Fine-Grained Complexity
Week 12

17.1.22

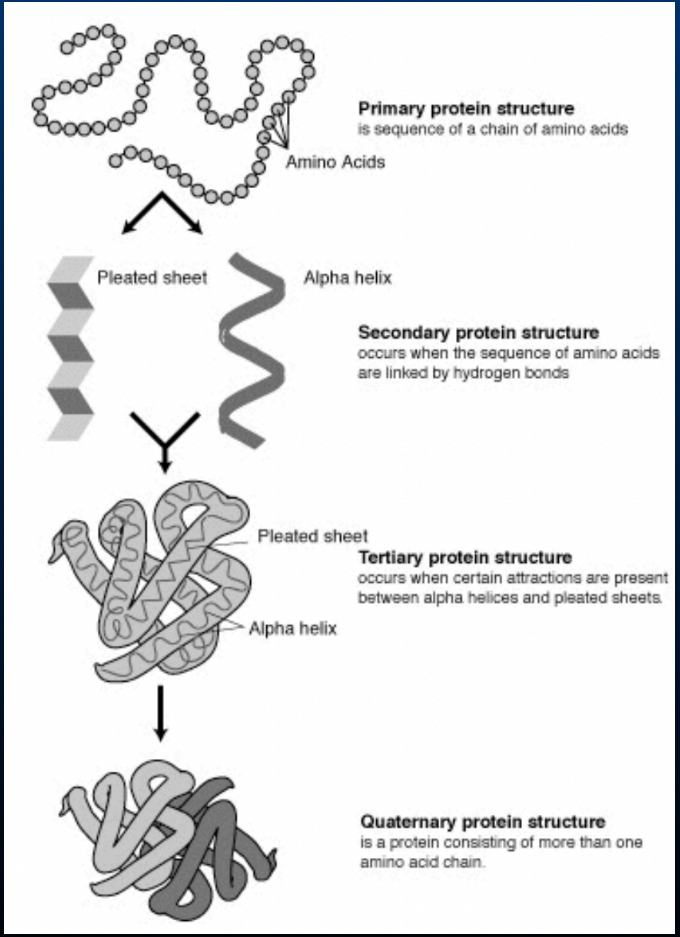
Input: Genome (1D)

Today: RNA Folding (2D)

Real Goal: Protein Folding (3D)

NP-Hard

"Solved" by AlphaFold



From Wikipedia

RNA Folding

"Maximum matching on a line"

Input: A sequence in $\{A,C,G,T\}^n$.

Output: Maximum number of **non-crossing** matches.

Matches:
A - T
C - G

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A C C G A A C T C C G G T A

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Matches:
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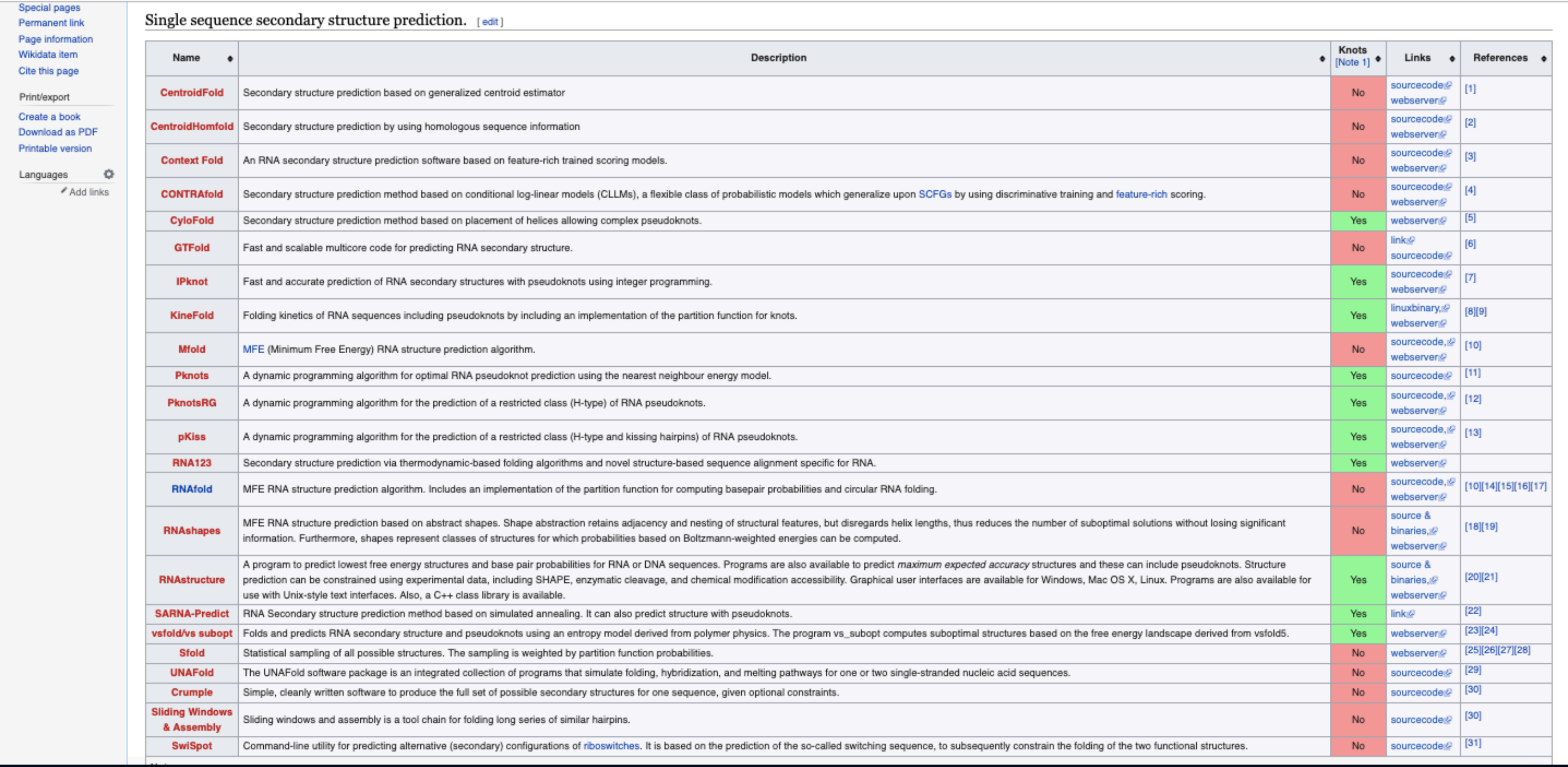
C - G

