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Representative Subgraph Sampling using MCMC Methods

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Graphs are growing...

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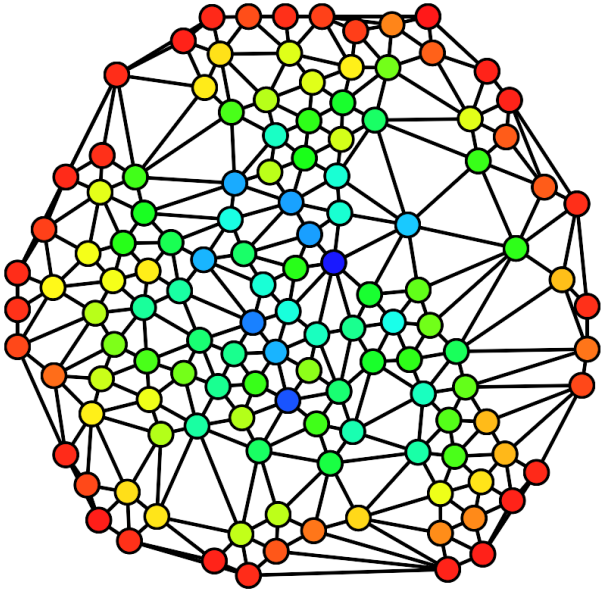
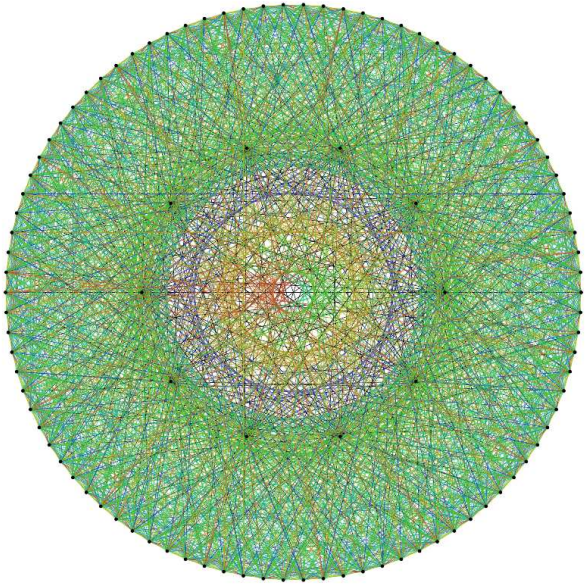
Increase in graph sizes

- Classic chemoinformatics: dozens of nodes
- Systems biology: thousands of nodes
- Internet and online communities: hundreds of thousands and millions of nodes





Graph size is a challenge

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Algorithmic challenge

- Basic operations on graphs are expensive:
  - graph isomorphism: Checking identity of two graphs
  - subgraph isomorphism: Checking if graph G includes graph S
- No polynomial runtime algorithm (in the number of nodes n) is known for any of these basic operations
- As a consequence, runtime for all algorithms that use these basic operations scales exponentially with the size of the graph

Potential solutions

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Make your algorithms more efficient

- look at special subclasses of graphs
- treat graphs as sets
- map graphs to feature vectors

Make your graphs smaller

- find a smaller graph S that preserves key characteristics of the original graph G.
- Strategy 1: generate S synthetically
- Strategy 2: sample S from G
- Strategy 2 is the topic of this talk.

Related work I

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Random Node Selection (Leskovec & Faloutsos, 2006)

- Randomly pick n' nodes from the graph
- Different Variants:
  - Uniform random sampling
  - Sampling according to PageRank weight
  - Sampling according to node degree

Random Edge Selection

- Randomly pick edges from the graph
  - Uniform random sampling
  - Pick combinations of nodes and edges
  - Combination of both

Related work II

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Sampling by exploration

- Different variants of picking a node randomly and then exploring its neighborhood
- Forest Fire
  - randomly pick a node v from the graph
  - randomly pick a random number x
  - select x neighbors of v: $w_1, \ldots, w_x$ (edges not visited before)
  - recursively repeat this for all $w_1, \ldots, w_x$
  - terminate when the desired number of nodes (n') nodes have been 'burnt'

State-of-the-art with respect to sample size: Good samples down to 15% of the original graph size

Optimisation problem

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Goal

- Optimal subgraph sample is

$$\text{argmin}_{|S|=n'} \Delta(\sigma(S), \sigma(G)) \tag{1}$$

- G is the original graph
- S the subgraph sample
- $\sigma(X)$ is a topological property of graph X
- Δ is a distance function on these topological properties
- n' is the desired size of the subgraph sample that has to be pre-specified

Metropolis graph sampling

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Algorithm

- Use Metropolis to search the space of subgraphs of G
- Initially pick one subgraph sample S with n' nodes randomly
- Iterate the following steps until convergence
  - Remove one node from S
  - Randomly add a new node to $S \rightarrow S'$
  - Compute the likelihood ratio $a = \frac{\varrho^*(S')}{\varrho^*(S)}$

    if $a \geq 1$: accept transition: $S := S'$
  - if $a < 1$: accept transition: $S := S'$ with probability a

    reject transition: $S := S$ with probability $1 - a$

How to define $\varrho^*(S)$ to get a 'good' subgraph sample?

