Topological implications of negative curvature for biological and social networks

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Joint work with

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- Nasim Mobasheri (UIC)

Outline of talk

1. **Introduction**
2. **Basic definitions and notations**
3. **Computing hyperbolicity for real networks**
4. **Implications of hyperbolicity of networks**
   - Hyperbolicity and crosstalk in regulatory networks
   - Geodesic triangles and crosstalk paths
   - Identifying essential edges and nodes in regulatory networks
   - A social network application

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Graph-theoretical analysis leads to useful insights for many complex systems, such as

- **World-Wide Web**
- **social network of jazz musicians**
- **metabolic networks**
- **protein-protein interaction networks**

Examples of useful network measures for such analyses

- **degree based** , *e.g.*
  - **maximum/minimum/average degree, degree distribution,** ......
- **connectivity based** , *e.g.*
  - **clustering coefficient, largest cliques or densest sub-graphs,** ......
- **geodesic based** , *e.g.*
  - **diameter, betweenness centrality,** ......
- **other more complex measures**

network measure for this talk

network curvature via (Gromov) hyperbolicity measure

- originally proposed by Gromov in 1987 in the context of group theory
  - observed that many results concerning the fundamental group of a Riemann surface hold true in a more general context
  - defined for infinite continuous metric space with bounded local geometry via properties of geodesics
  - can be related to standard scalar curvature of Hyperbolic manifold
- adopted to finite graphs using a so-called 4-node condition

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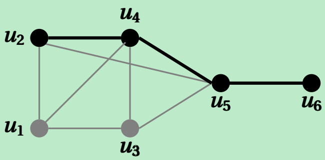
Graphs, geodesics and related notations

$G=(V,E)$	connected undirected graph of $n \geq 4$ nodes
$u \overset{\mathcal{P}}{\leftrightsquigarrow} v$	path $\mathcal{P} \equiv (\underbrace{u_0}_{=u}, u_1, \ldots, u_{k-1}, \underbrace{u_k}_{=v})$ between nodes u and v
$\ell(\mathcal{P})$	length (number of edges) of the path $u \overset{\mathcal{P}}{\leftrightsquigarrow} v$
$u_i \overset{\mathcal{P}}{\leftrightsquigarrow} u_j$	sub-path $(u_i, u_{i+1}, \ldots, u_j)$ of $\mathcal{P}$ between nodes u_i and u_j
$u \overset{s}{\leftrightsquigarrow} v$	a shortest path between nodes u and v
$d_{u,v}$	length of a shortest path between nodes u and v



$u_2 \overset{\mathcal{P}}{\leftrightsquigarrow} u_6$ is the path $\mathcal{P} \equiv (u_2, u_4, u_5, u_6)$

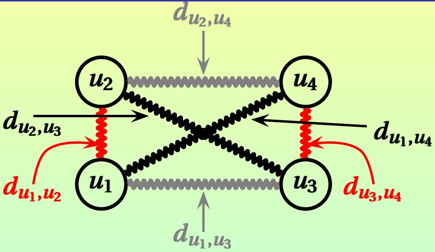
$\ell(\mathcal{P}) = 3$

$d_{u_2,u_6} = 2$

Basic definitions and notations

4 node condition (Gromov, 1987)

Consider four nodes u_1, u_2, u_3, u_4 and the six shortest paths among pairs of these nodes



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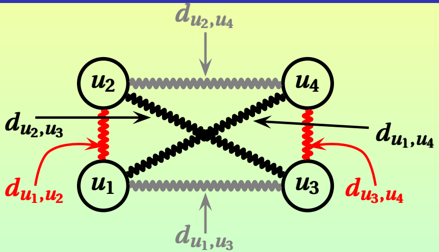
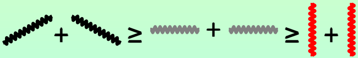


Assume, without loss of generality, that

$$\underbrace{d_{u_1,u_4}+d_{u_2,u_3}}_{=L} \geq \underbrace{d_{u_1,u_3}+d_{u_2,u_4}}_{=M} \geq \underbrace{d_{u_1,u_2}+d_{u_3,u_4}}_{=S}$$



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Basic definitions and notations

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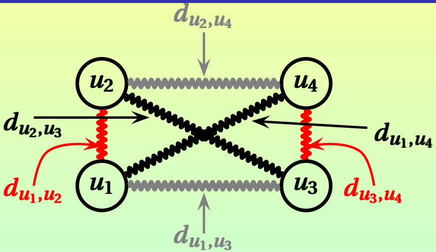

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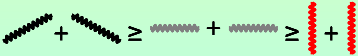
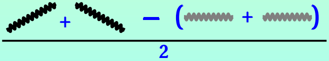


Let $\delta_{u_1,u_2,u_3,u_4} = \frac{L-M}{2}$



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Basic definitions and notations

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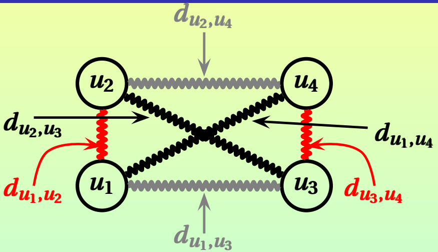
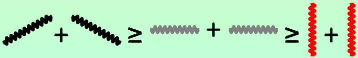
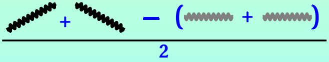


Assume, without loss of generality, that

$$\underbrace{d_{u_1,u_4} + d_{u_2,u_3}}_{=L} \geq \underbrace{d_{u_1,u_3} + d_{u_2,u_4}}_{=M} \geq \underbrace{d_{u_1,u_2} + d_{u_3,u_4}}_{=S}$$



Let $\delta_{u_1,u_2,u_3,u_4} = \frac{L-M}{2}$



Definition (hyperbolicity of G)

$$\delta(G) = \max_{u_1,u_2,u_3,u_4} \left\{ \delta_{u_1,u_2,u_3,u_4} \right\}$$

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Definition (Δ-hyperbolic graphs)

G is Δ-hyperbolic provided $\delta(G) \leq \Delta$

Definition (Hyperbolic graphs)

If Δ is a constant independent of graph parameters, then a Δ-hyperbolic graph is simply called a hyperbolic graph

Basic definitions and notations

Hyperbolic graphs (graphs of negative curvature)

Definition (Δ-hyperbolic graphs)

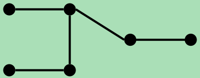
G is Δ-hyperbolic provided $\delta(G) \leq \Delta$

Definition (Hyperbolic graphs)

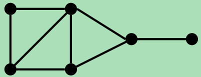
If Δ is a constant independent of graph parameters, then a Δ-hyperbolic graph is simply called a hyperbolic graph

Example (Hyperbolic and non-hyperbolic graphs)

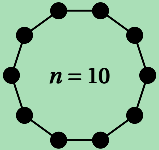
Tree: $\Delta(G) = 0$
hyperbolic graph



Chordal (triangulated) graph:
$\Delta(G) = 1/2$
hyperbolic graph



Simple cycle: $\Delta(G) = \lceil n/4 \rceil$
non-hyperbolic graph



Are there real-world networks that are hyperbolic?

Yes, for example:

- **Preferential attachment networks were shown to be scaled hyperbolic**
  - [Jonckheere and Lohsoonthorn, 2004; Jonckheere, Lohsoonthorn and Bonahon, 2007]
- **Networks of high power transceivers in a wireless sensor network were empirically observed to have a tendency to be hyperbolic**
  - [Ariaei, Lou, Jonckeere, Krishnamachari and Zuniga, 2008]
- **Communication networks at the IP layer and at other levels were empirically observed to be hyperbolic**
  - [Narayan and Saniee, 2011]
- **Extreme congestion at a very limited number of nodes in a very large traffic network was shown to be caused due to hyperbolicity of the network together with minimum length routing**
  - [Jonckheerea, Loua, Bonahona and Baryshnikova, 2011]
- **Topology of Internet can be effectively mapped to a hyperbolic space**
  - [Bogun, Papadopoulos and Krioukov, 2010]

Definition (average hyperbolicity)

$$\delta_{\text{ave}}(G) = \frac{1}{\binom{n}{4}} \sum_{u_1,u_2,u_3,u_4} \delta_{u_1,u_2,u_3,u_4}$$

expected value of δ_{u_1,u_2,u_3,u_4} if u_1, u_2, u_3, u_4 are picked uniformly at random

Computation of $\delta(G)$ and $\delta_{\text{ave}}(G)$

- Trivially in $O\left(n^4\right)$ time
  - Compute all-pairs shortest paths — Floyd–Warshall algorithm $O\left(n^3\right)$ time
  - For each combination u_1, u_2, u_3, u_4, compute δ_{u_1,u_2,u_3,u_4} — $O\left(n^4\right)$ time
- Open problem: can we compute in $O\left(n^{4-\varepsilon}\right)$ time?

