- Total of 20 cases tested.
- Size of images is small due to spectral method software limitations.

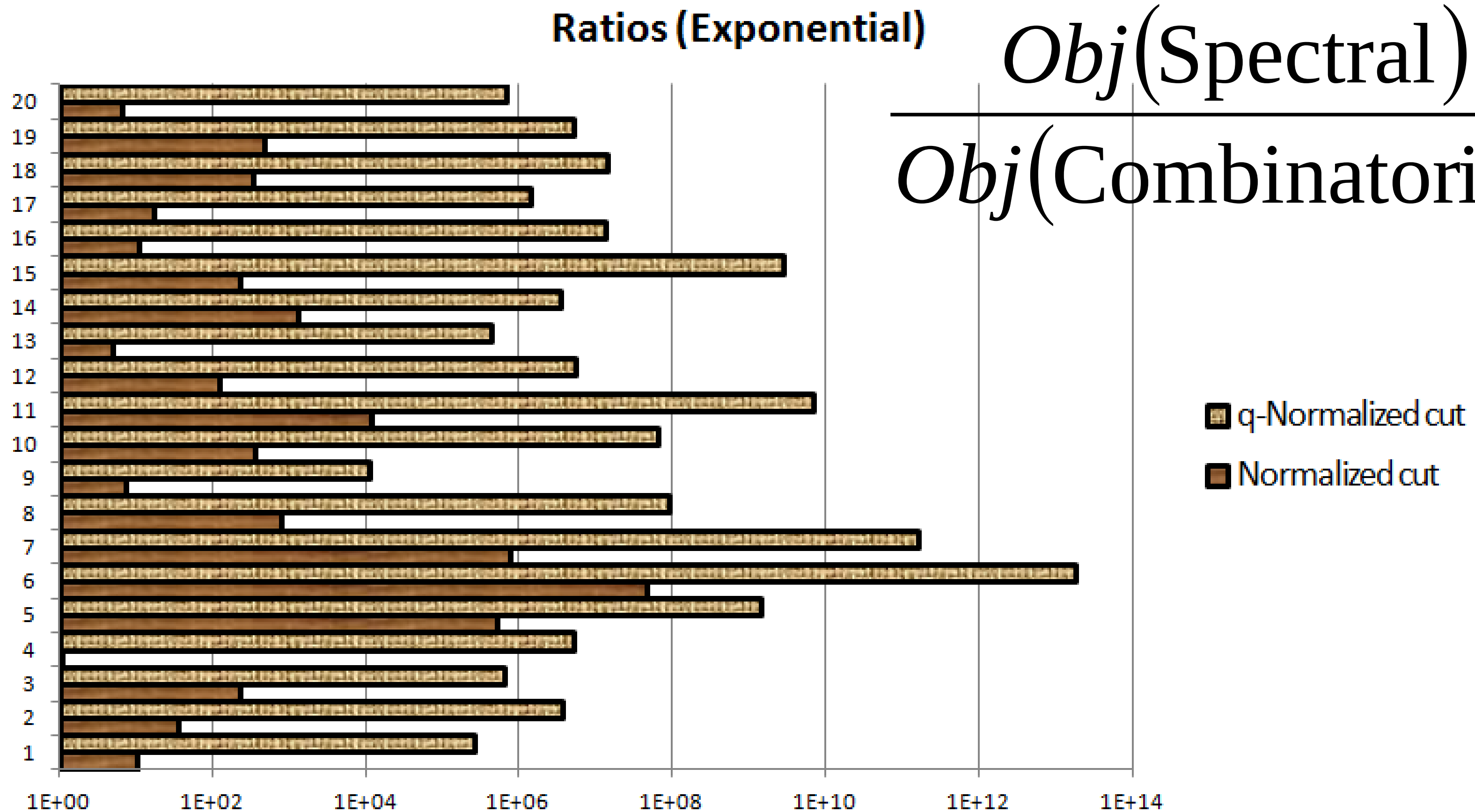
The 20 images

Scalability of NC' versus the spectral algorithm (Shi)



