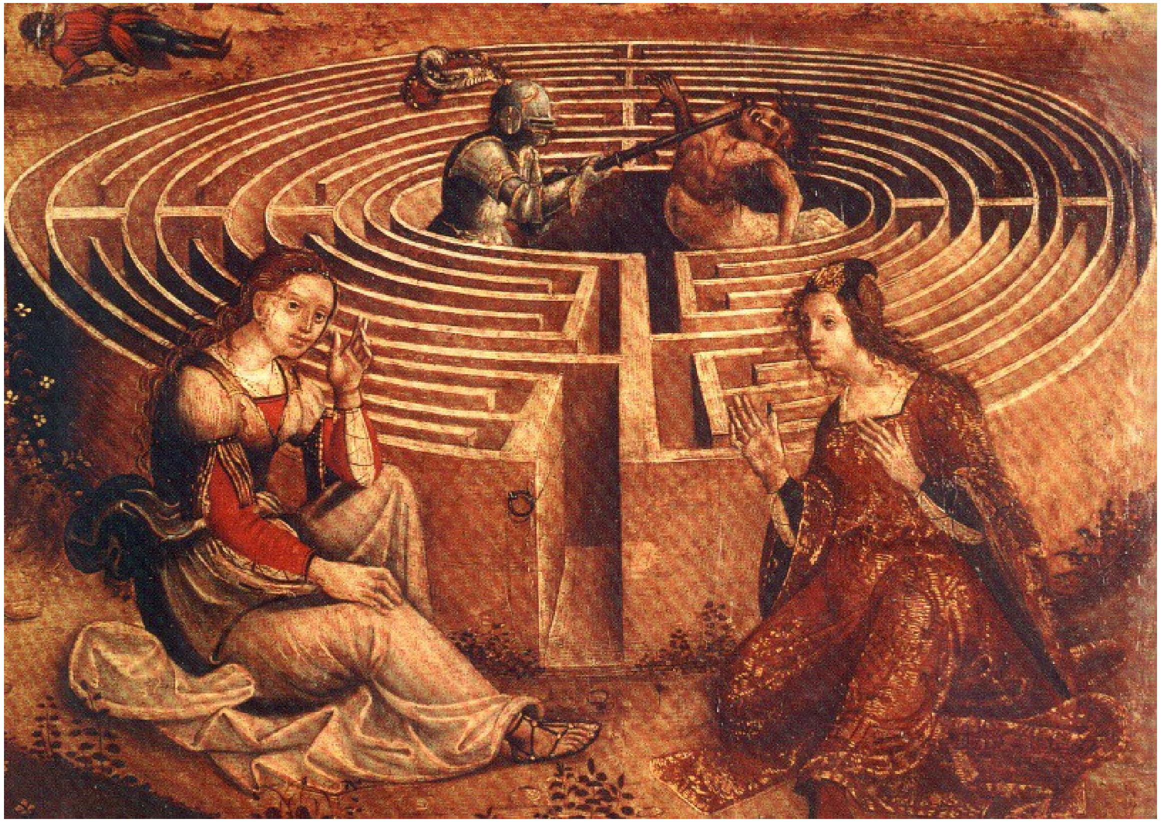
VC-dimension: Ariadne's Thread in the Big Data Labyrinth

(was: Using VC-dimension for faster computation and tighter analysis)



Matteo Riondato

Thesis Defense

April 18, 2014

Outline

Introduction

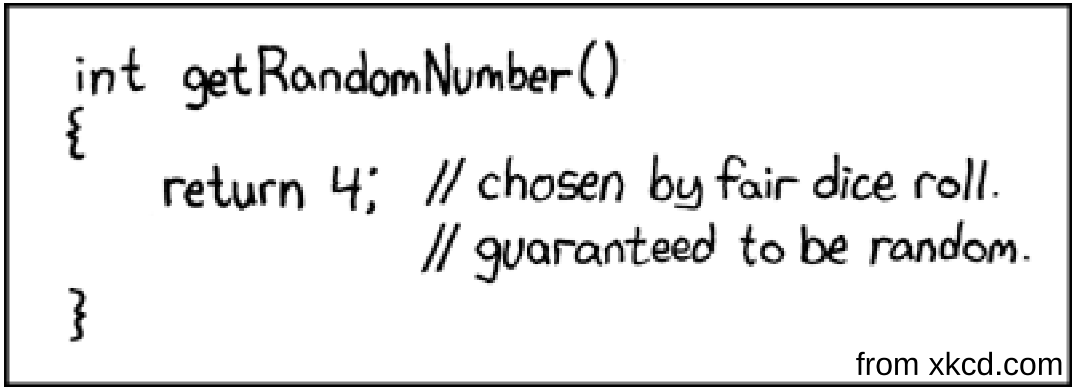
- Problem
- Thesis statement
- Contributions
- VC-dimension

Estimating betweenness centrality

Conclusions

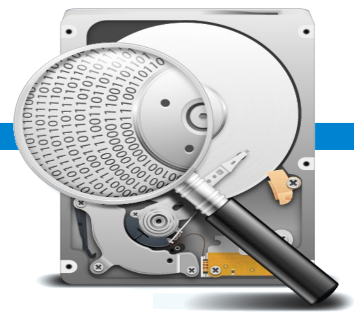
What am I talking about?

Sampling-based Randomized Algorithms for Big Data Analytics



What is data analytics?

Data



Data analytics

=

cleaning, inspecting, transforming, modeling, ...

Information

Needs fast algorithms → challenging due to Big Data

Why is Big Data a challenge?

Volume: data size is large and grows

Variety: no. of "questions" is large

cost(analytics algorithm) = cost(Volume) + cost(Variety)

E.g., cost(APriori) = cost(size dataset) + cost(no. of patterns)

Smart algorithms may cut cost(Variety)

- cost(Volume) always takes over

Thesis statement

We use VC-dimension to obtain high-quality approximations for many data analytics tasks by processing a small random sample of the data

- Probabilistic guarantees on quality of approximations
- Tasks from data mining, graph analysis, database management
- In 1 line:

  "Hey guys, you forgot about this theorem. Here's how to use it."

What are our contributions?