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Outline of talk

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Real networks used for empirical validation

20 well-known biological and social networks

- 11 biological networks that include 3 transcriptional regulatory, 5 signalling, 1 metabolic, 1 immune response and 1 oriented protein-protein interaction networks
- 9 social networks range from interactions in dolphin communities to the social network of jazz musicians
- hyperbolicity of the biological and directed social networks was computed by ignoring the direction of edges
- hyperbolicity values were calculated by writing codes in C using standard algorithmic procedures

Next slide: List of 20 networks ▸

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Computing hyperbolicity for real networks

Direct calculation

11 biological networks

	# nodes	# edges
1. *E. coli* transcriptional	311	451
2. Mammalian signaling	512	1047
3. *E. coli* transcriptional	418	544
4. T-LGL signaling	58	135
5. *S. cerevisiae* transcriptional	690	1082
6. *C. elegans* metabolic	453	2040
7. Drosophila segment polarity (6 cells)	78	132
8. ABA signaling	55	88
9. Immune response network	18	42
10. T cell receptor signaling	94	138
11. Oriented yeast PPI	786	2445

9 social networks

	# nodes	# edges
1. Dolphin social network	62	160
2. American College Football	115	612
3. Zachary Karate Club	34	78
4. Books about US politics	105	442
5. Sawmill communication network	36	62
6. Jazz Musician network	198	2742
7. Visiting ties in San Juan	75	144
8. World Soccer Data, Paris 1998	35	118
9. Les Miserables characters	77	251

Computing hyperbolicity for real networks

Direct calculation

Biological networks

	Average degree	δ_{ave}	δ
1. *E. coli* transcriptional	1.45	0.132	2
2. Mammalian Signaling	2.04	0.013	3
3. *E. Coli* transcriptional	1.30	0.043	2
4. T LGL signaling	2.32	0.297	2
5. *S. cerevisiae* transcriptional	1.56	0.004	3
6. *C. elegans* Metabolic	4.50	0.010	1.5
7. *Drosophila* segment polarity	1.69	0.676	4
8. ABA signaling	1.60	0.302	2
9. Immune Response Network	2.33	0.286	1.5
10. T Cell Receptor Signalling	1.46	0.323	3
11. Oriented yeast PPI	3.11	0.001	2

social networks

	Average degree	δ_{ave}	δ
1. Dolphins social network	5.16	0.262	2
2. American College Football	10.64	0.312	2
3. Zachary Karate Club	4.58	0.170	1
4. Books about US Politics	8.41	0.247	2
5. Sawmill communication	3.44	0.162	1
6. Jazz musician	27.69	0.140	1.5
7. Visiting ties in San Juan	3.84	0.422	3
8. World Soccer data, 1998	3.37	0.270	2.5
9. Les Miserable	6.51	0.278	2

- Hyperbolicity values of almost all networks are small
- For all networks δ_{ave} is one or two orders of magnitude smaller than δ
  - Intuitively, this suggests that value of δ may be a rare deviation from typical values of δ_{u_1,u_2,u_3,u_4} for most combinations of nodes $\{u_1, u_2, u_3, u_4\}$
- No systematic dependence of δ on number of nodes/edges or average degree

Computing hyperbolicity for real networks

Direct calculation

Definition (Diameter of a graph)

$\mathcal{D} = \max_{u,v} \{d_{u,v}\}$ **longest shortest path**

Fact

$\delta \leq \mathcal{D}/2$ **small diameter implies small hyperbolicity**

We found no systematic dependence of δ on $\mathcal{D}$

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Computing hyperbolicity for real networks

Direct calculation

Definition (Diameter of a graph)

$\mathscr{D} = \max_{u,v} \{d_{u,v}\}$ longest shortest path

Fact

$\delta \leq \mathscr{D}/2$ small diameter implies small hyperbolicity

We found no systematic dependence of δ on $\mathscr{D}$

For more rigorous checks of hyperbolicity of finite graphs
and
for evaluation of statistical significance of the hyperbolicity measure
see our paper

R. Albert, B. DasGupta and N. Mobasheri,
Topological implications of negative curvature for biological and social networks.
Physical Review E 89(3), 032811 (2014)

Outline of talk

Implications of hyperbolicity

We discuss topological implications of hyperbolicity somewhat informally

Precise Theorems and their proofs are available in our paper

R. Albert, B. DasGupta and N. Mobasheri,

Topological implications of negative curvature for biological and social networks.

Physical Review E 89(3), 032811 (2014)

Outline of talk

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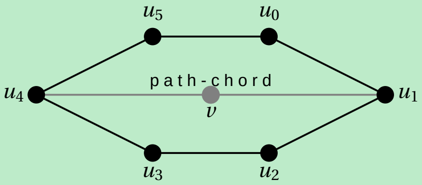
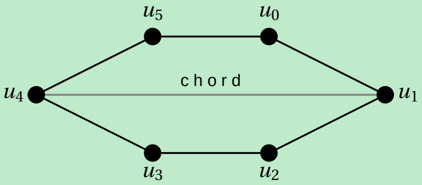
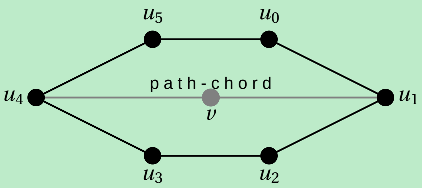
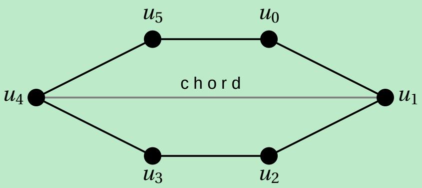
Definition (**Path chord and chord**)





Definition (**Path chord and chord**)





Theorem (**large cycle without path-chord imply large hyperbolicity**)

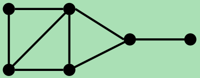
G has a cycle of k nodes which has no path-chord $\implies$ $\delta \geq \lceil k/4 \rceil$

Corollary

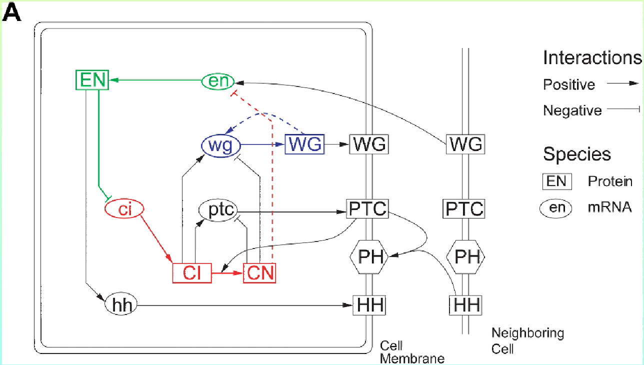
Any cycle containing more than 4δ nodes must have a path-chord

Example

$\delta < 1 \implies G$ **is chordal graph**



An example of a regulatory network



Network associated to the Drosophila segment polarity

G. von Dassow, E. Meir, E. M. Munro and G. M. Odell, Nature 406, 188-192 (2000)

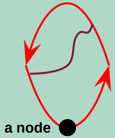
Hyperbolicity and crosstalk in regulatory networks

short-cuts in long feedback loops

node regulates itself through a long feedback loop

⇒ this loop must have a path-chord

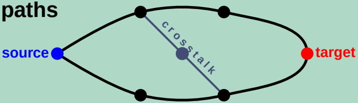
⇒ a shorter feedback cycle through the same node



interpreting chord or short path-chord as crosstalk

"source" regulates "target" through two long paths

⇒ must exist a crosstalk path between these two paths



number of crosstalk paths increases at least linearly with total length of two paths

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R. Albert, B. DasGupta and N. Mobasheri, Physical Review E 89(3), 032811 (2014)

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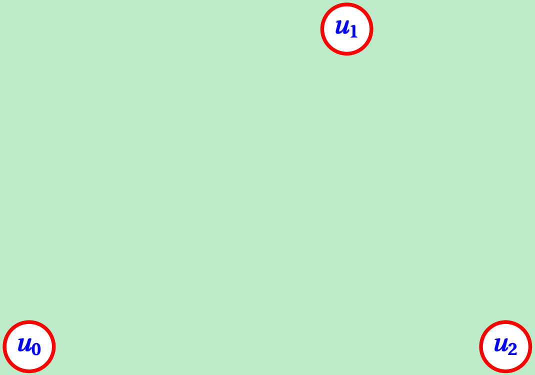
Geodesic triangles and crosstalk paths



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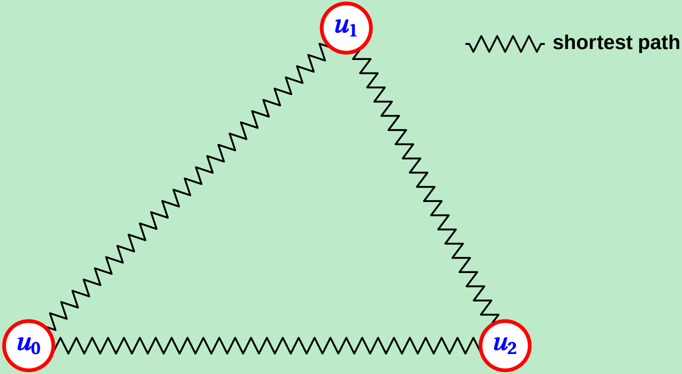
Geodesic triangles and crosstalk paths