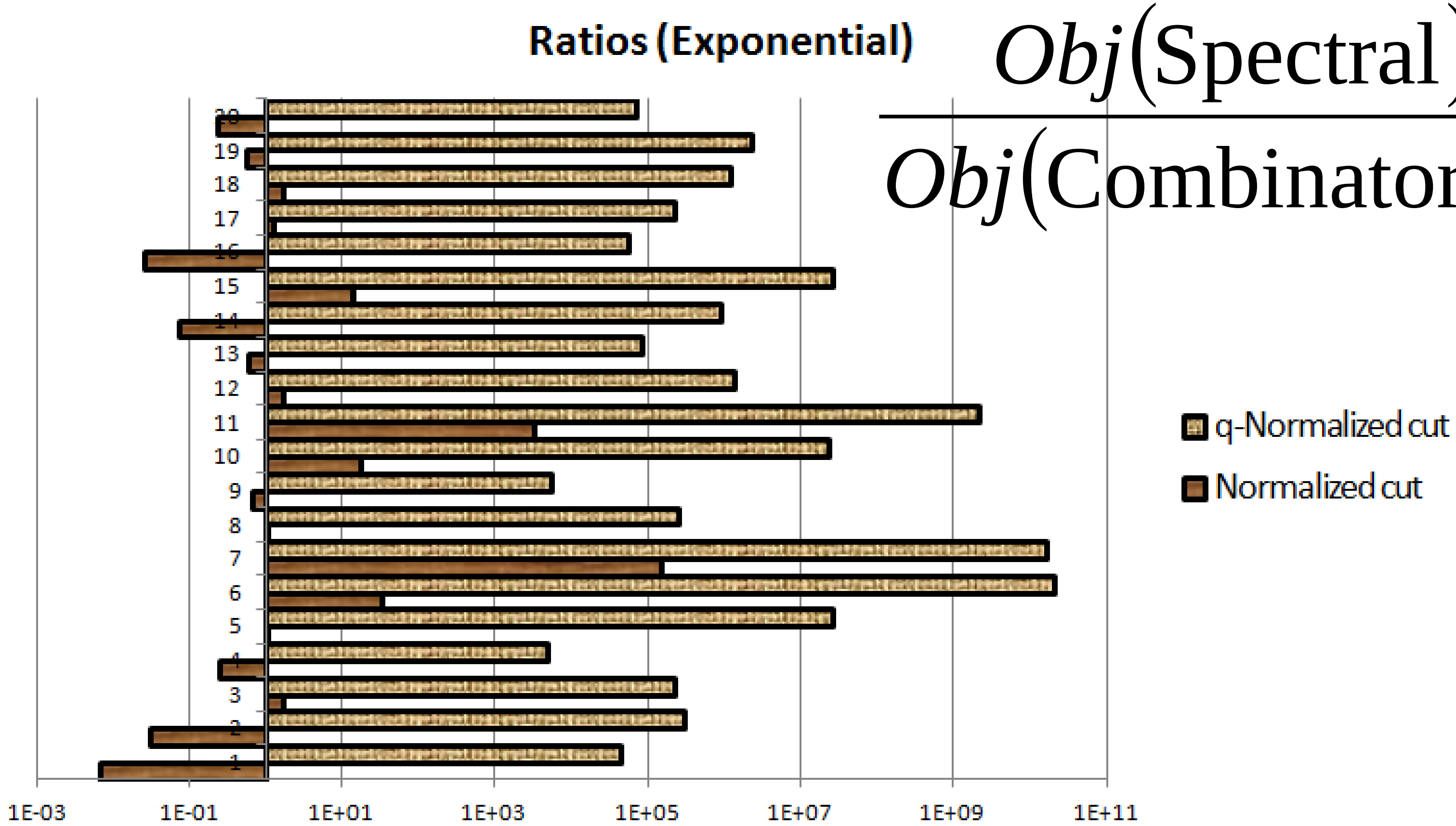
A comparison of NC values of NC' with the spectral algorithm

$$\frac{Obj(\text{Spectral})}{Obj(\text{Combinatorial})}$$



A comparison of NC values of NC' with the sweep spectral algorithm

$$\frac{Obj(\text{Spectral})}{Obj(\text{Combinatorial})}$$



The performance for spectral sweep [H,Cheng, Bertelli13]

For h_G the Cheeger Constant, λ_1 the Fielder eigenvalue,

$$\frac{\lambda_1}{2} \leq h_G \leq \sqrt{2\lambda_1}. \tag{1}$$

The proof of the second inequality of the above bound, introduces a bipartition generated by applying the spectral sweep technique to the Fiedler eigenvector to find a lowest value bipartition for the Cheeger constant's objective. Let the Cheeger constant objective value for this bipartition be denoted by h_{SWEEP}, then at best the sweep solution has the same upper bound as the optimal solution:

$$h_G \leq h_{SWEEP} \leq \sqrt{2\lambda_1} \leq 2\sqrt{h_G}. \tag{2}$$

For NC_{SWEEP} be the lowest value of a bipartition for the normalized cut objective, generated by the spectral sweep technique on the Fiedler eigenvector in the spectral method. (Note: NC_{SWEEP} and h_{SWEEP} may not correspond to the same bipartition.) Let $NC(h_{SWEEP})$ be the objective value of normalized cut for the bipartition that generates the value of h_{SWEEP}, then the following inequality holds

$$NC_{SWEEP} \leq NC(h_{SWEEP}) \leq 2h_{SWEEP}, \quad (3)$$

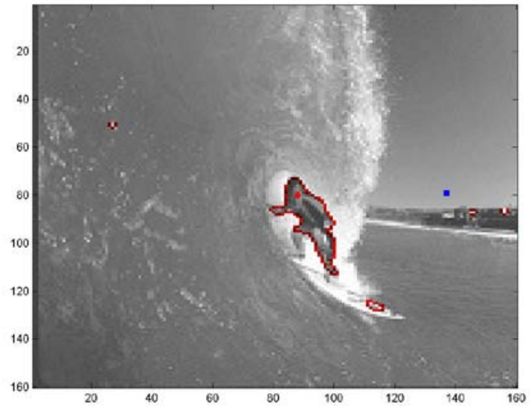
Combining $h_{SWEEP} \leq 2\sqrt{h_G}$ from (2) with (3),