Defining $\varrho^*(S)$

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Two roles

- ϱ is a probability distribution that Metropolis samples from (ϱ^* proportional to ϱ)
- ϱ^* shall reflect subgraph quality

Definition

- We define $\varrho^*(S)$ to be the inverse of a distance Δ between the sample S and the original graph G wrt to some graph property σ (to the power of p):

$$\varrho^*(S) := \frac{1}{\Delta_{G,\sigma}(S)^p} = \frac{1}{\Delta(\sigma(S), \sigma(G))^p}, \tag{2}$$

where $p \in \mathbb{R}^+$ and $p \gg 0$.

Chaining

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Strategy

- Observation: Good samples are often connected subgraphs
- Idea: Restrict search space to connected subgraphs
- Allow transition from S to S' only if S' is connected

Runtime

- Size of search space is reduced
- Additional check of connectivity is required for each transition

Simulated annealing

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Strategy (Kirkpatrick et al., 1983)

- Metropolis-variant for global optimization
- ϱ^* is controlled by temperature parameter T (in denominator):
- T slowly decreases to zero ('initially huge jumps, later on small steps')

We define the temperature-dependent density as

$$\varrho^*_{p,T}(S) = e^{\frac{\log \varrho^*_p(S)}{T}} = e^{log\Delta_{G,\sigma}(S)^{(-\frac{p}{T})}} = \Delta_{G,\sigma}(S)^{(-\frac{p}{T})}$$

so that a new acceptance-probability follows

$$a(S, S') = min(1, \frac{\varrho^*_{p,T}(S')}{\varrho^*_{p,T}(S)}) = min(1, (\frac{\Delta_{G,\sigma}(S)}{\Delta_{G,\sigma}(S')})^{\frac{p}{T}})$$

assuming a symmetric proposal distribution.

Experiments

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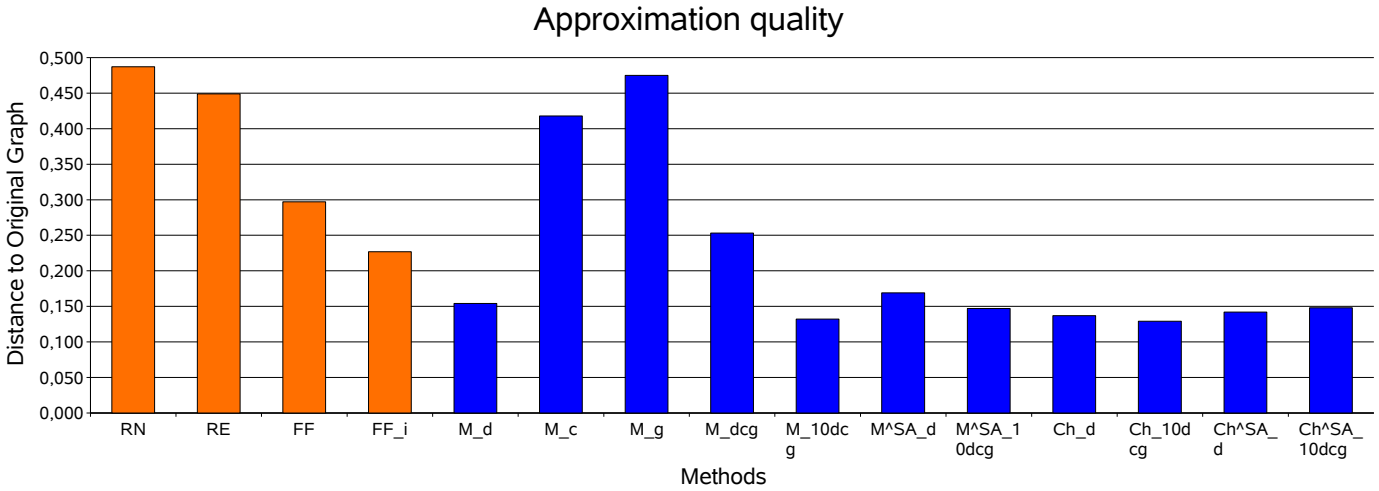
Setup