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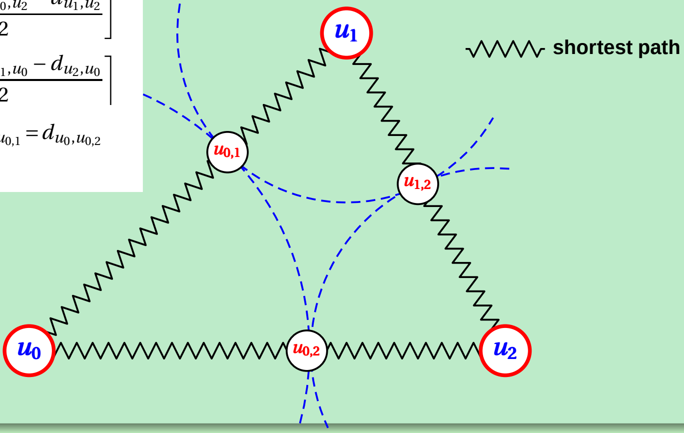
Geodesic triangles and crosstalk paths

$$d_{u_0,u_{0,1}} = \left\lfloor \frac{d_{u_0,u_1} + d_{u_0,u_2} - d_{u_1,u_2}}{2} \right\rfloor$$

$$d_{u_1,u_{0,1}} = \left\lceil \frac{d_{u_1,u_2} + d_{u_1,u_0} - d_{u_2,u_0}}{2} \right\rceil$$

$$d_{u_1,u_{0,1}} = d_{u_1,u_{1,2}} \quad d_{u_0,u_{0,1}} = d_{u_0,u_{0,2}}$$

$$d_{u_2,u_{0,2}} = d_{u_2,u_{1,2}}$$



R. Albert, B. DasGupta and N. Mobasheri, Physical Review E 89(3), 032811 (2014)

Geodesic triangles and crosstalk paths

$\forall\, v$ **in one path** $\exists\, v'$ **in the other path such that** $d_{v,v'} \le \max\{6\delta, 2\}$

$$d_{u_0,u_{0,1}} = \left\lfloor \frac{d_{u_0,u_1} + d_{u_0,u_2} - d_{u_1,u_2}}{2} \right\rfloor$$

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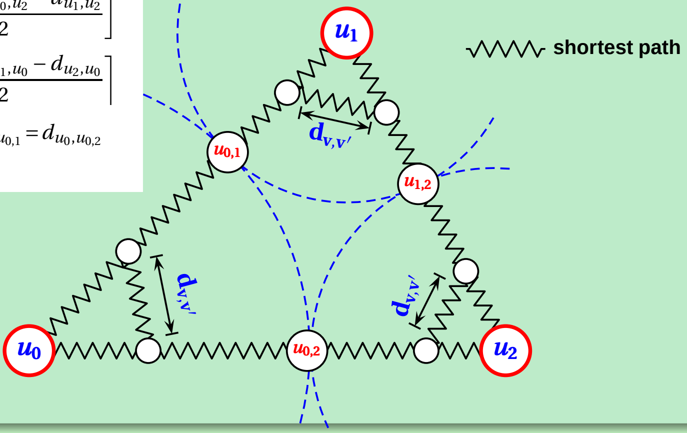


R. Albert, B. DasGupta and N. Mobasheri, Physical Review E 89(3), 032811 (2014)

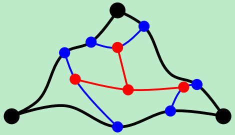
Implications of geodesic triangles for regulatory networks

Consider feedback or feed-forward loop formed by the shortest paths among three nodes

We can expect short cross-talk paths between these shortest paths

⇓

Feedback/feed-forward loop is nested with additional feedback/feed-forward loops



Implications of hyperbolicity

Implications of geodesic triangles and crosstalk paths for regulatory networks

Implications of geodesic triangles for regulatory networks

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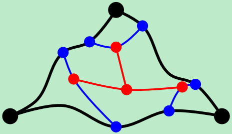
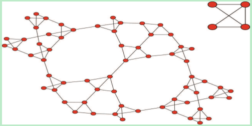


Empirical evidence [R. Albert, Journal of Cell Science 118, 4947-4957 (2005)]

Network motifs[a] are often nested

Two generations of nested assembly for a common *E. coli* motif [DeDeo and Krakauer, 2012]



[a] *e.g.*, feed-forward or feedback loops of small number of nodes

Definition (Hausdorff distance between two paths $\mathscr{P}_1$ and $\mathscr{P}_2$)

$$d_H(\mathscr{P}_1,\mathscr{P}_2) \stackrel{\text{def}}{=} \max\left\{ \max_{v_1\in\mathscr{P}_1} \min_{v_2\in\mathscr{P}_2} \left\{d_{v_1,v_2}\right\}, \max_{v_2\in\mathscr{P}_2} \min_{v_1\in\mathscr{P}_1} \left\{d_{v_1,v_2}\right\} \right\}$$

small Hausdorff distance implies every node of either path is close to some node of the other path

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R. Albert, B. DasGupta and N. Mobasheri, Physical Review E 89(3), 032811 (2014)

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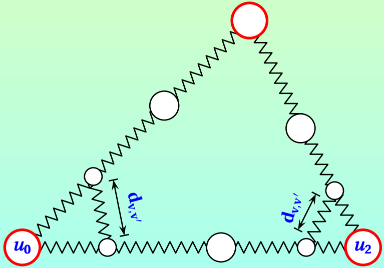
$$d_H(\mathscr{P}_1,\mathscr{P}_2) \stackrel{\text{def}}{=} \max\left\{ \max_{v_1\in\mathscr{P}_1} \min_{v_2\in\mathscr{P}_2} \left\{d_{v_1,v_2}\right\},\ \max_{v_2\in\mathscr{P}_2} \min_{v_1\in\mathscr{P}_1} \left\{d_{v_1,v_2}\right\} \right\}$$

small Hausdorff distance implies every node of either path is close to some node of the other path



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Definition (Hausdorff distance between two paths $\mathscr{P}_1$ and $\mathscr{P}_2$)

$$d_H(\mathscr{P}_1,\mathscr{P}_2) \stackrel{\text{def}}{=} \max\left\{ \max_{v_1\in\mathscr{P}_1} \min_{v_2\in\mathscr{P}_2} \left\{d_{v_1,v_2}\right\}, \max_{v_2\in\mathscr{P}_2} \min_{v_1\in\mathscr{P}_1} \left\{d_{v_1,v_2}\right\} \right\}$$

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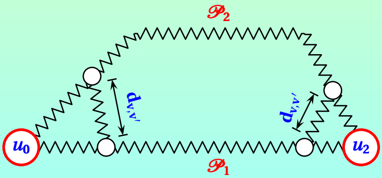

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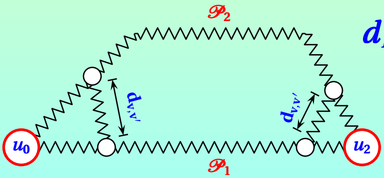

$$d_H(\mathscr{P}_1,\mathscr{P}_2) \leq \max\{6\delta,\ 2\}$$

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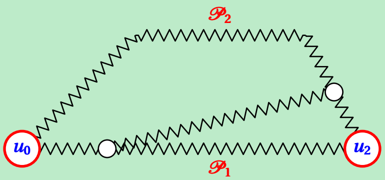
Implications of hyperbolicity

Hausdorff distance between shortest paths

this result versus our previous path-chord result

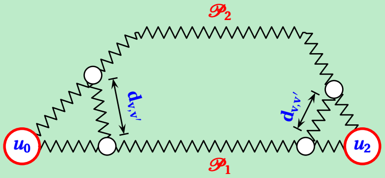
path-chord result



long cycle $\Rightarrow$ there is a path chord

this result

$$d_H(\mathscr{P}_1, \mathscr{P}_2) \leq \max\{6\delta, 2\}$$



Which result is more general in nature ?

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Implications of hyperbolicity

Hausdorff distance between shortest paths

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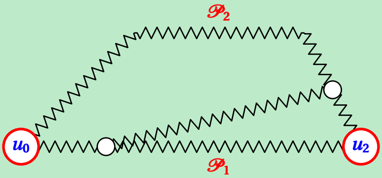

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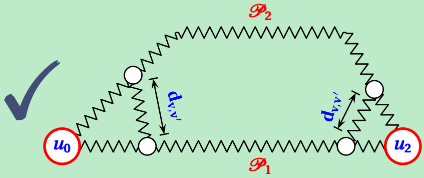
$$d_H(\mathcal{P}_1, \mathcal{P}_2) \leq \max\{6\delta, 2\}$$



Which result is more general in nature ?