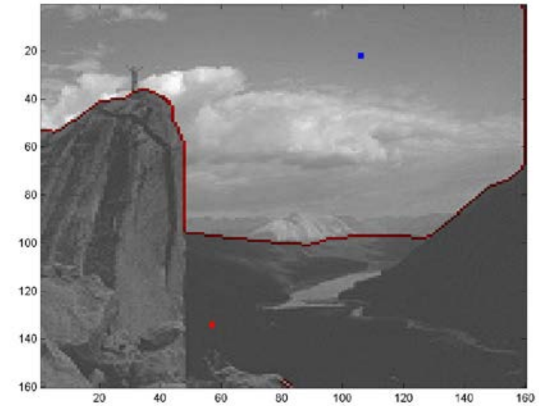
$$NC_{SWEEP} \leq 2h_{SWEEP} \leq 4\sqrt{h_G} \leq 4\sqrt{NC_G} \leq 4\sqrt{NC_{NC'}}.$$

Subjective Visual Segmentation Quality Comparison

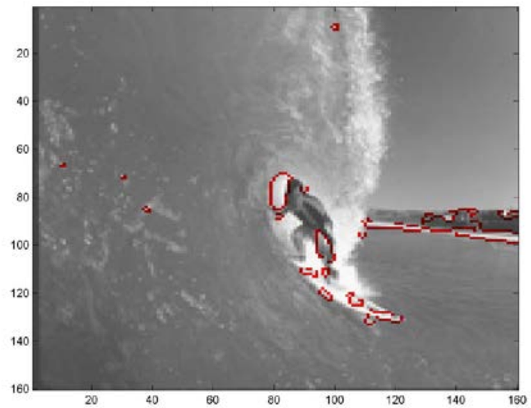
- Normalized Cut

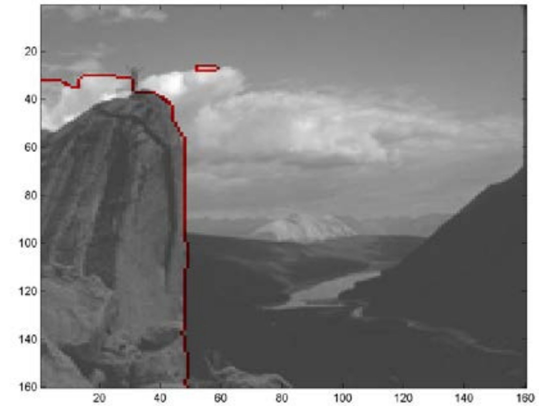
Combinatorial