Database query selectivity

- characterization of VC-dimension of SQL queries
- sampling-based algorithm – smallest sample size

Frequent Itemsets / Association Rules

- sampling-based algorithm – smallest sample size
- MapReduce algorithm – fastest and most scalable
- statistical test – more statistical power than available solutions

Betweenness centrality

- sampling-based algorithm – fastest available
- tighter analysis of existing sampling-based algorithm

Why sampling?

Natural solution to cut cost(Volume)

Implies approximations

- OK: data analytics is exploratory

Trade-off:

- larger sample = better approximation but slower algorithm
  - quantified by deviation bounds (Chernoff, Azuma, VC-dimension, …)

Why VC-dimension?

Chernoff+Union too weak for Big Data analytics

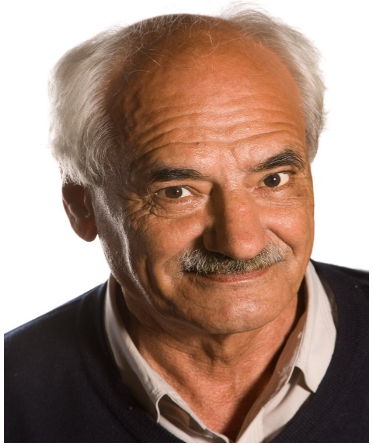
- Chernoff: guarantee on answer to single question
- Union: guarantee extended to all questions
- Sample size depends on no. of questions (Variety):

$$|\mathcal{S}| = \frac{1}{\varepsilon^2}\left(\log_2 |Q| + \ln\frac{1}{\delta}\right)$$

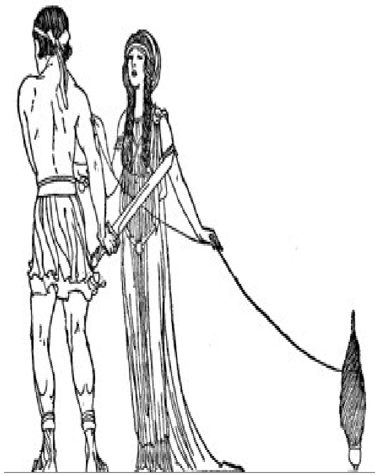
VC-dimension overcomes this issue:

$$|\mathcal{S}| = \frac{1}{\varepsilon^2}\left(\mathsf{VC}(Q) + \ln\frac{1}{\delta}\right)$$

Vladimir N. Vapnik



Aleksey J. Chervonenkis



What is VC-dimension?

D : set of points

F : collection of subsets of D (ranges)

$\Big\}$ (D, F) rangeset

VC-dimension of (D, F) measures "richness" of F

For any $C \subseteq D$, let $P_C = \{C \cap r \ : \ r \in F\} (\subseteq 2^C)$

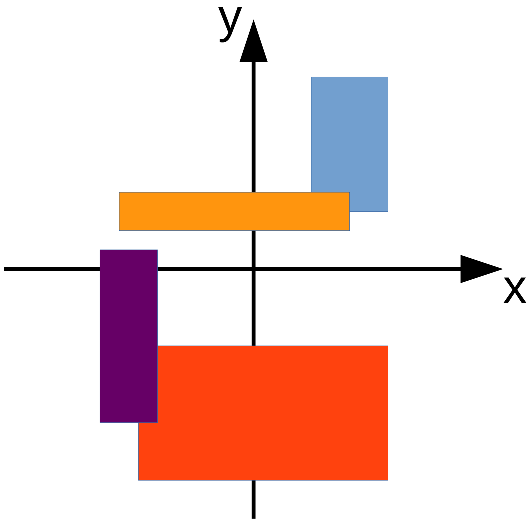
If $P_C = 2^C$, then C is shattered by F

$$\boxed{\mathrm{VC}(D, F) = \sup\left\{|C| \ : \ C \subseteq D \wedge P_C = 2^C\right\}}$$