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A notational simplification

unless G is a tree or a complete graph (K_n), $\delta > 0$

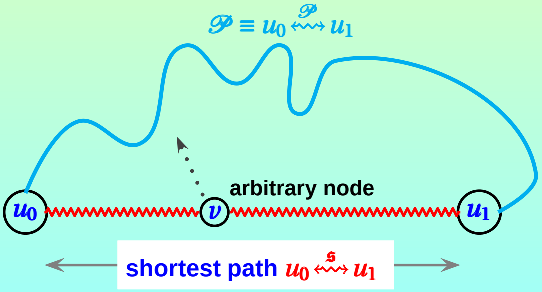
$$\delta > 0 \;\equiv\; \delta \geq 1/2$$

$$\delta \geq 1/2 \;\Rightarrow\; \max\{6\delta, 2\} = 6\delta$$

Hence, we will simply write 6δ instead of $\max\{6\delta, 2\}$

Distance from a shortest path $u_0 \overset{\mathfrak{s}}{\leftrightsquigarrow} u_1$ to another arbitrary path $u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$

n is the number of nodes in the graph **$\ell(\mathscr{P})$ is length of path $\mathscr{P}$**



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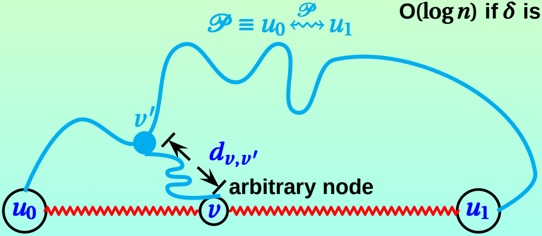
n is the number of nodes in the graph **$\ell(\mathscr{P})$ is length of path $\mathscr{P}$**

$$\exists v' \; d_{v,v'} \leq \underbrace{6\delta \log_2 \ell(\mathscr{P})}_{< \, 6\delta \log_2 n}$$

O($\log n$) if δ is constant



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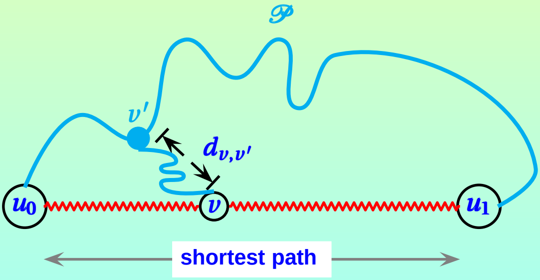
An interesting implication of this bound

$$\exists v' \;\; d_{v,v'} \le 6\delta \log_2 \ell(\mathscr{P})$$



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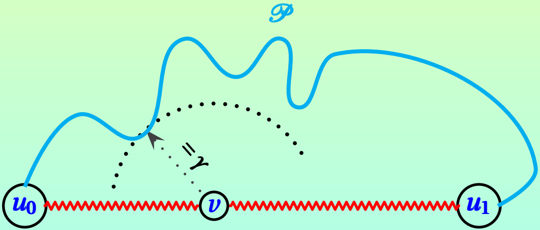
An interesting implication of this bound

assume $\forall\, v' \in \mathscr{P}\ \ d_{v,v'} \geq \gamma$



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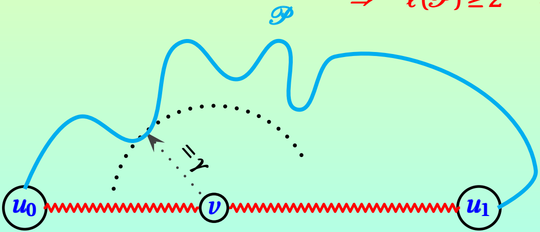
An interesting implication of this bound

assume $\forall\, v' \in \mathscr{P}\;\; d_{v,v'} \geq \gamma$

$$\Rightarrow \quad \ell(\mathscr{P}) \geq 2^{\frac{\gamma}{6\delta}} = \Omega\left(2^{\Omega(\gamma)}\right)$$

if δ is constant



Next: better bounds for approximately short paths ▸

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Implications of hyperbolicity

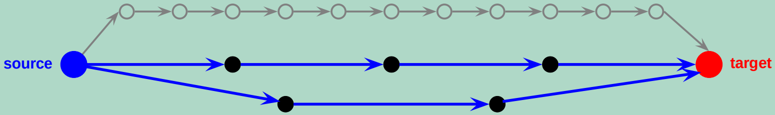
Approximately short path

Why consider approximately short paths ?

Regulatory networks

Up/down-regulation of a target node is mediated by two or more "close to shortest" paths starting from the same regulator node

Additional "very long" paths between the same regulator and target node do *not* contribute significantly to the target node's regulation



Definition ε-additive-approximate short path $\mathscr{P}$

$$\underbrace{\ell(\mathscr{P})}_{\text{length of } \mathscr{P}} \leq \text{length of shortest path } + \varepsilon$$

Why consider approximately short paths ?

Algorithmic efficiency reasons

Approximate short path may be faster to compute as opposed to exact shortest path

Routing and navigation problems (traffic networks)

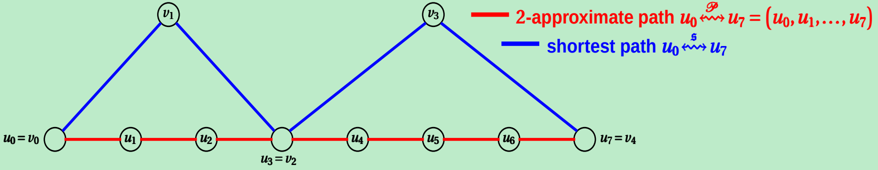
Routing via approximate short path

Definition μ-approximate short path $u_0 \overset{\mathcal{P}}{\leftrightsquigarrow} u_k = (u_0, u_1, \dots, u_k)$

$$\ell(u_i \overset{\mathcal{P}}{\leftrightsquigarrow} u_j) \leq \mu \;\; d_{u_i,u_j} \quad \text{for all } 0 \leq i < j \leq k$$

length of sub-path from u_i to u_j

distance between u_i and u_j

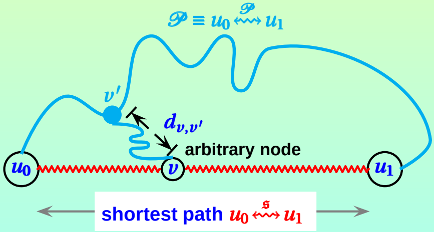


Implications of hyperbolicity

Distance between geodesic and approximately short path

Distance from shortest path to an approximately short path $u_0 \overset{\mathcal{P}}{\leftrightsquigarrow} u_1$

(approximately short: ε-additive approximate or, μ-approximate)



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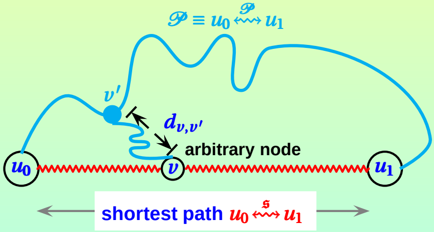

$u_0 \overset{\mathcal{P}}{\leftrightsquigarrow} u_1$ is ε-additive approximate

$$\forall\, v\ \exists\, v' \quad d_{v,v'} \leq \left(6\delta+2\right)\log_2\left(8\left(6\delta+2\right)\log_2\left[\left(6\delta+2\right)\left(4+2\varepsilon\right)\right]+1+\frac{\varepsilon}{2}\right)$$

$$O\left(\delta\log\left(\varepsilon+\delta\log\varepsilon\right)\right)$$

depends only on δ and ε

short crosstalk path for small ε and δ

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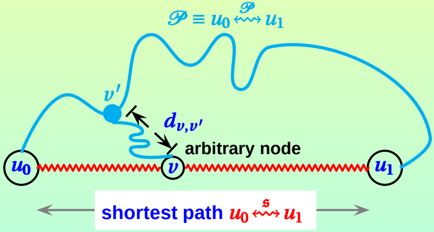
Distance from shortest path to an approximately short path $u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$

(approximately short: ε-additive approximate or, μ-approximate)



$u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$ is μ-approximate

$$\forall\, v\ \exists\, v' \quad d_{v,v'} \leq \left(6\delta+2\right)\log_2\left(\left(6\mu+2\right)\left(6\delta+2\right)\log_2\left[\left(6\delta+2\right)\left(3\mu+1\right)\mu\right]+\mu\right)$$

$O\left(\delta\log\left(\mu\delta\right)\right)$ — **depends only on δ and μ**

short crosstalk path for small μ and δ

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Contrast the new bounds with the old bound of $d_{v,v'} = O(\delta \log \ell(\mathscr{P}))$

d_{u_0,u_1} is the length of a shortest path between u_0 and u_1

$u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$ is ε-additive approximate

$\ell(\mathscr{P}) \leq d_{u_0,u_1} + \varepsilon$

Old bound

$O(\delta \log(\varepsilon + d_{u_0,u_1}))$

New bound

$O(\delta \log(\varepsilon + \delta \log \varepsilon))$ no dependency on d_{u_0,u_1}

$u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$ is μ-approximate

$\ell(\mathscr{P}) \leq \mu \, d_{u_0,u_1}$

Old bound

$O(\delta (\log(\mu \, d_{u_0,u_1})))$

New bound

$O(\delta \log(\mu\delta))$ no dependency on d_{u_0,u_1}

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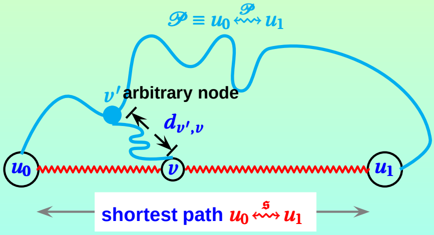
Distance between geodesic and approximately short path