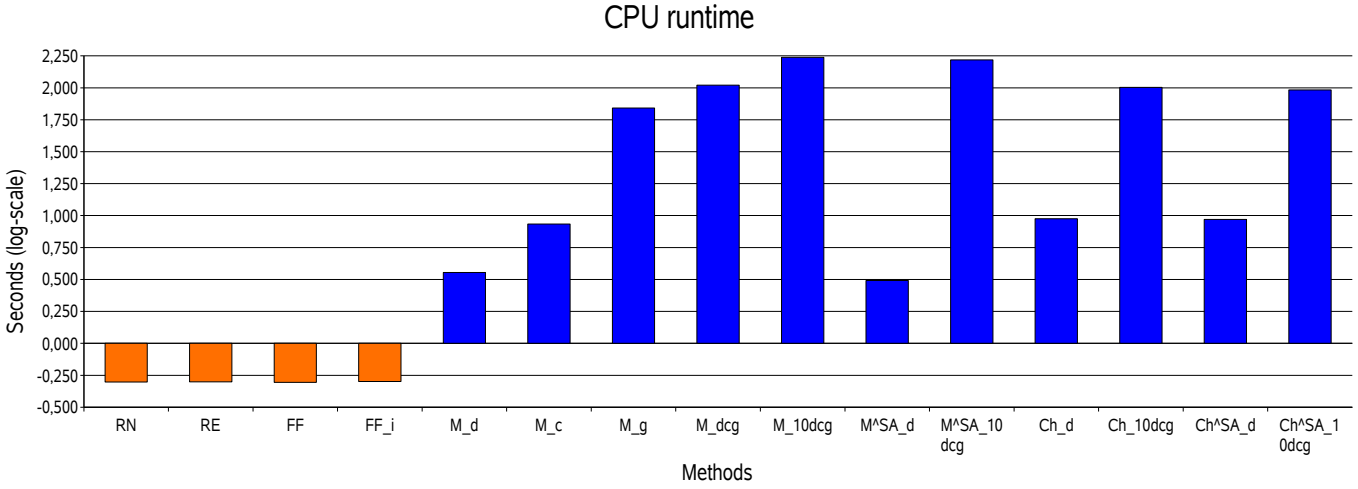
- Data: 5 datasets (329 to 75,879 nodes)
- Goal: Find representative subgraph with $n' = 100$ nodes
- Our Methods:
  - Metropolis M
  - Simulated Annealing SA
  - Chaining Ch
- Graph properties σ (for sampling):
  - degree distribution d
  - clustering coefficient c
  - graphlet distribution g
  - weighted combination of all three dcg
- Compare to Random Edge (RE), Random Node (RN), Forest Fire (FF,FF$_i$)