In general: A sequence in $(\Sigma \cup \Sigma')^n$.

$\forall \sigma \in \Sigma$: there is a unique match $\sigma' \in \Sigma'$.

List of RNA Folding Algorithms



Single sequence secondary structure prediction.

Name	Description	Knots [Note 1]	Links	References
CentroidFold	Secondary structure prediction based on generalized centroid estimator	No	sourcecode webserver	[1]
CentroidHomfold	Secondary structure prediction by using homologous sequence information	No	sourcecode webserver	[2]
Context Fold	An RNA secondary structure prediction software based on feature-rich trained scoring models.	No	sourcecode webserver	[3]
CONTRAfold	Secondary structure prediction method based on conditional log-linear models (CLLMs), a flexible class of probabilistic models which generalize upon SCFGs by using discriminative training and feature-rich scoring.	No	sourcecode webserver	[4]
CyloFold	Secondary structure prediction method based on placement of helices allowing complex pseudoknots.	Yes	webserver	[5]
GTFold	Fast and scalable multicore code for predicting RNA secondary structure.	No	link sourcecode	[6]
IPknot	Fast and accurate prediction of RNA secondary structures with pseudoknots using integer programming.	Yes	sourcecode webserver	[7]
KineFold	Folding kinetics of RNA sequences including pseudoknots by including an implementation of the partition function for knots.	Yes	linuxbinary, webserver	[8][9]
Mfold	MFE (Minimum Free Energy) RNA structure prediction algorithm.	No	sourcecode, webserver	[10]
Pknots	A dynamic programming algorithm for optimal RNA pseudoknot prediction using the nearest neighbour energy model.	Yes	sourcecode	[11]
PknotsRG	A dynamic programming algorithm for the prediction of a restricted class (H-type) of RNA pseudoknots.	Yes	sourcecode, webserver	[12]
pKiss	A dynamic programming algorithm for the prediction of a restricted class (H-type and kissing hairpins) of RNA pseudoknots.	Yes	sourcecode, webserver	[13]
RNA123	Secondary structure prediction via thermodynamic-based folding algorithms and novel structure-based sequence alignment specific for RNA.	Yes	webserver	
RNAfold	MFE RNA structure prediction algorithm. Includes an implementation of the partition function for computing basepair probabilities and circular RNA folding.	No	sourcecode, webserver	[10][14][15][16][17]
RNAshapes	MFE RNA structure prediction based on abstract shapes. Shape abstraction retains adjacency and nesting of structural features, but disregards helix lengths, thus reduces the number of suboptimal solutions without losing significant information. Furthermore, shapes represent classes of structures for which probabilities based on Boltzmann-weighted energies can be computed.	No	source & binaries, webserver	[18][19]
RNAstructure	A program to predict lowest free energy structures and base pair probabilities for RNA or DNA sequences. Programs are also available to predict *maximum expected accuracy* structures and these can include pseudoknots. Structure prediction can be constrained using experimental data, including SHAPE, enzymatic cleavage, and chemical modification accessibility. Graphical user interfaces are available for Windows, Mac OS X, Linux. Programs are also available for use with Unix-style text interfaces. Also, a C++ class library is available.	Yes	source & binaries, webserver	[20][21]
SARNA-Predict	RNA Secondary structure prediction method based on simulated annealing. It can also predict structure with pseudoknots.	Yes	link	[22]
vsfold/vs subopt	Folds and predicts RNA secondary structure and pseudoknots using an entropy model derived from polymer physics. The program vs_subopt computes suboptimal structures based on the free energy landscape derived from vsfold5.	Yes	webserver	[23][24]
Sfold	Statistical sampling of all possible structures. The sampling is weighted by partition function probabilities.	No	webserver	[25][26][27][28]
UNAFold	The UNAFold software package is an integrated collection of programs that simulate folding, hybridization, and melting pathways for one or two single-stranded nucleic acid sequences.	No	sourcecode	[29]
Crumple	Simple, cleanly written software to produce the full set of possible secondary structures for one sequence, given optional constraints.	No	sourcecode	[30]
Sliding Windows & Assembly	Sliding windows and assembly is a tool chain for folding long series of similar hairpins.	No	sourcecode	[30]
SwiSpot	Command-line utility for predicting alternative (secondary) configurations of riboswitches. It is based on the prediction of the so-called switching sequence, to subsequently constrain the folding of the two functional structures.	No	sourcecode	[31]