VC-dimension – Example

$D = \mathbb{R}^2$

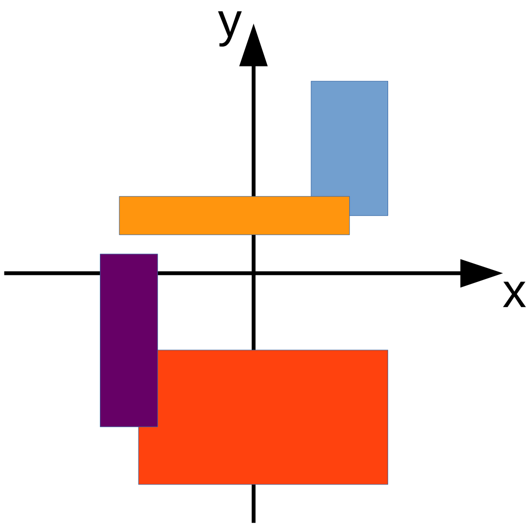
F = all axis-aligned rectangles



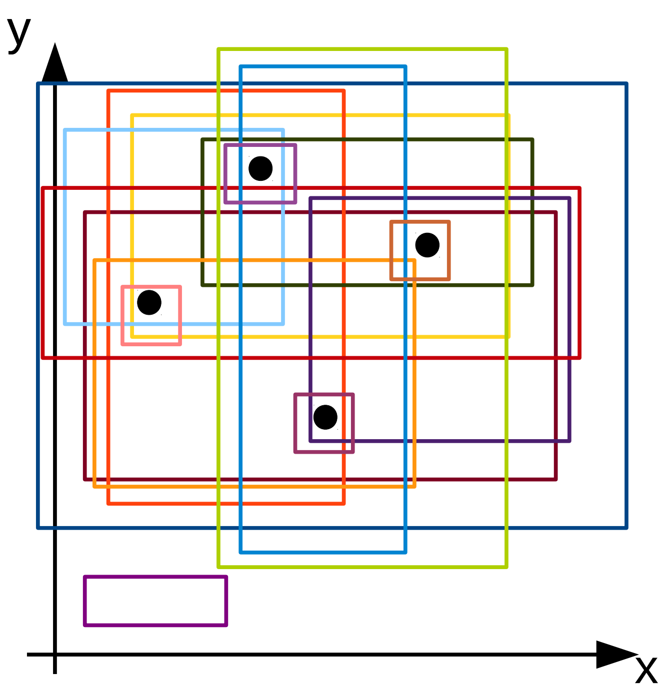
VC-dimension – Example

$D = \mathbb{R}^2$

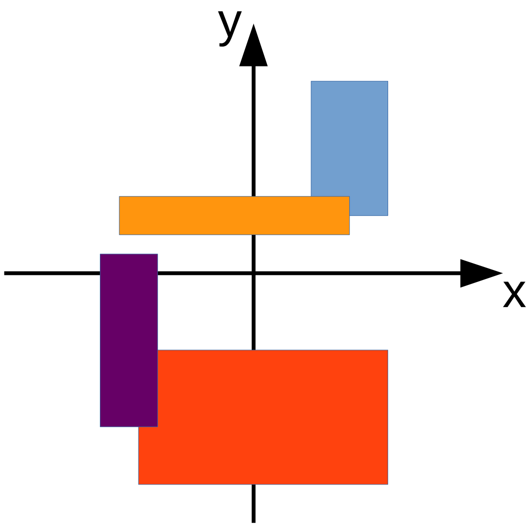
F = all axis-aligned rectangles



Shattering 4 points? easy! Need 16 rectangles



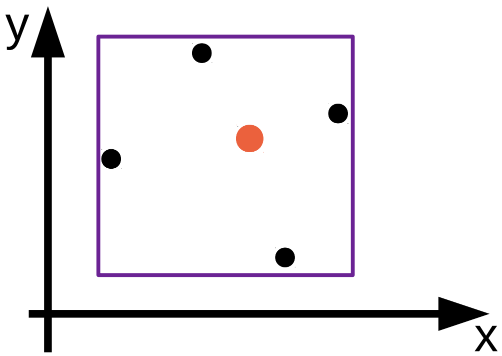
VC-dimension – Example



$D = \mathbb{R}^2$

F = all axis-aligned rectangles

Shattering 5 points? impossible!



One point is contained in all rectangles containing the other four

$\mathsf{VC}(D, F) = 4$

How does it relate to sampling?

Theorem ([Vapnik and Chervonenkis '71] [Li et al. '08])

- Fix $0 < \varepsilon, \delta < 1$, and assume $\mathsf{VC}(D, F) \leq d$
- π : probability distribution on D
- $\mathcal{S}$: collection of samples from D, according to π, with

$$\boxed{|\mathcal{S}| \geq \frac{1}{\varepsilon^2}\left(d + \log\frac{1}{\delta}\right)}$$

- Then, with probability $\geq 1 - \delta$

$$\boxed{\left|\pi(R) - \frac{1}{|\mathcal{S}|}\sum_{a \in \mathcal{S}} \mathbb{1}_R(a)\right| \leq \varepsilon, \text{ for any } R \in F}$$

What do we need to use it?

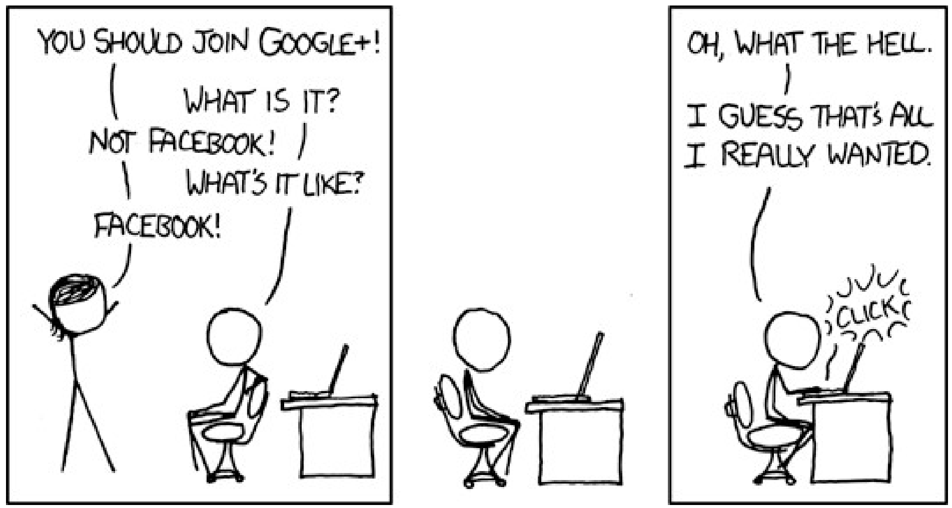
- analytics task as probability estimation problem
- definition of D and F
- probability distribution π on D
- efficient procedure to sample from π
- upper bound to $\mathrm{VC}(D, F)$
  - must be efficient to compute

Outline

- ✓ Introduction
  - ✓ Problem
  - ✓ Thesis statement
  - ✓ Contributions
  - ✓ VC-dimension
- Estimating betweenness centrality
  - Rangeset and bounds
  - Algorithms
- Conclusions

What's the setting?

Take a social network. Even Google+



from xkcd.com

What do you do with it? You analyze it

- If the NSA does it, it must be useful, right?

What are you analyzing about?

What vertices in a graph are important?

Betweenness centrality: measure of vertex importance

- fraction of shortest paths that go through vertex

Graph $G = (V, E)$ $|V| = n$ $|E| = m$

$$\boxed{\mathsf{b}(v) = \frac{1}{n(n-1)} \sum_{p_{uw} \in \mathbb{S}_G} \frac{\mathbb{1}_{\mathcal{T}_v}(p_{uw})}{\sigma_{uw}}}$$

$\mathbb{S}_G$ = all shortest paths in G

$\mathcal{S}_{uv}$= set of shortest paths from u to v ($\sigma_{uv} = |\mathcal{S}_{uv}|$)

$\mathcal{T}_v = \{p \in \mathbb{S}_G \ : \ v \in \mathsf{Int}(p)\}$

How can we compute it?

Naïve algorithm: all pairs shortest paths + aggregation

- Aggregation part dominates. Complexity: $\Theta(n^3)$

[Brandes '01]:

- aggregation after each Single Source Shortest Path computation
- Complexity: $O(nm)$ or $O(nm + n^2 \log n)$

Too much for networks with 10^9 vertices, 10^{10} edges

what to sample?
how much?

Solution: fewer SP computations using sampling!

What do we want to get?