Distance from an approximately short path $u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$ to a shortest path

approximately short: ε-additive approximate
or, μ-approximate

for simplified exposition, we show bounds only in asymptotic $O(\cdot)$ notation
please refer to our paper for more precise bounds



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Implications of hyperbolicity

Distance between geodesic and approximately short path

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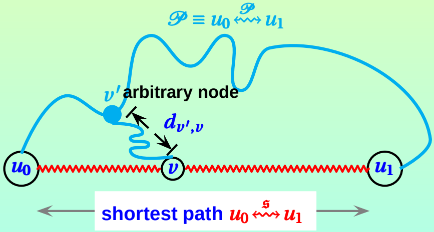

$u_0 \overset{\mathscr{P}}{\leftrightsquigarrow} u_1$ is ε-additive approximate

$\forall v' \, \exists v \;\; d_{v',v} \leq O(\varepsilon + \delta \log(\varepsilon + \delta \log \varepsilon))$ depends only on δ and ε

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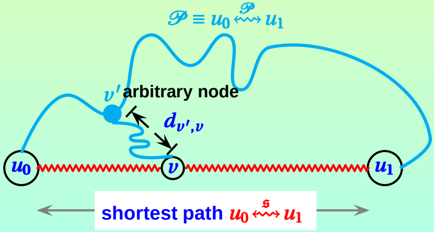
Distance from an approximately short path $u_0 \overset{\mathscr{P}}{\rightsquigarrow} u_1$ to a shortest path

ε-additive approximate

or, μ-approximate

for simplified exposition, we show bounds only in asymptotic $O(\cdot)$ notation

please refer to our paper for more precise bounds



$u_0 \overset{\mathscr{P}}{\rightsquigarrow} u_1$ is μ-approximate

$\forall v' \, \exists v \;\; d_{v',v} \leq O(\mu\delta \log(\mu\delta))$ **depends only on δ and μ**

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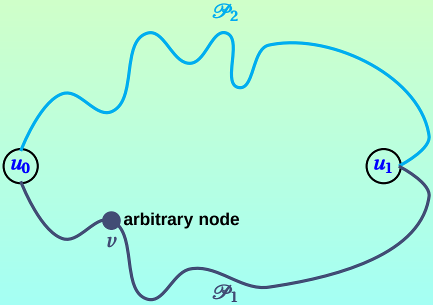
Distance between geodesic and approximately short path

Distance from approximate short path $\mathcal{P}_1$ (arbitrary node v) to approximate short path $\mathcal{P}_2$ (nearest node v')



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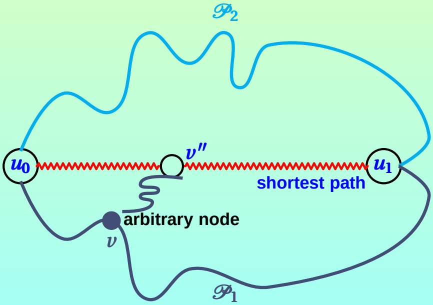
Implications of hyperbolicity

Distance between geodesic and approximately short path

Distance **from approximate short path $\mathscr{P}_1$** (arbitrary node v) **to approximate short path $\mathscr{P}_2$** (nearest node v')



go to any shortest path

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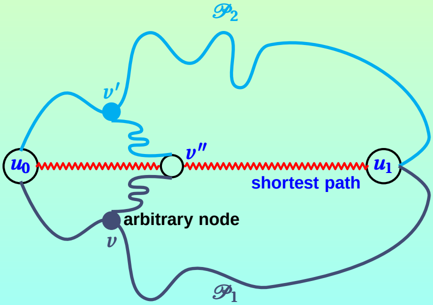
Distance from approximate short path $\mathscr{P}_1$ (arbitrary node v) to approximate short path $\mathscr{P}_2$ (nearest node v')



continue to the other path

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Implications of hyperbolicity

Distance between geodesic and approximately short path

Distance $\underbrace{\text{from approximate short path } \mathscr{P}_1}_{\text{arbitrary node } v}$ $\underbrace{\text{to approximate short path } \mathscr{P}_2}_{\text{nearest node } v'}$

we sometimes overestimate quantities to simplify expression

$\mathscr{P}_1$ is ε_1-additive approximate
$\mathscr{P}_2$ is ε_2-additive approximate

$$O\left(\varepsilon_1 + \delta \log(\varepsilon_1 \varepsilon_2) + \delta \log \delta\right)$$

$\mathscr{P}_1$ is ε-additive approximate
$\mathscr{P}_2$ is μ-approximate

$$O\left(\varepsilon + \delta \log(\varepsilon\mu) + \delta^2 \log\log \varepsilon\right)$$

$\mathscr{P}_1$ is μ-approximate
$\mathscr{P}_2$ is ε-additive approximate

$$O\left(\mu\delta \log(\mu\delta) + \varepsilon + \delta \log \varepsilon\right)$$

$\mathscr{P}_1$ is μ_1-approximate
$\mathscr{P}_2$ is μ_2-approximate

$$O\left(\mu_1\delta \log(\mu_1\delta) + \delta \log \mu_2\right)$$

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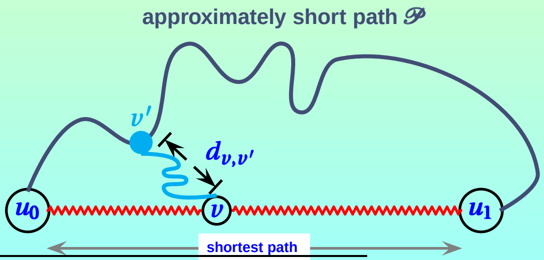
Interesting implications of these improved bounds



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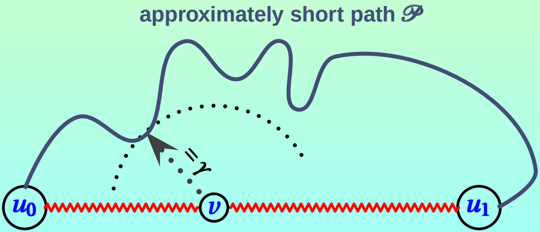
Interesting implications of these improved bounds

assume $\forall\, v' \in \mathscr{P} \;\; d_{v,v'} \geq \gamma$



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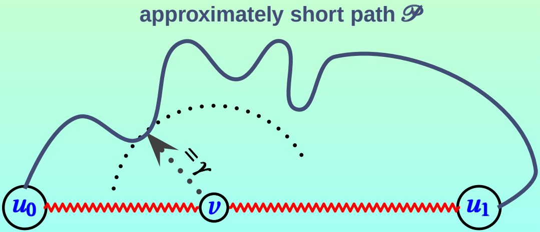
Interesting implications of these improved bounds

assume $\forall\, v' \in \mathscr{P}\;\; d_{v,v'} \geq \gamma \quad \Rightarrow$

if $\mathscr{P}$ is ε-additive-approximate short then

$$\varepsilon = \Omega\left(\frac{2^{\gamma/\delta}}{\delta} - \log\delta\right)$$



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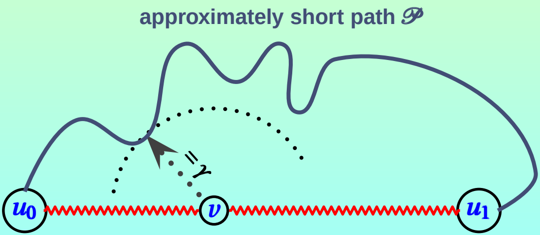
Interesting implications of these improved bounds

assume $\forall\, v' \in \mathscr{P}\;\; d_{v,v'} \geq \gamma$ $\Rightarrow$ if $\mathscr{P}$ is μ-approximate short then

$$\mu = \Omega\left(\frac{2^{\gamma/\delta}}{\gamma}\right)$$



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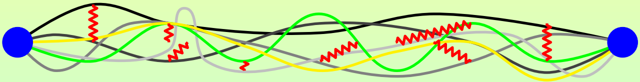
Implications of hyperbolicity

Distance between geodesic and approximately short path

To wrap it up, approximate shortest paths look like the following cartoon



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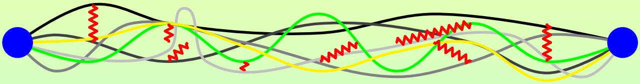

Interpretation for regulatory networks

- **It is reasonable to assume that, when up- or down-regulation of a target node is mediated by two or more approximate short paths starting from the same regulator node, additional very long paths between the same regulator and target node do not contribute significantly to the target node's regulation**
- **We refer to the short paths as relevant, and to the long paths as irrelevant**
- **Then, our finding can be summarized by saying that**

  almost all relevant paths between two nodes have crosstalk paths between each other