Sample quality

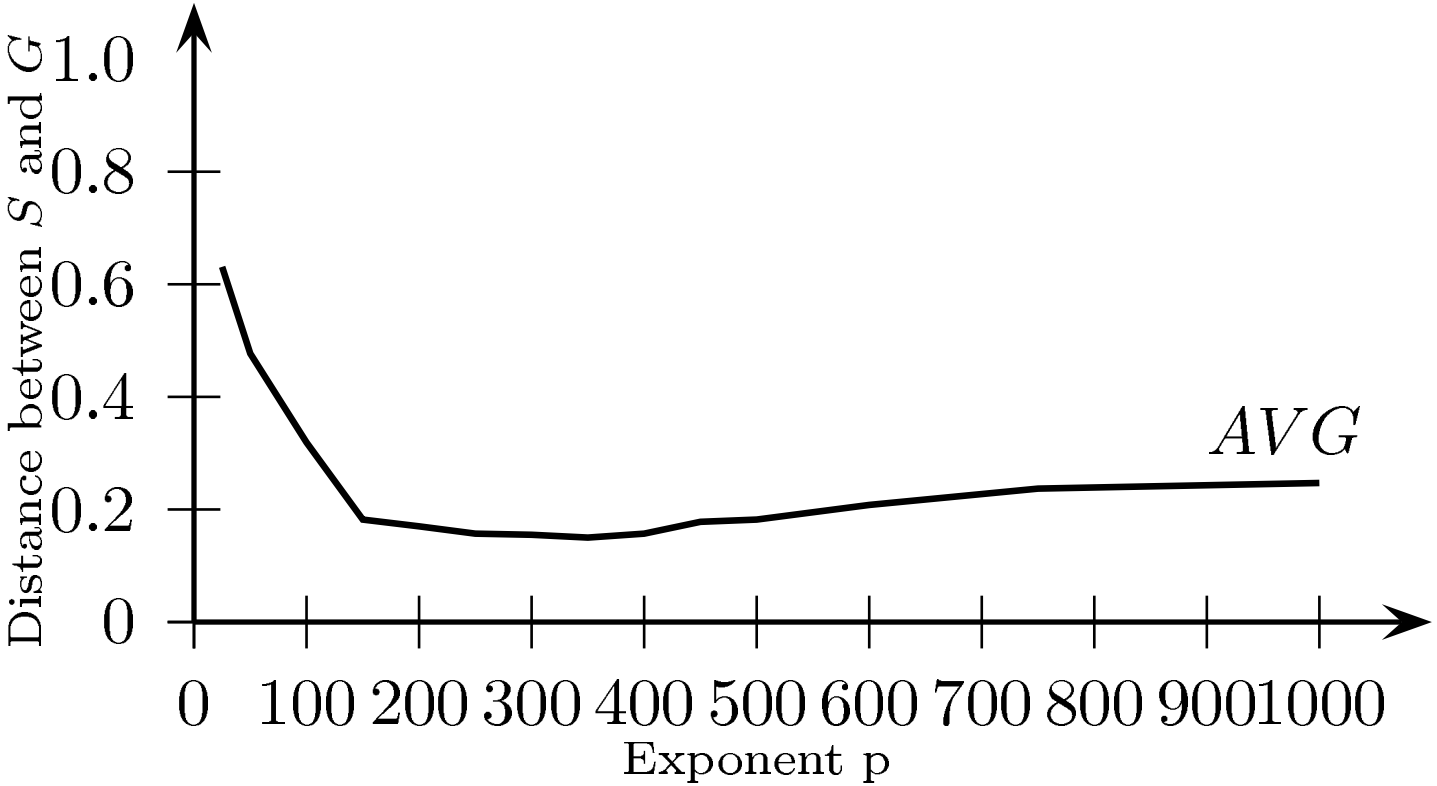
- measured in terms of graph properties (degree distribution, diameter, clustering coefficient, graphlet distribution)
- Results here are averages over all these four criteria