Probabilistic guarantees on approximation

(ε, δ)-approximation: values $(\tilde{\mathrm{b}}(v))_{v \in V}$ such that

$$\Pr\left(\exists v \in V \ : \ |\tilde{\mathrm{b}}(v) - \mathrm{b}(v)| > \varepsilon\right) < \delta$$

accuracy

confidence

Trade-off: smaller ε or δ, higher number of samples

A first sampling algorithm

[BrandesPich '08]:

- $r \leftarrow \frac{1}{2\varepsilon^2}\left(\ln n + \ln 2 + \ln \frac{1}{\delta}\right)$
- for $i \leftarrow 1, \ldots, r$
  - $v_i \leftarrow$ random vertex
  - Perform SSSP from v_i
  - Perform partial aggregation for $\tilde{\mathrm{b}}(u), u \in V$ (like in exact algorithm)
- output $\tilde{\mathrm{b}}(v), \forall v \in V$

How do they compute the sample size?

- Hoeffding bound for single vertex

$$\Pr(|\tilde{\mathsf{b}}(v) - \mathsf{b}(v)| > \varepsilon) < 2e^{-2r\varepsilon^2}$$

Wassily Hoeffding

- union bound over n vertices: we want

$$2e^{-2r\varepsilon^2} \leq \frac{\delta}{n}$$

- sample size for (ε, δ)-approximation:

$$r \geq \frac{1}{2\varepsilon^2}\left(\ln n + \ln 2 + \ln \frac{1}{\delta}\right)$$

What's wrong with this?

Size depends on $\ln n$

- loose, due to union bound
- not the right quantity
- should be characteristic quantity of graph

At each iteration, algorithm performs SSSP

- full exploration of the graph (no locality)

What can we do?

Our algorithm [RiondatoK14]

- uses VC-dimension
- sample size depends on vertex-diameter of G
- at each step, single s-t shortest path computation
  - fewer edges touched
  - more locality
  - can use bidirectional search

Our algorithm

- $\mathsf{VD}(G) \leftarrow$ vertex-diameter of G
- $r \leftarrow (1/2\varepsilon^2)(\lfloor \log_2(\mathsf{VD}(G) - 2) \rfloor + 1 + \ln(1/\delta))$
- $\tilde{\mathsf{b}}(v) \leftarrow 0, \forall v \in V$
- for $i \leftarrow 1, \ldots, r$
  - $(u, v) \leftarrow$ random pair of vertices
  - $\mathcal{S}_{uv} \leftarrow$ all SPs from u to v (Dijkstra, trunc. BFS, bidirect. Search)
  - $p \leftarrow$ random element of $\mathcal{S}_{uv}$
  - $\tilde{\mathsf{b}}(w) \leftarrow \tilde{\mathsf{b}}(w) + 1/r, \forall w \in \mathsf{Int}(p)$
- output $\tilde{\mathsf{b}}(v), \forall v \in V$

What is the vertex-diameter?

$\mathsf{VD}(G)$: max no. of vertices in a SP

$$\mathsf{VD}(G) = \max\{|p| \ : \ p \in \mathbb{S}_G\}$$

- small in social networks

G not weighted: $\mathsf{VD}(G) = \Delta_G + 1$

- otherwise no relationship in general

Computation:

- G unweighted, undirected: 2-approx via SSSP
- otherwise: size of largest WCC

What do we get?

- $\mathsf{VD}(G) \leftarrow$ vertex-diameter of G
- $r \leftarrow (1/2\varepsilon^2)(\lfloor \log_2(\mathsf{VD}(G)-2)\rfloor + 1 + \ln(1/\delta))$
- $\tilde{\mathsf{b}}(v) \leftarrow 0, \forall v \in V$
- for $i \leftarrow 1, \ldots, r$
  - $(u, v) \leftarrow$ random pair of vertices
  - $\mathcal{S}_{uv} \leftarrow$ all SPs from u to v (Dijkstra, trunc. BFS, bidirect. Search)
  - $p \leftarrow$ random element of $\mathcal{S}_{uv}$
  - $\tilde{\mathsf{b}}(w) \leftarrow \tilde{\mathsf{b}}(w) + 1/r, \forall w \in \mathsf{Int}(p)$
- output $\tilde{\mathsf{b}}(v), \forall v \in V$

Theorem: $(\tilde{\mathsf{b}}(v))_{v\in V}$ is a (ε, δ)-approximation

How can we prove it?

Define rangeset

Define probability distribution

Define betweenness as probability estimation problem

Show upper bound to VC-dimension

- Bonus: show tightness + variants

Apply VC-dimension sampling theorem

What are the rangeset and the probability?

$D = \mathbb{S}_G$ = all SPs in G

Let $T_v = \{p \in \mathbb{S}_G \ : \ v \in \mathsf{Int}(p)\}$

$F = \{T_v, v \in V\}$

Probability distribution π on $\mathbb{S}_G$:

$$\pi(p_{uw}) = \frac{1}{n(n-1)} \frac{1}{\sigma_{uw}}$$

- algorithm samples paths according to π
- $\pi(T_v) = \frac{1}{n(n-1)} \sum_{p_{uw} \in T_v} \frac{1}{\sigma_{uw}} = \frac{1}{n(n-1)} \sum_{p_{uw} \in \mathbb{S}_G} \frac{\mathbb{1}_{\mathsf{p_{uw}}}(v)}{\sigma_{uw}} = \mathsf{b}(v)$

What is the VC-dimension of our rangeset?

Theorem: $\mathsf{VC}(\mathbb{S}_G, F) \leq \lfloor \log_2 \mathsf{VD}(G) - 2 \rfloor + 1$

Proof

- To shatter $A \subseteq \mathbb{S}_G$, $|A| = d$,
  - need 2^d different ranges
  - any $p \in A$ must appear in 2^{d-1} different ranges
- Any p appears only in the ranges T_v such that $v \in \mathsf{Int}(p)$
- i.e., it appears in $|\mathsf{Int}(p)| \leq \mathsf{VD}(G) - 2$ ranges
- To shatter A, must be $2^{d-1} \leq \mathsf{VD}(G) - 2$

How to use the bound?