Spectral

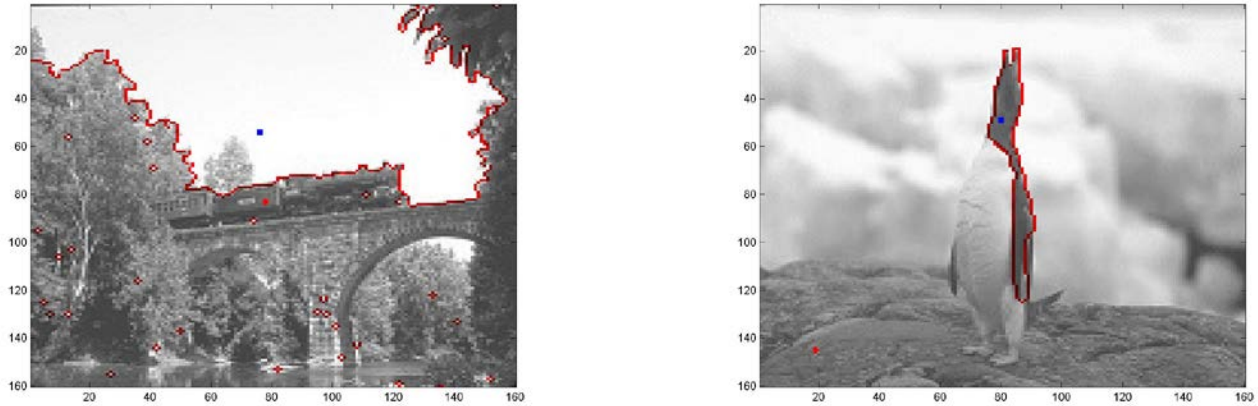




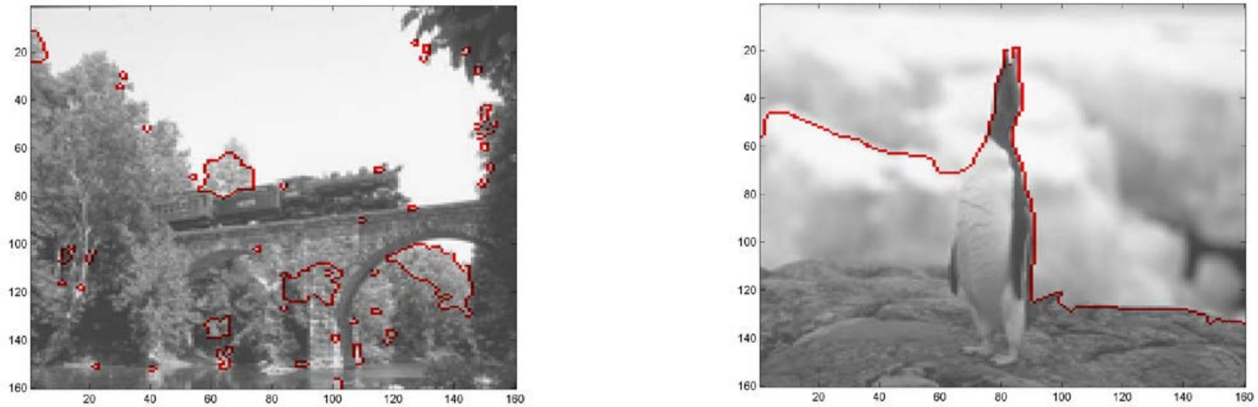
Subjective Visual Segmentation Quality Comparison (cont.)

- Normalized Cut (cont.)

Combinatorial



Spectral

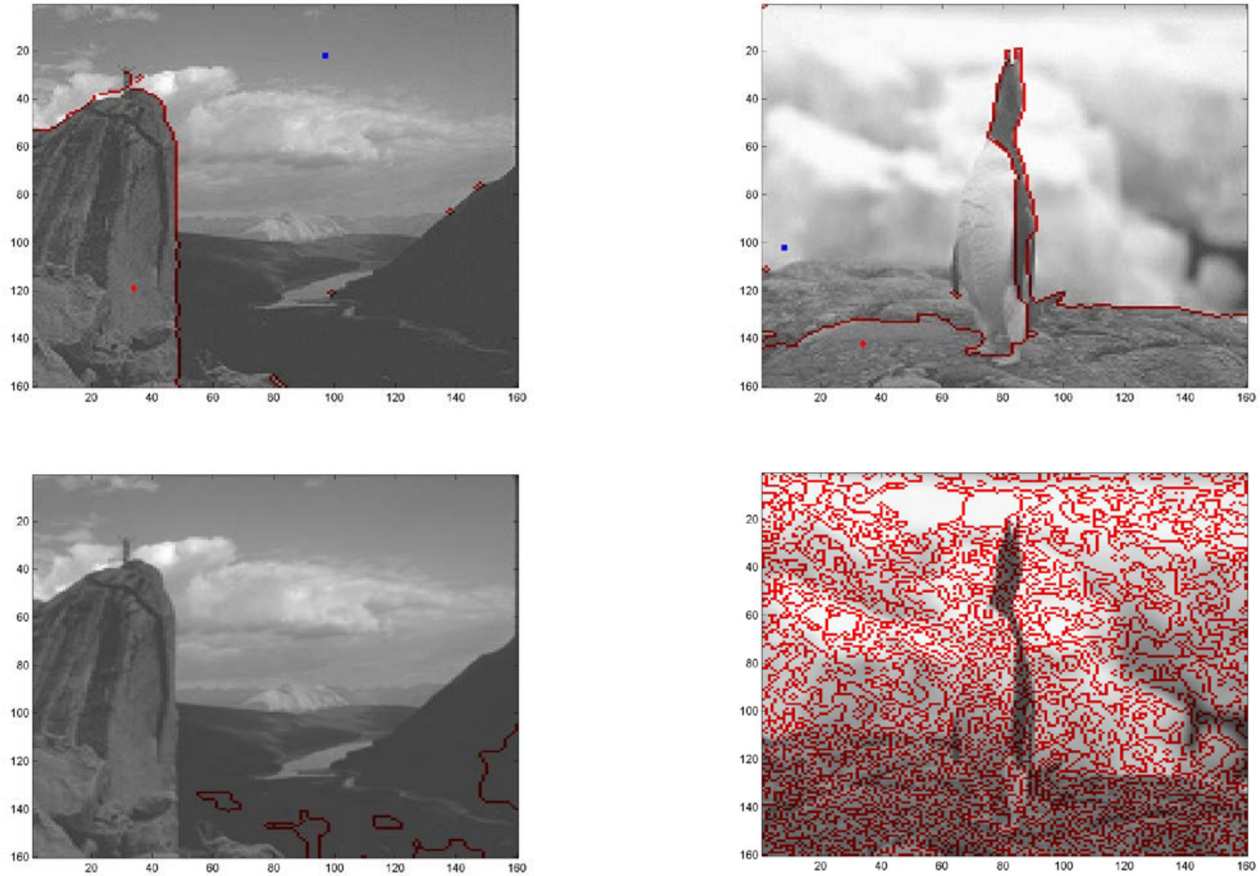


Subjective Visual Segmentation Quality Comparison (cont.)