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Outline of talk

UIC

Influence of a node on the geodesics between other pair of nodes

integer parameters used in this result

	$\kappa \geq 4$	$\alpha > 0$	$r > 3(\kappa - 2)\delta$
Example:	5	1	$9\delta + 1$

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Implications of hyperbolicity

Identifying essential edges and nodes in regulatory networks

Influence of a node on the geodesics between other pair of nodes

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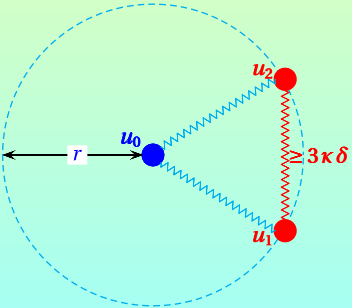

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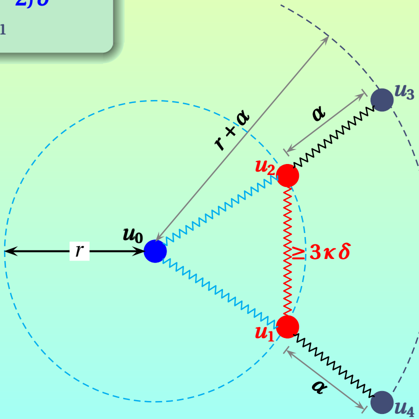

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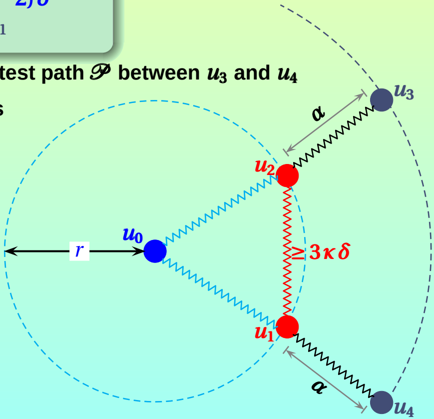
consider any shortest path $\mathscr{P}$ between u_3 and u_4

$\mathscr{P}$ must look like this



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Influence of a node on the geodesics between other pair of nodes

integer parameters used in this result

	$\kappa \geq 4$	$\alpha > 0$	$r > 3(\kappa - 2)\delta$
Example:	5	1	$9\delta + 1$

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$$\gamma = d_{u_0,v} \leq \quad r - \left(\tfrac{3}{2}\kappa - 1\right)\delta$$

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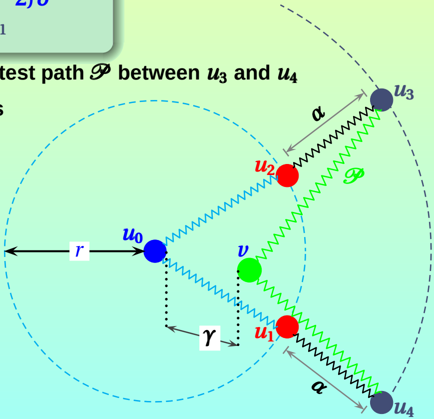

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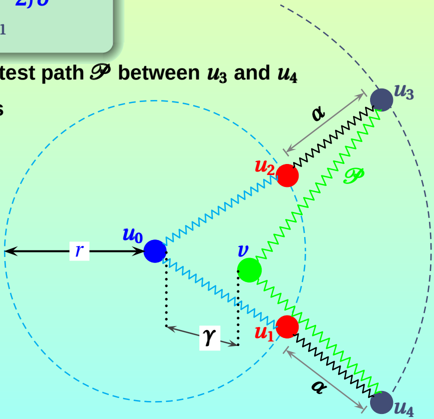
$$r - \Theta(\kappa\delta)$$

$$\ell(\mathscr{P}) \geq \quad (3\kappa-2)\delta + 2\alpha$$

$$\Omega(\kappa\delta + \alpha)$$



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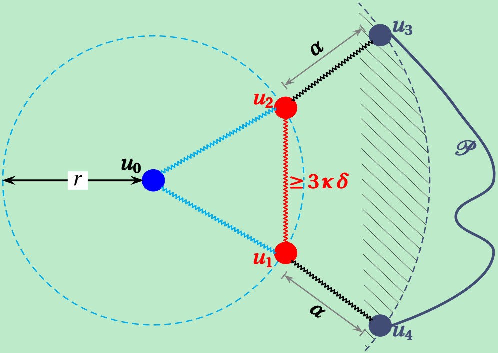
Influence of a node on the geodesics between other pair of nodes

Corollary (of previous results)

consider any path $\mathscr{P}$ between u_3 and u_4

suppose that $\mathscr{P}$ does not intersect the shaded region



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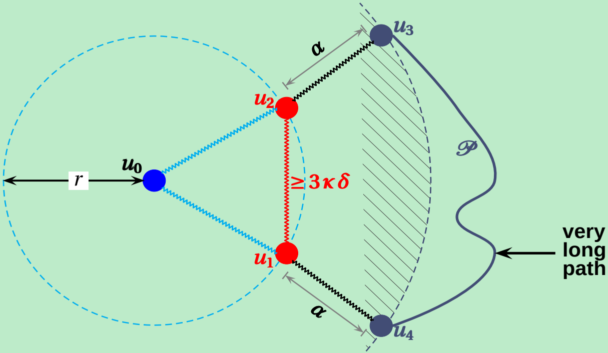
$$\ell(\mathscr{P}) \geq 2^{\frac{\alpha}{6\delta}+\frac{\kappa}{4}}$$

$$2^{\Omega\left(\frac{\alpha}{\delta}+\kappa\right)}$$



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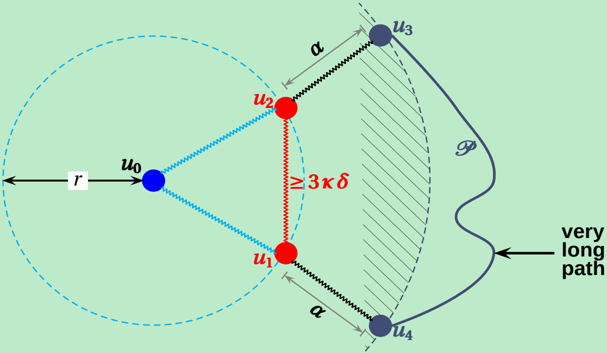
$\mathscr{P}$ ε-additive-approximate $\Rightarrow$

$\varepsilon > \frac{2^{\frac{\alpha}{6\delta}+\frac{\kappa}{4}}}{48\delta} - \log_2(48\delta)$

$\Omega\left(2^{\Theta(\alpha+\kappa)}\right)$ **if δ is constant**



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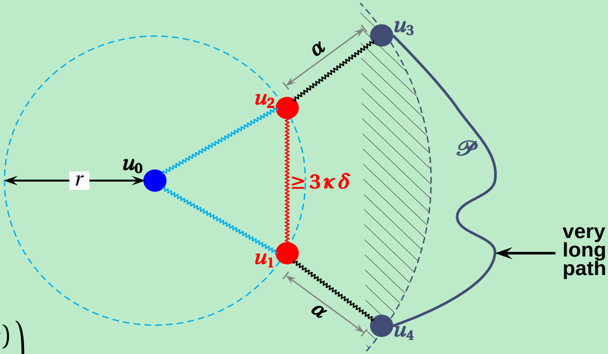
$\mathscr{P}$ **μ-approximate $\Rightarrow$**

$$\mu \geq \frac{2^{\frac{\alpha}{6\delta}}+\frac{\kappa}{4}}{12\alpha+6\delta\left(3\kappa-26\right)}$$

$$\Omega\left(\frac{2^{\Theta\left(\frac{\alpha}{\delta}+\kappa\right)}}{\alpha+\kappa\delta}\right)$$



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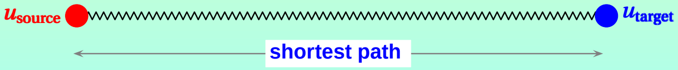
Interesting implications of these bounds for regulatory networks



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Implications of hyperbolicity

Identifying essential edges and nodes in regulatory networks

Interesting implications of these bounds for regulatory networks

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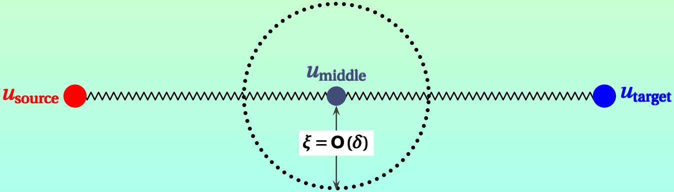

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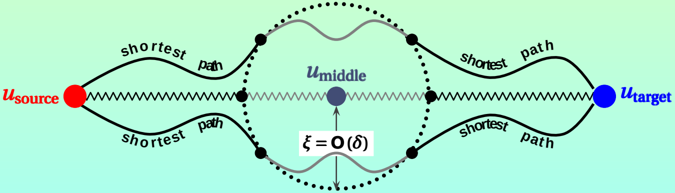
Interesting implications of these bounds for regulatory networks

All shortest paths between u_{source} and u_{target} must intersect the ξ-neighborhood

Therefore, "knocking out" nodes in ξ-neighborhood cuts off all shortest regulatory paths between u_{source} and u_{target}



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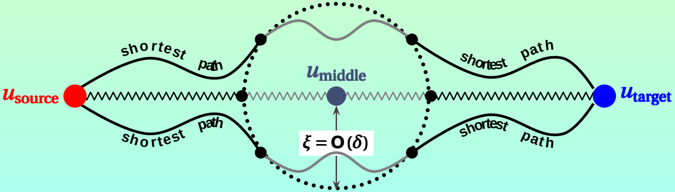
Interesting implications of these bounds for regulatory networks

But, it gets even more interesting !