$\tilde{\mathsf{b}}(v)$ = empirical average for $\mathsf{b}(v)$
Sampling done according to π
Know upper bound to $\mathsf{VC}(\mathbb{S}_G, F)$

We can apply the **VC sample theorem**

If $r \geq \frac{1}{\varepsilon^2}\left(\lfloor \log_2(\mathsf{VD}(G)-2)\rfloor + 1 + \ln\frac{1}{\delta}\right)$

then $(\tilde{\mathsf{b}}(v))_{v\in V}$ is an (ε,δ)-approximation:

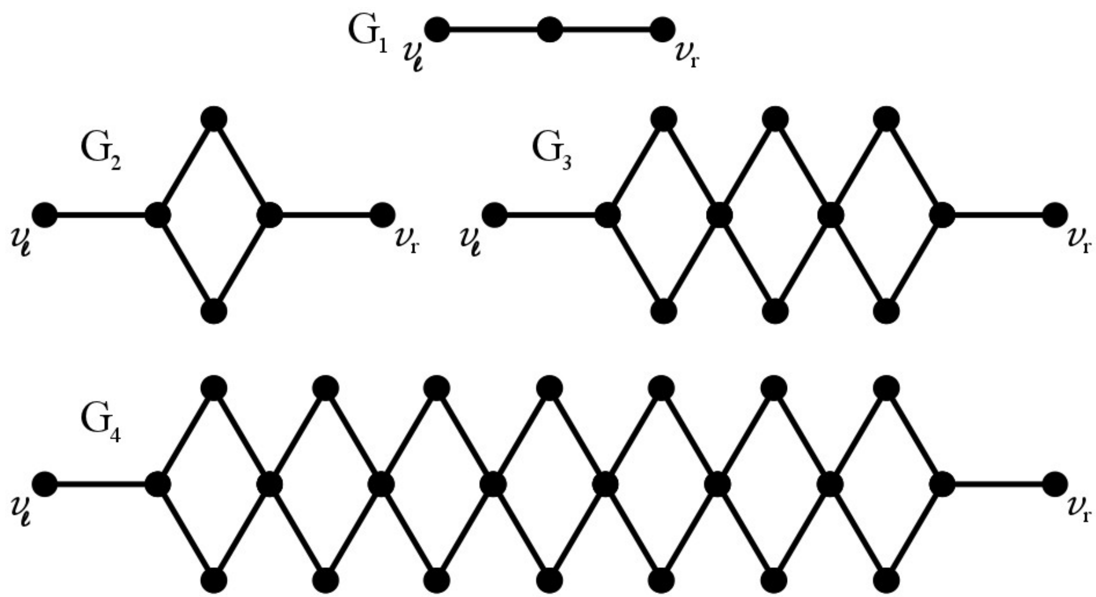
$$\Pr\left(\exists v \in V \ : \ |\tilde{\mathsf{b}}(v) - \mathsf{b}(v)| > \varepsilon\right) < \delta$$

Roadmap

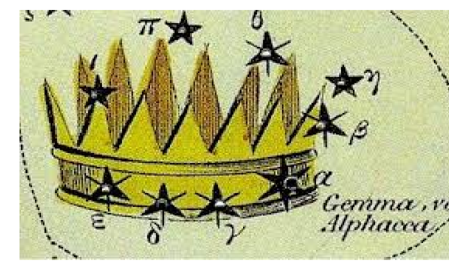
- ✓ Define rangeset
- ✓ Define probability distribution
- ✓ Define betweenness as probability estimation problem
- ✓ Show upper bound to VC-dimension
  - Bonus: show tightness + variants
- ✓ Apply VC-dimension sampling theorem

Is the bound tight?

Concertina graphs $(G_i)_{i\in\mathbb{N}}$



Concertina, musical instrument



Corona Borealis

Theorem: $\mathsf{VC}(\mathbb{S}_{G_i}) = \lfloor \log_2(\mathsf{VD}(G_i) - 2) \rfloor + 1 = i$

Is the vertex diameter the right quantity?

No.

If

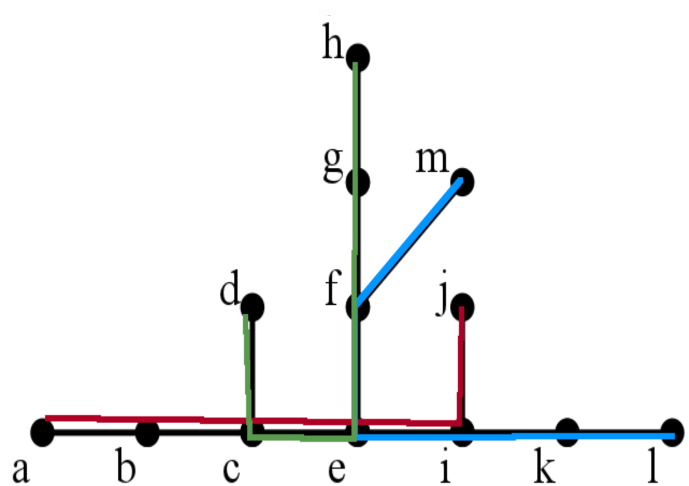
- G is undirected
- for every connected pair (u, v) there is a unique SP, then