- q-Normalized Cut (Entropy)

Combinatorial

Spectral



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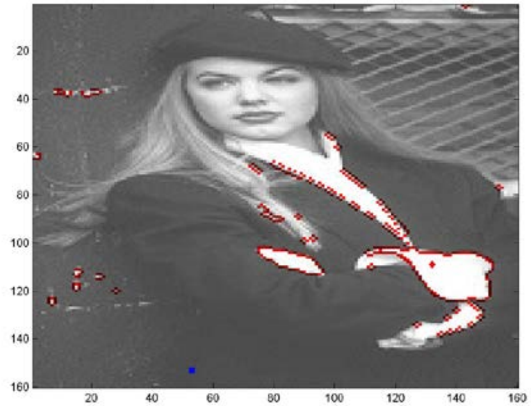
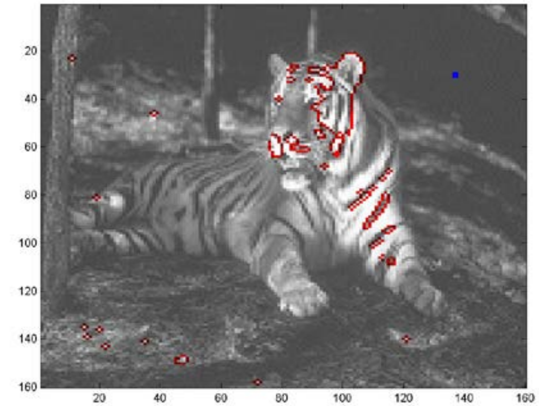
Subjective Visual Segmentation Quality Comparison (cont.)

- q-Normalized Cut (Entropy) (cont.)

Combinatorial



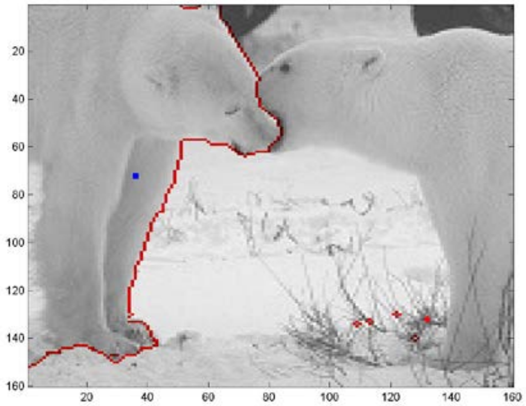


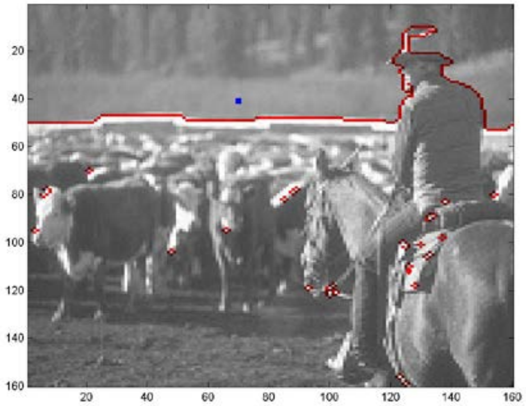
Spectral

The benefit of nested cuts in providing better segmentation quality

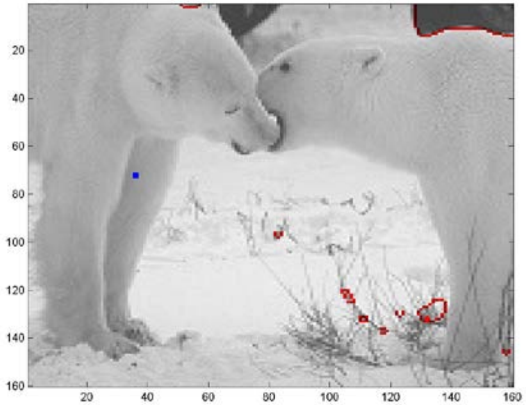
- Normalized Cut

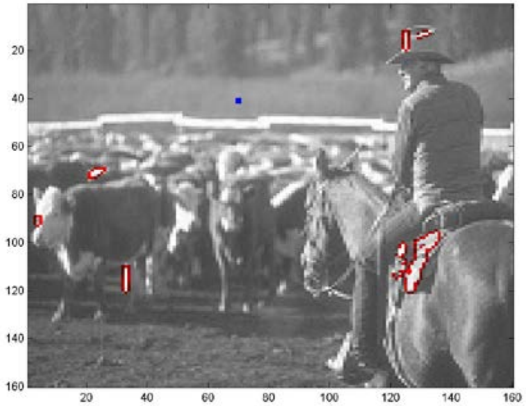
Cut presenting subjectively better visual segmentation