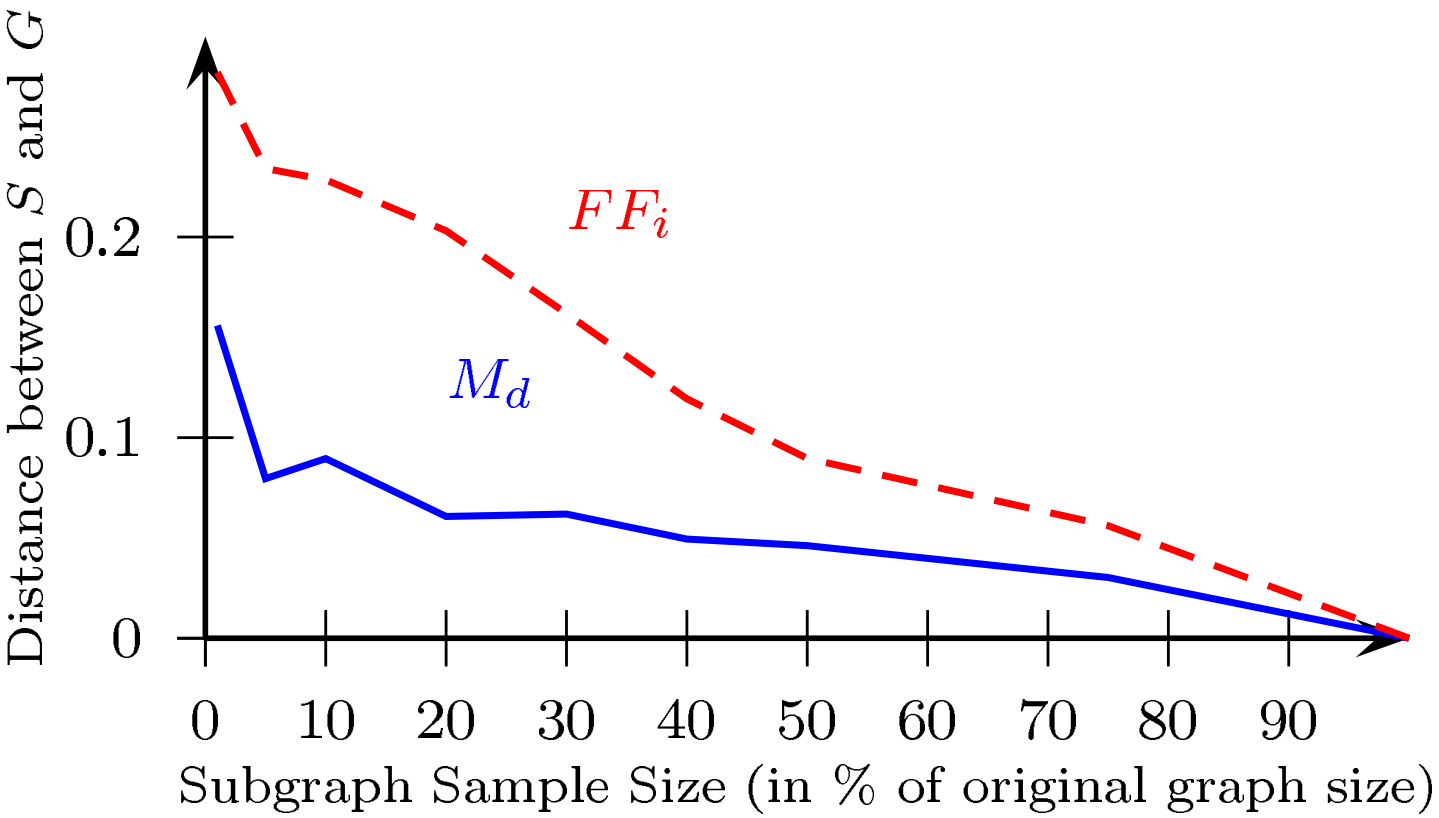
CPU runtime


CPU runtime
Seconds (log-scale)
2,250
2,000
1,750
1,500
1,250
1,000
0,750
0,500
0,250
0,000
-0,250
-0,500
RN
RE
FF
FF_i
M_d
M_c
M_g
M_dcg
M_10dcg
M^SA_d
M^SA_10 dcg
Ch_d
Ch_10dcg
Ch^SA_d
Ch^SA_1 0dcg
Methods

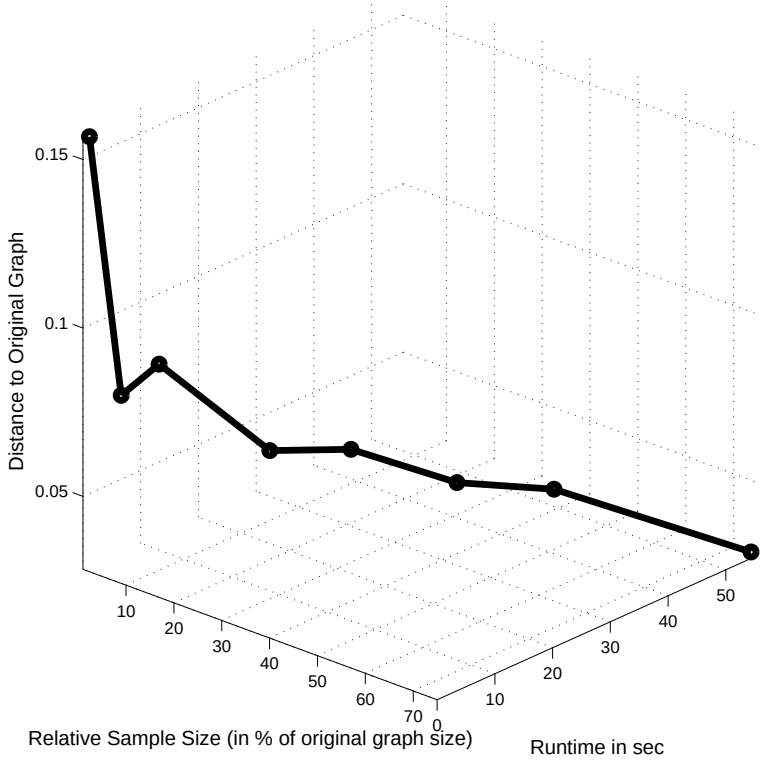
Impact of exponent



Impact of sample size



Distance vs. Runtime vs. Size



Summary

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Results and Observations

- Metropolis methods for Representative Subgraph Sampling
- High-quality samples down to 0.15% of original graph size
- Metropolis algorithm approximating the degree distribution best combines efficiency and sample quality

Applications and Future Work

- Subgraph samples can be used directly for visualization, graph kernel computation, and frequent subgraph mining
- Future work will look into representative subgraph mining for tasks that only indirectly rely on topol. properties (community detection, graph clustering)

The End

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THANK YOU! QUESTIONS?