$$\boxed{\mathsf{VC}(\mathbb{S}_G, F) \leq 3}$$

Proof: two SPs that meet and separate can't meet again

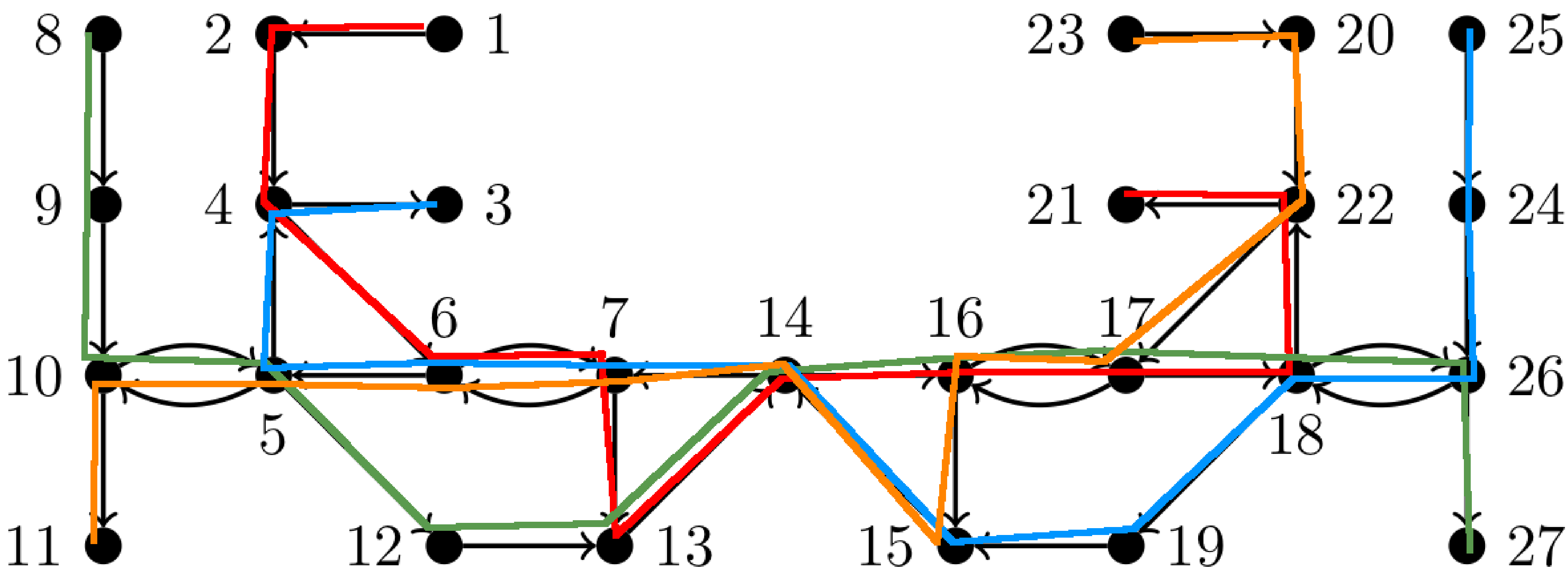
- + case analysis

Tight? Yes



Is this true for directed graphs?

No. Can shatter 4 SP!



Open question: still a constant for directed graphs? (6?)

What about relative guarantees?

$\mathsf{b}^{(K)}$: K^{th} highest betweenness, ties broken arbitrarily

Top-K vertices: $T(K,G) = \{v \in V \ : \ \mathsf{b}(v) \geq \mathsf{b}^{(K)}\}$

Relative approximation: $C = \{(v, \tilde{\mathsf{b}}(v))\}$ s.t.

$$(1-\varepsilon)\mathsf{b}(v) \leq \tilde{\mathsf{b}}(v) \leq (1+\varepsilon)\mathsf{b}(v), \forall v \in C$$

Algorithm:

- run additive approximation algorithm
- $\tilde{\mathsf{b}}^{(K)} \leftarrow$ lower bound to $\mathsf{b}^{(K)}$
- use $\tilde{\mathsf{b}}^{(K)}$ and relative-guarantees version of VC sample theorem to compute sample size for relative approximation for $T(K,G)$

How good is the algorithm in practice?

C implementation as patch to igraph

Graphs: real (snap.stanford.edu) + artificial BarabasiAlbert

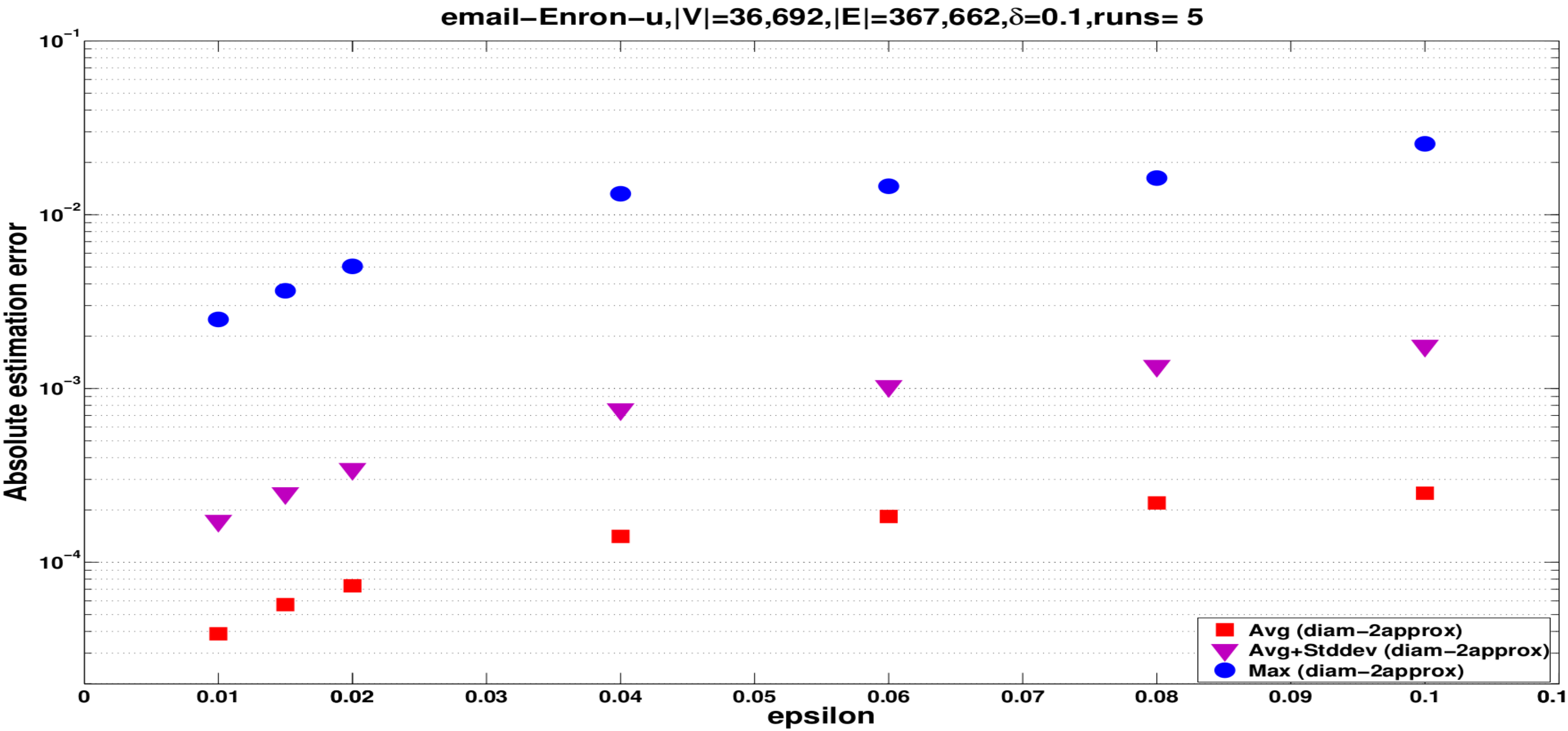
- social networks, road networks, …

Goals: evaluate $\left\{\begin{array}{l}\text{accuracy}\\\text{speed}\\\text{scalability}\end{array}\right.$