Cut minimizing objective function value

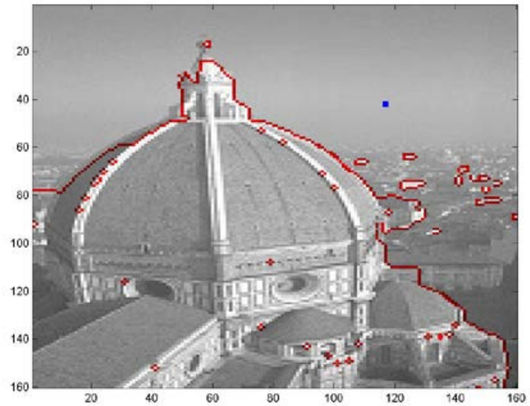


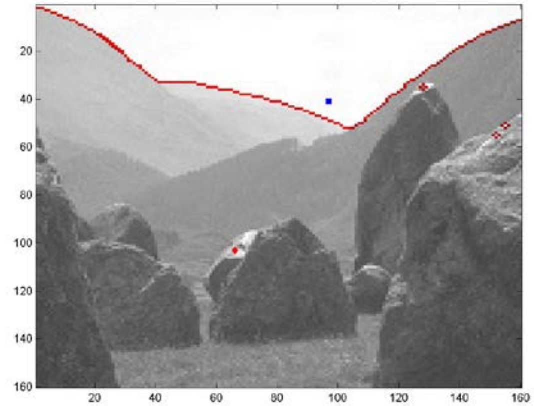


The benefit of nested cuts in providing better segmentation quality (cont.)

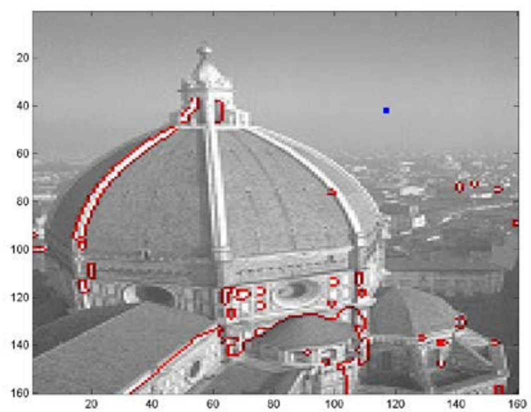
- Normalized Cut (cont.)

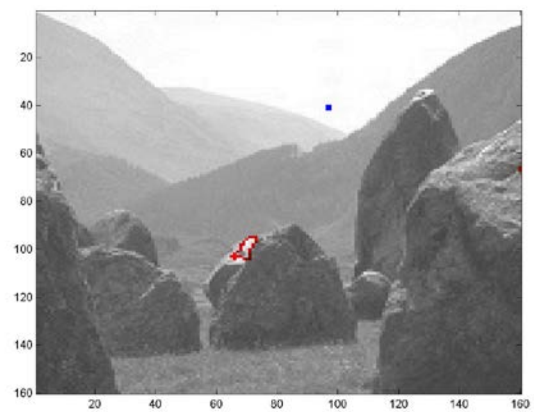
Cut presenting subjectively better visual segmentation





Cut minimizing objective function value



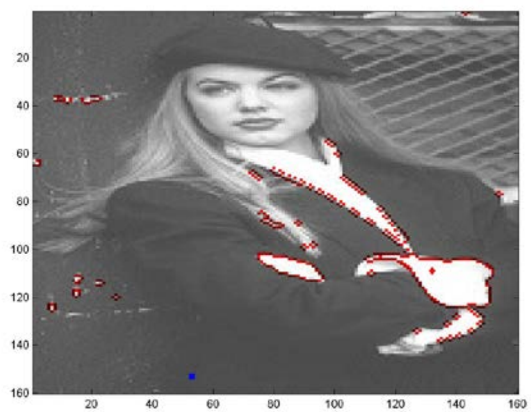


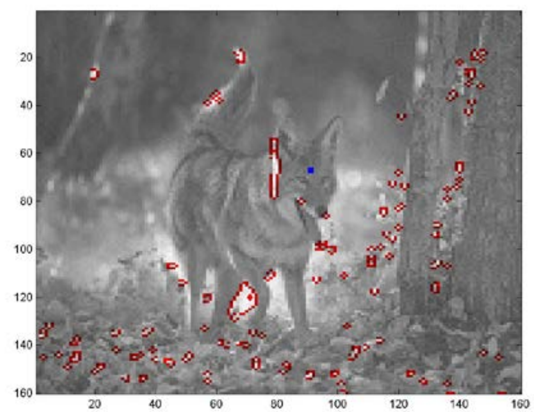
The benefit of nested cuts in providing better segmentation quality (cont.)

- q-Normalized Cut (Entropy)

Cut presenting subjectively better visual segmentation

Cut minimizing objective function value

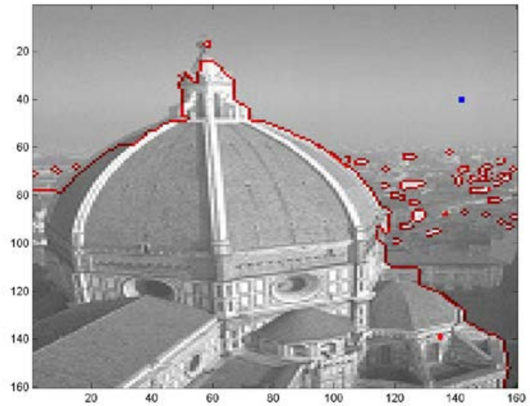


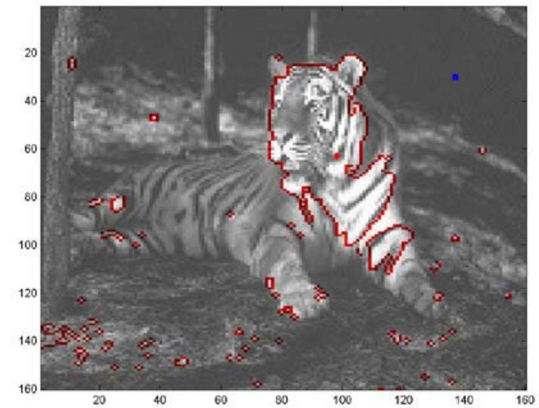


The benefit of nested cut in providing better segmentation quality (cont.)