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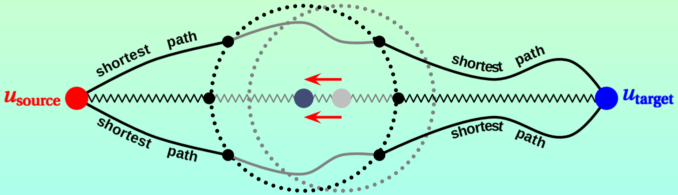
Interesting implications of these bounds for regulatory networks

But, it gets even more interesting !

shifting the ξ-neighborhood does not change claim



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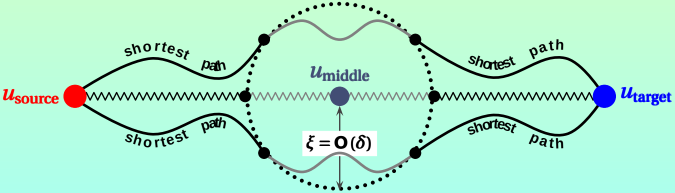
Interesting implications of these bounds for regulatory networks

how about enlarging the ξ-neighborhood ?



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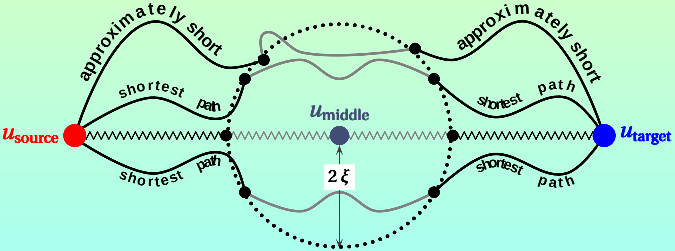
Interesting implications of these bounds for regulatory networks

how about enlarging the ξ-neighborhood ?

approximately short paths start intersecting the neighborhood



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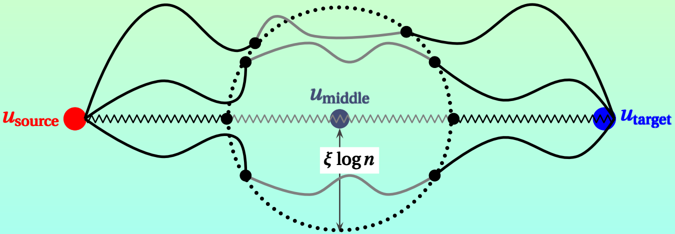
Interesting implications of these bounds for regulatory networks

Consider a ball (neighborhood) of radius $\xi \log n$ **(n is the number of nodes)**



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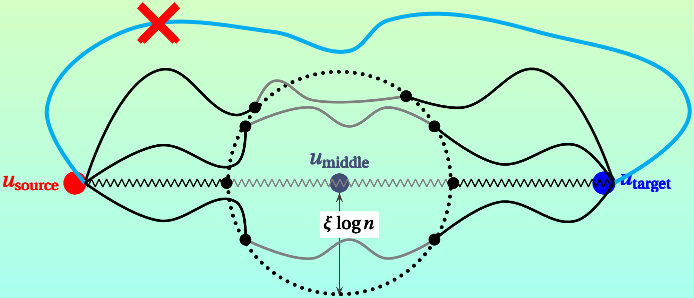
Interesting implications of these bounds for regulatory networks

Consider a ball (neighborhood) of radius $\xi \log n$ (n is the number of nodes)

All paths intersect the neighborhood



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Implications of hyperbolicity

Identifying essential edges and nodes in regulatory networks

Empirical estimation of neighborhoods and number of essential nodes

We empirically investigated these claims on relevant paths passing through a neighborhood of a central node for the following two biological networks:

- ***E. coli* transcriptional**
- **T-LGL signaling**

by selecting a few biologically relevant source-target pairs

Our results show much better bounds for real networks compared to the worst-case pessimistic bounds in the mathematical theorems

see our paper for further details

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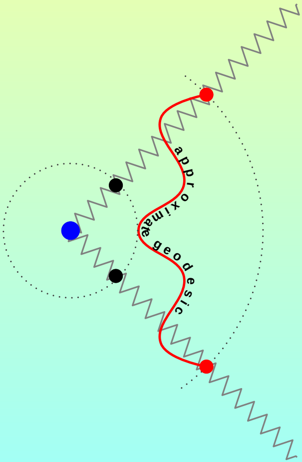
The following cartoon informally depicts some of the preceding discussions



Implications of hyperbolicity

Identifying essential edges and nodes in regulatory networks

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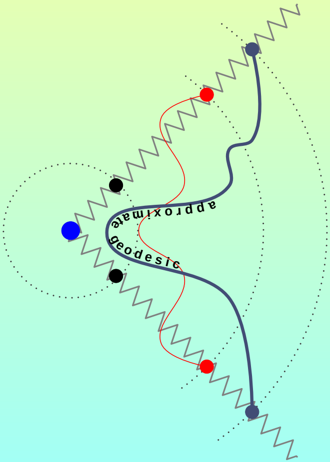

Implications of hyperbolicity

Identifying essential edges and nodes in regulatory networks

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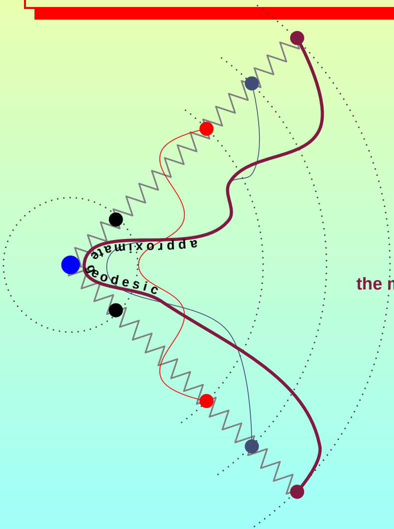
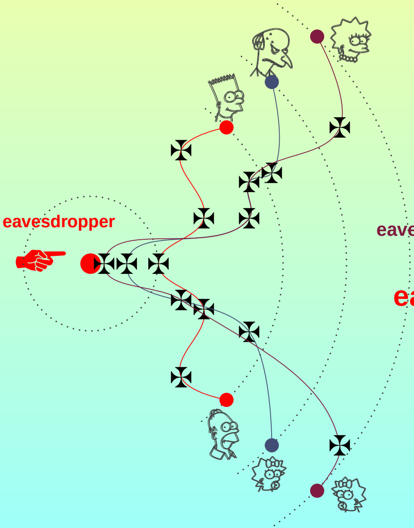


the further we move from the central node

the more a shortest path bends inward towards the central node

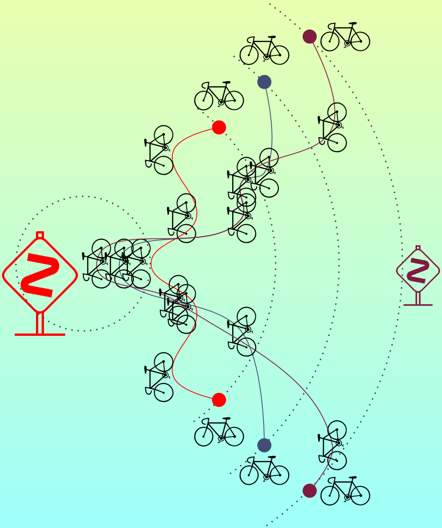


eavesdropper may succeed with limited sensor range

eavesdropper need not be a hub

Implications of hyperbolicity

Identifying essential edges and nodes in regulatory networks



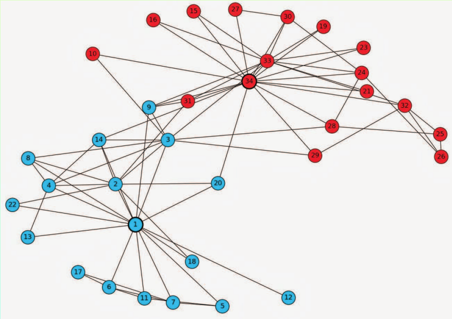
Traffic network

need not be a hub

Outline of talk

UIC

Visual illustration of a well-known social network



Zachary's Karate Club (http://networkdata.ics.uci.edu/data.php?id=105)

Structural hole in a social network [Burt, 1995; Borgatti, 1997]

Definition (Adjacency matrix of an undirected unweighted graph)

$$\begin{array}{c|ccccc|} & & & u & & \\ & \cdots & \cdots & \cdots & \cdots & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots \\ v & \cdots & \cdots & a_{u,v} & \cdots & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \vdots \\ & \cdots & \cdots & \cdots & \cdots & \cdots \end{array}$$

$$a_{u,v} = \begin{cases} 1, & \text{if } \{u,v\} \text{ is an edge} \\ 0, & \text{otherwise} \end{cases}$$