How accurate is our algorithm?

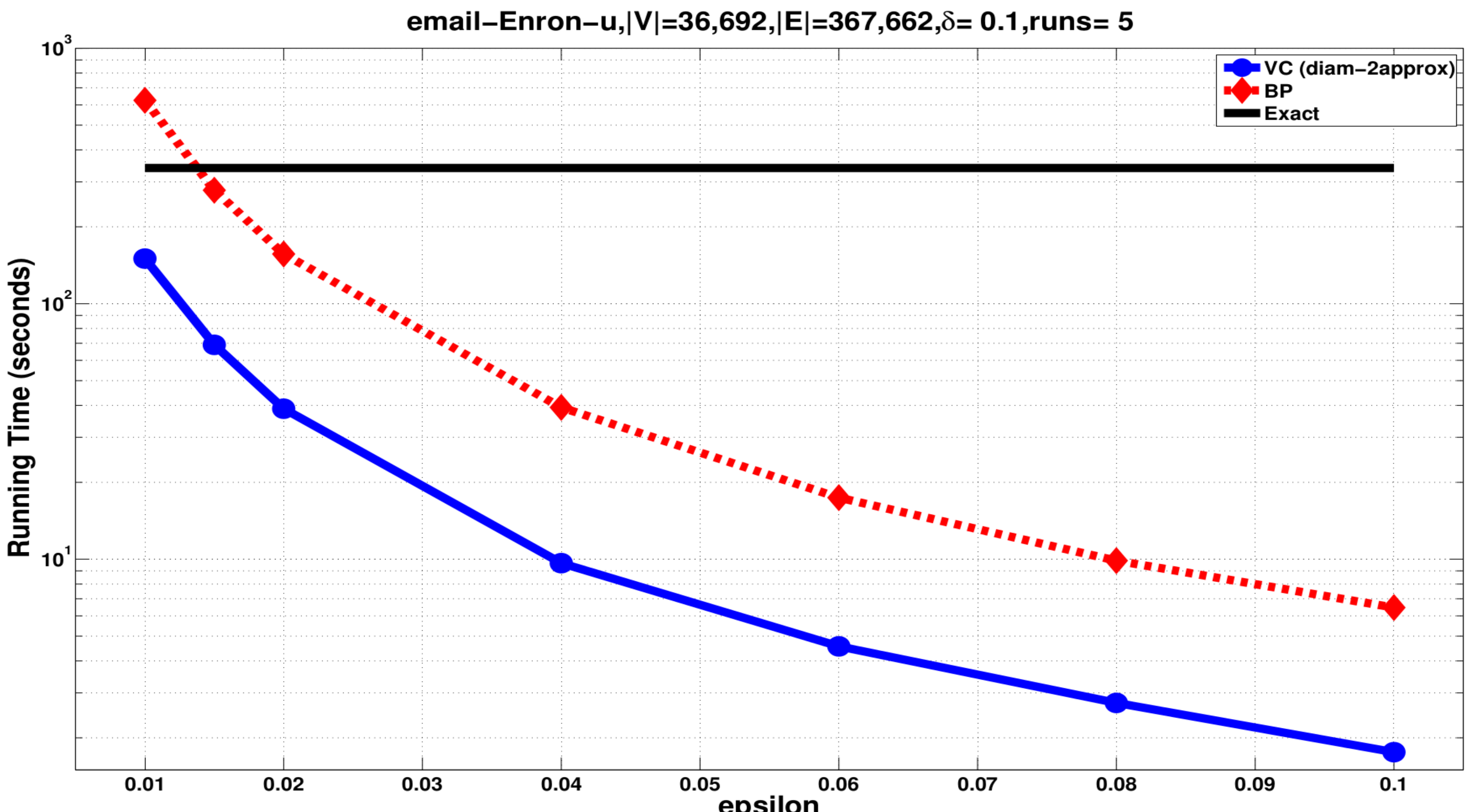
$|\tilde{\mathrm{b}}(v) - \mathrm{b}(v)|$ always $\leq \varepsilon$ (O(10³) runs on different graphs)