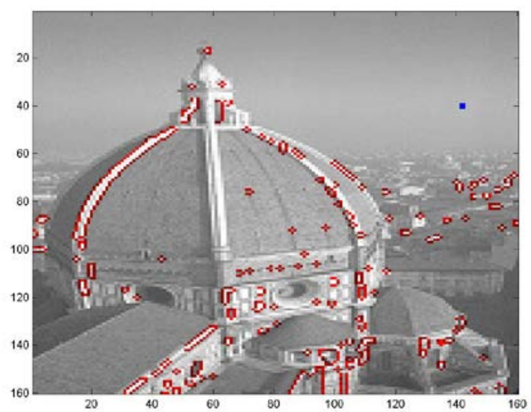
- q-Normalized Cut (Entropy) (cont.)

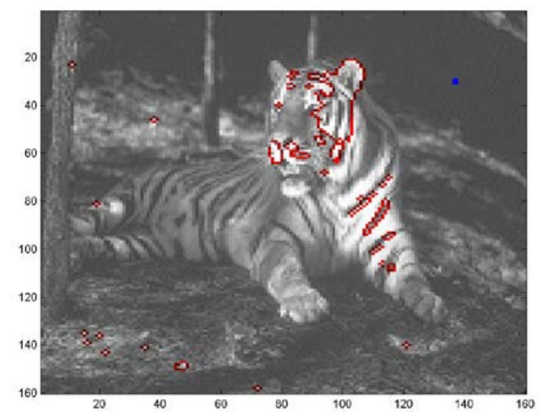
Cut presenting subjectively better visual segmentation





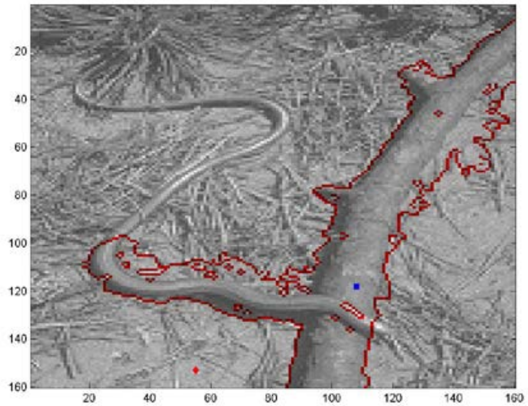
Cut minimizing objective function value

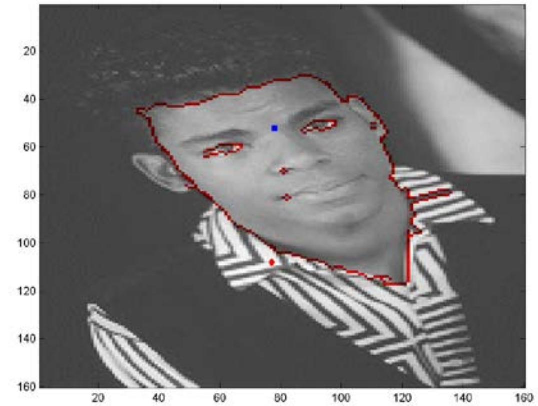




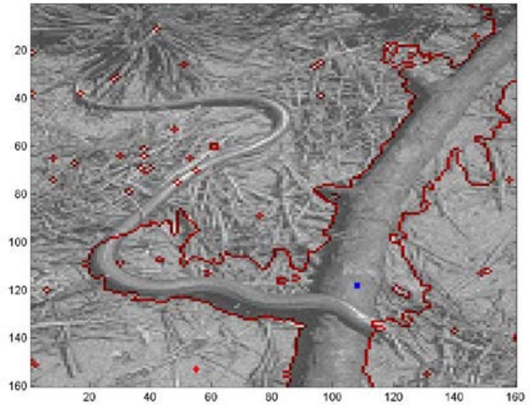
The benefit of defining node weights as entropy

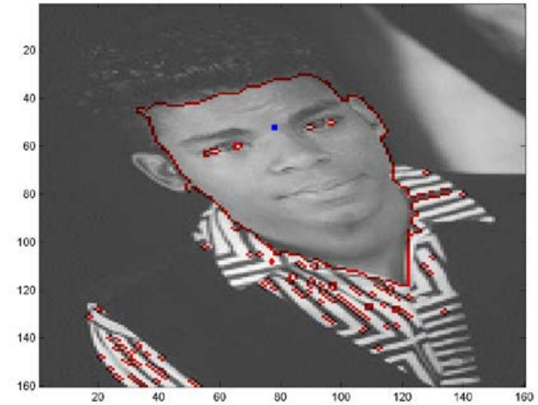
Cut presenting subjectively best visual segmentation using q-normalized cut