Definition (measure of structural hole at node u [Burt, 1995; Borgatti, 1997])

(assume u has degree at least 2)

$$\mathfrak{M}_u \stackrel{\text{def}}{=} \sum_{v \in V} \left(\frac{a_{u,v} + a_{v,u}}{\max_{x \neq u} \{a_{u,x} + a_{x,u}\}} \left[1 - \sum_{\substack{y \in V \\ y \neq u,v}} \left(\frac{a_{u,y} + a_{y,u}}{\sum_{x \neq u} (a_{u,x} + a_{x,u})} \right) \left(\frac{a_{v,y} + a_{y,v}}{\max_{z \neq y} \{a_{v,z} + a_{z,v}\}} \right) \right] \right)$$

too complicated ☹

Structural hole in a social network [Burt, 1995; Borgatti, 1997]

Definition (Adjacency matrix of an undirected unweighted graph)

$$v \begin{pmatrix} \cdots & \cdots & \overset{u}{\cdots} & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & \cdots & a_{u,v} & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} \qquad a_{u,v} = \begin{cases} 1, & \text{if } \{u,v\} \text{ is an edge} \\ 0, & \text{otherwise} \end{cases}$$

Definition (measure of structural hole at node u [Burt, 1995; Borgatti, 1997])

(assume u has degree at least 2)

Let $\text{Nbr}(u)$ be set of nodes adjacent to u

$$\mathfrak{M}_u = \left|\text{Nbr}(u)\right| - \frac{\sum_{v,y \in \text{Nbr}(u)} a_{v,y}}{\left|\text{Nbr}(u)\right|}$$

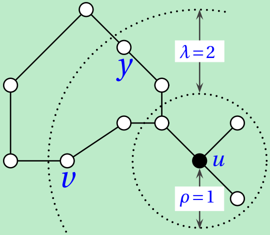
Next: An intuitive interpretation of $\mathfrak{M}_u$ ►

An intuitive interpretation of $\mathfrak{M}_u$

Definition (weak dominance $\prec_{\text{weak}}^{\rho,\lambda}$)

Nodes v, y are weakly (ρ,λ)-dominated by node u provided

- $\rho < d_{u,v}, d_{u,y} \leq \rho+\lambda$, and
- for at least one shortest path $\mathscr{P}$ between v and y, $\mathscr{P}$ contains a node z such that $d_{u,z} \leq \rho$



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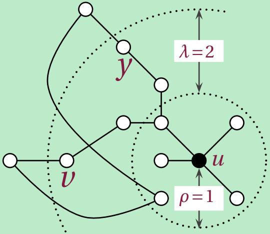


An intuitive interpretation of $\mathfrak{M}_u$

Notation (boundary of the ξ-neighborhood of node u)

$\mathcal{B}_\xi(u) = \{ v \mid d_{u,v} = \xi \}$ — the set of all nodes at a distance of precisely ξ from u

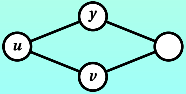
Observation

$$\mathfrak{M}_u = \mathbb{E}\left[\text{number of pairs of nodes } v,y \text{ such that } v,y \text{ is weakly } (\underset{\rho}{0},\underset{\lambda}{1})\text{-dominated by } u \;\middle|\; v \text{ is selected uniformly randomly from } \bigcup_{\underset{\rho}{0} < j \le \underset{\lambda}{1}} \mathcal{B}_j(u) \right]$$

$$\geq \mathbb{E}\left[\text{number of pairs of nodes } v,y \text{ such that } v,y \text{ is strongly } (0,1)\text{-dominated by } u \;\middle|\; v \text{ is selected uniformly randomly from } \bigcup_{0 < j \le 1} \mathcal{B}_j(u) \right]$$

always true

equality does not hold in general



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Generalize $\mathfrak{M}_u$ to $\mathfrak{M}_{u,\rho,\lambda}$ for larger ball of influence of a node
replace $(0,1)$ by (ρ,λ)

$$\mathfrak{M}_u = \mathbb{E}\left[\text{number of pairs of nodes } v,y \text{ such that } v,y \text{ is weakly } (\underset{\rho}{0},\underset{\lambda}{1})\text{-dominated by } u \;\middle|\; v \text{ is selected uniformly randomly from } \bigcup_{\underset{\rho}{0}<j\leq\underset{\lambda}{1}} \mathscr{B}_j(u) \right]$$

$$\mathfrak{M}_{u,\rho,\lambda} = \mathbb{E}\left[\text{number of pairs of nodes } v,y \text{ such that } v,y \text{ is weakly } (\rho,\lambda)\text{-dominated by } u \;\middle|\; v \text{ is selected uniformly randomly from } \bigcup_{\rho<j\leq\lambda} \mathscr{B}_j(u) \right]$$

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Generalize $\mathfrak{M}_u$ to $\mathfrak{M}_{u,\rho,\lambda}$ for larger ball of influence of a node

replace $(0,1)$ by (ρ,λ)

Lemma (equivalence of strong and weak domination)

If $\lambda \geq 6\delta \log_2 n$ then

$$\mathfrak{M}_{u,\rho,\lambda} \stackrel{\text{def}}{=} \mathbb{E}\left[\text{number of pairs of nodes } v,y \text{ such that } v,y \text{ is weakly } (\rho,\lambda)\text{-dominated by } u \;\middle|\; v \text{ is selected uniformly randomly from } \bigcup_{\rho<j\leq\lambda} \mathcal{B}_j(u) \right]$$

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↑ **equality holds now**

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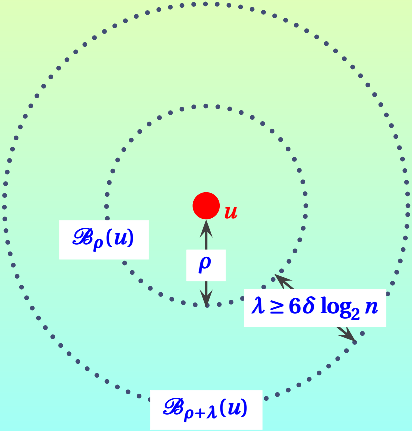

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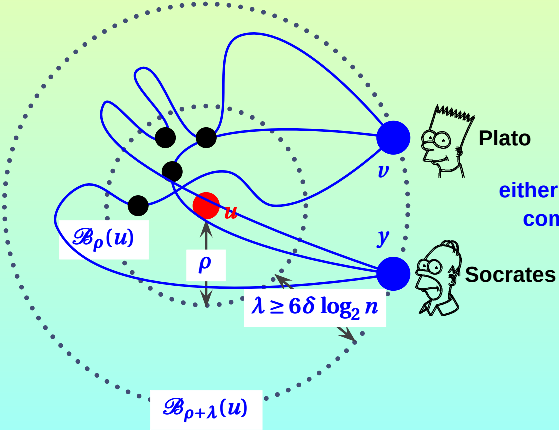
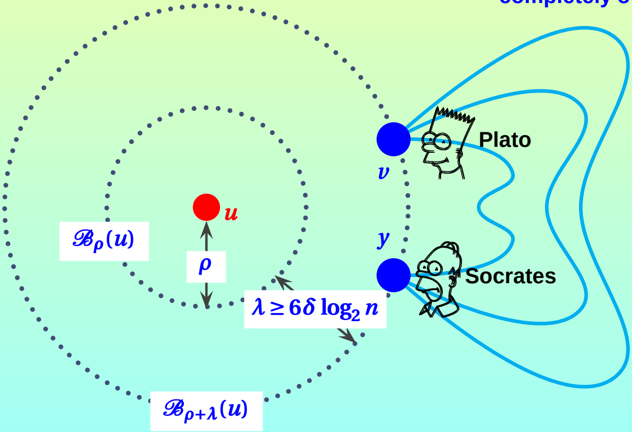


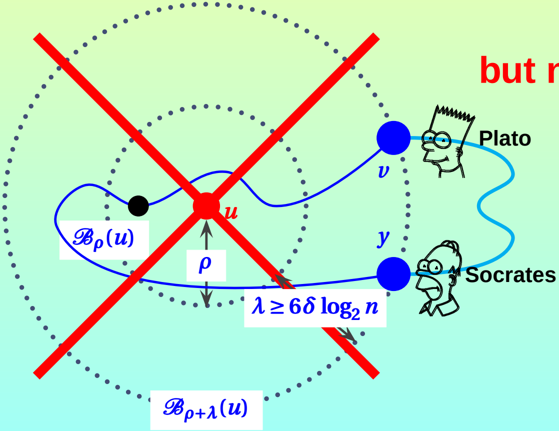
either all the shortest paths are completely inside $\mathcal{B}_{\rho+\lambda}(u)$

What does this lemma mean intuitively ?

or all the shortest paths are completely outside of $\mathscr{B}_{\rho+\lambda}(u)$



What does this lemma mean intuitively ?



but not both !

Thank you for your attention

Questions??

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