Accuracy ~8x better than guaranteed

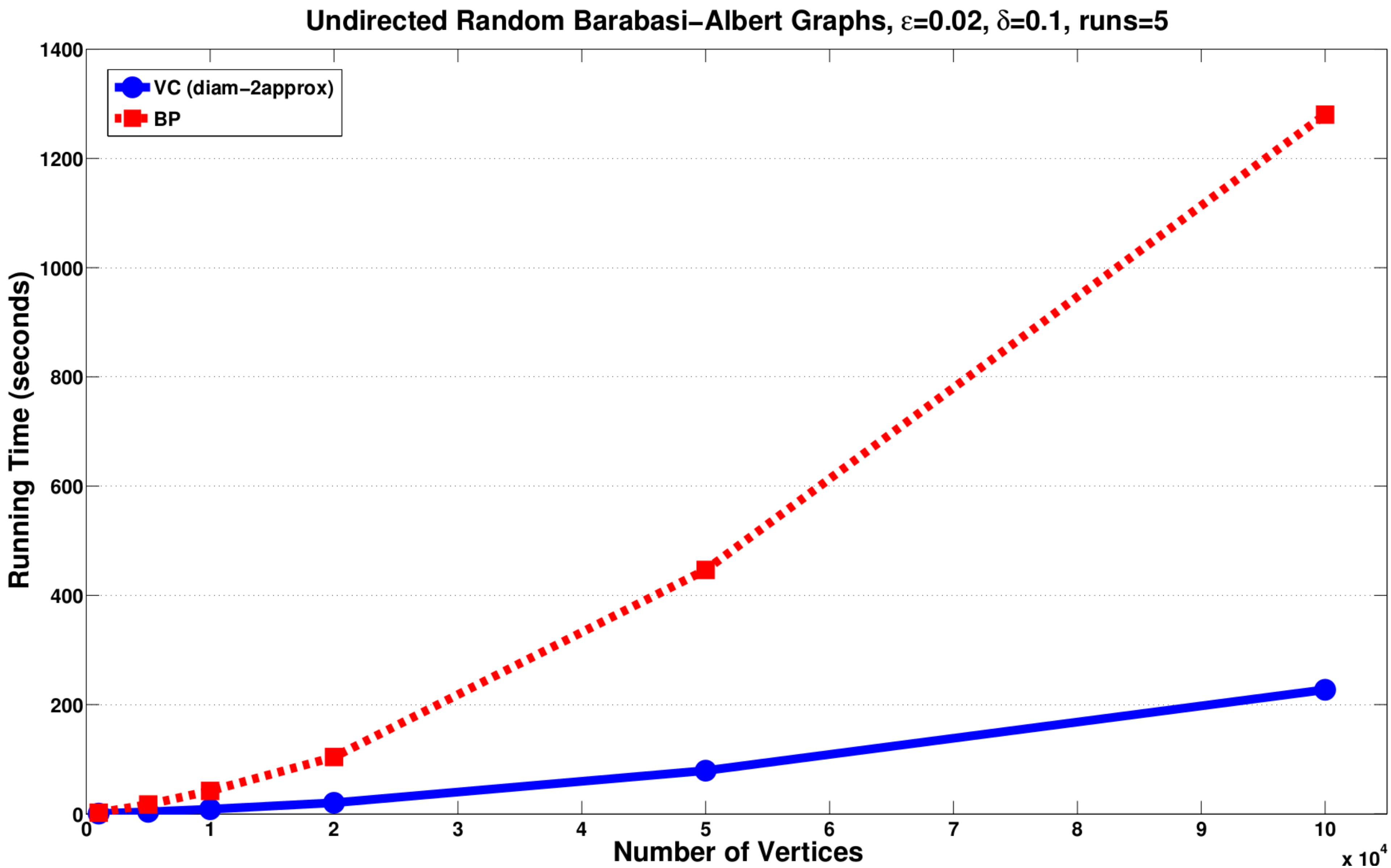


How fast is our algorithm?

~8x faster than simple sampling algorithm



How well does it scale?



Am I telling the truth?

Yes, but.

- $\tilde{\mathrm{b}}_{\mathsf{s}}(v)$: estimator of simple sampling alg. w/ same no. of samples

- Theorem: $\mathrm{Var}[\tilde{\mathrm{b}}_{\mathsf{s}}(v)] \leq \mathrm{Var}[\tilde{\mathrm{b}}(v)], \forall v \in V$
  - does not imply that it computes a (ε, δ)-approximation

- Emphasis on different aspects:
  - Ours: speed and scalability
  - Theirs: accuracy

What did I show you?

Two sampling based algorithms for betweenness estimation

- Top-K algo is first to achieve high relative guarantees
- Much smaller sample size than previously known
- Fewer computations than existing work = faster

Characterizing graph problems through VC-dimension is challenging, but interesting

- and rewarding

Published at ACM WSDM'14, journal subm. in preparation

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  - ✓ Algorithms
- Conclusions
  - Limitations of sampling
  - Directions for further research

What did we learn?

We can approximate many data analytics tasks using sampling

- size depends on bound to VC-dim., not no. of questions (Variety)
  - characteristic quantity of the dataset / problem
- lower cost(Volume)

- sample fits into memory of single machine
  - can use MapReduce for boosting-like approach (many samples in parallel)
- can use "backwards" to derive statistical tests for false positives

What are the limitations?

Need efficient-to-compute bound on VC-dimension

Need efficient sampling procedure

Need for independent sampling

- some new developments here

Dependency on ε

Where to go from here?

Smaller samples

- pseudodimension, shatter coefficients, covering numbers, …

Progressive sampling

- Rademacher averages bounds

Statistical testing

- False Discovery Rate rather than Family-Wide Error Rate

New technology / computational platforms

- Spark, Pregel, …

Did we publish?

- R., Akdere, Çetintemel, Zdonik, Upfal. "The VC-dimension of SQL queries and selectivity estimation through sampling". ECML-PKDD'11.
- R., Upfal. "Efficient discovery of Association Rules and Frequent Itemsets through sampling with tight performance guarantees". ECML-PKDD'12, ACM TKDD'14.
- R., DeBrabant, Fonseca, Upfal. "PARMA: a parallel randomized algorithm for approximate association rule mining in MapReduce". ACM CIKM'12.
- R., Vandin. "Finding the True Frequent Itemsets". SIAM SDM'14.
- R., Kornaropoulos. "Fast approximation of betweenness centrality through sampling". ACM WSDM'14
- Others:
  - Pietracaprina, R., Upfal, Vandin. "Mining top-k Frequent Itemsets through progressive sampling". DMKD'10.
  - Akdere, Cetintemel, R., Upfal, Zdonik."The case for predictive database systems: opportunities and challenges". CIDR'11
  - Akdere, Cetintemel, R., Upfal, Zdonik. "Learning-based query performance modeling and prediction". IEEE ICDE'12.
  - Pietracaprina, Pucci, R., Silvestri, Upfal. "Space-round tradeoffs for MapReduce computations". ACM ICS'12

Who deserves all the credit?

- Eli
- Uğur, Basilis
- Andrea, Geppino, Stan, Rodrigo, Fabio, Francesco, Aris, Luca
- Olya, Andy, Justin, Evgenios, and all other PhDs
- Mackenzie, Michela, Marco, Bernardo, Robyn, Andrew, …
- Lauren and astaff@
- tstaff@ for the grid + problems@

"Not he who begins, but he who keeps going"
Leonardo da Vinci