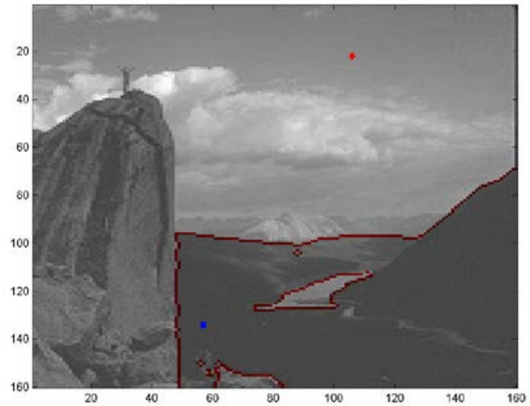
Cut presenting subjectively best visual segmentation using normalized cut





The benefit of defining node weights as entropy (cont.)

Cut presenting subjectively best visual segmentation using q-normalized cut



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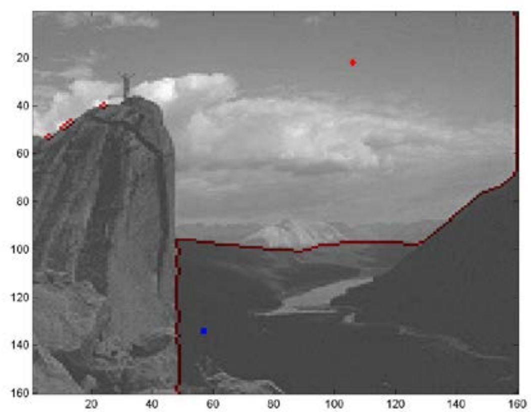

Conclusions

- The combinatorial technique provides better visual results in image segmentation.
- The combinatorial technique is faster than the spectral method (and requires substantially less storage)
- The combinatorial technique gives, on average, better quality solutions to several clustering problems.
- We used $$\min_{S \subset V} \frac{C_1(S,\bar{S})}{C_2(S,S)}$$ for: gene expression; knee cartilage volume computation (OA); pattern recognition; video tracking; enhancing nuclear detectors capabilities; drug efficacy studies, and general data mining.

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Questions

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Lemma 1's Proof

- Proof:

$$y_i = \begin{cases} 1 & \text{if } i \in S \\ -b & \text{if } i \in T = \bar{S} \end{cases}$$

$$y^T Q y = q(S) + b^2 q(T) \qquad y^T Q \mathbf{1} = 0 \Leftrightarrow b = \frac{q(S)}{q(T)}$$

$$y^T \mathcal{L} y = y^T D y - y^T W y$$

$$= \sum_{i \in S} d_i + b^2 \sum_{i \in \bar{S}} d_i - [C(S,S) - 2bC(S,\bar{S}) + b^2 C(\bar{S},\bar{S})]$$

$$= C(S,S) + C(S,\bar{S}) + b^2 C(S,\bar{S}) + b^2 C(\bar{S},\bar{S})$$

$$-[C(S,S) - 2bC(S,\bar{S}) + b^2 C(\bar{S},\bar{S})]$$

$$= (1 + b^2 + 2b) C(S,\bar{S}) = (1+b)^2 C(S,\bar{S})$$

Lemma 1's Proof

$$y^T \mathcal{L} y = (1+b)^2 C(S,\bar{S}) \qquad y^T Q y = q(S) + b^2 q(T)$$

$$\min_{\substack{y^T Q \vec{1}=0 \\ y\in\{-b,1\}}} \frac{y^T \mathcal{L} y}{y^T Q y} = \min_{\substack{y^T Q \vec{1}=0 \\ S\subset V}} \frac{(1+b)^2 C(S,\bar{S})}{q(S)+b^2 q(\bar{S})}$$

$$y^T Q \mathbf{1} = 0 \Leftrightarrow b = \frac{q(S)}{q(T)}$$

$$\frac{(1+b)^2 C(S,\bar{S})}{q(S)+b^2 q(\bar{S})} = \frac{(1+\frac{q(S)}{q(\bar{S})})^2 C(S,\bar{S})}{q(S)+(\frac{q(S)}{q(\bar{S})})^2 q(\bar{S})} = \frac{(1+\frac{q(S)}{q(\bar{S})})^2 C(S,\bar{S})}{q(S)(1+\frac{q(S)}{q(\bar{S})})}$$

$$= \frac{(1+\frac{q(S)}{q(\bar{S})}) C(S,\bar{S})}{q(S)}.$$

Lemma 1's proof

$$\min_{\substack{y^T Q \vec{1}=0 \\ y\in\{-b,1\}}} \frac{y^T \mathcal{L} y}{y^T Q y} = \min_{S\subset V} C(S,\bar{S})[\frac{1}{q(S)} + \frac{1}{q(\bar{S})}]$$

$\square$