RNA Folding is in P

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Output: Maximum number of **non-crossing** matches.

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A - T
C - G

$$A\ C\ C\ \boxed{\overset{i}{G}\ A\ A\ C\ T\ C\ C\ A\ C\ \overset{j}{C}}\ G\ G\ T\ A$$

$$D[i,j] = OPT(x[i,\ldots,j]) =$$

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$$\mathrm{A\ C\ C}\boxed{\mathrm{G\ A\ A\ C\ T\ C\ C\ A\ C\ C}}\mathrm{G\ G\ T\ A}$$

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$n^2 \cdot n$

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Thm: RNA Folding is in $O(n^3)$ time.

Quadratic Lower Bound?

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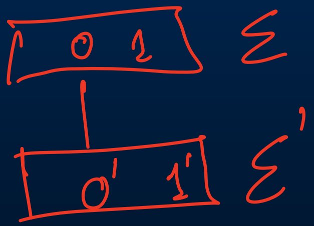
Longest Common Subsequence (LCS) → RNA Folding

n

$2n$



$\Sigma \cup \Sigma'$

$0 - 0'$

Thm: $O(n^{2-\varepsilon})$ for RNA Folding refutes SETH.

Quadratic Lower Bound?

Longest Common Subsequence (LCS) → RNA Folding

x

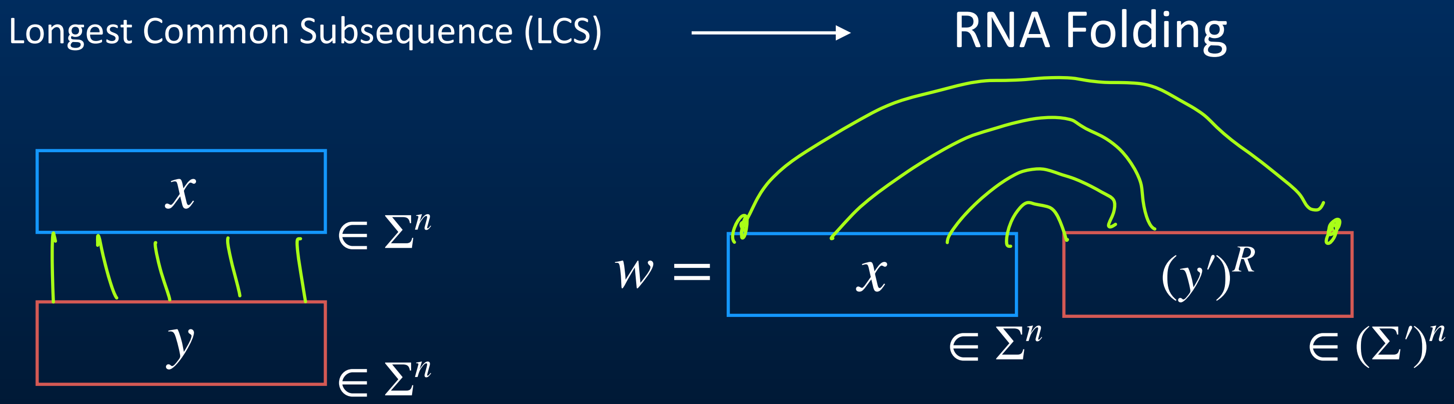
y

$w =$

$$OPT_{RNA}(w) = LCS(x, y)$$

Thm: $O(n^{2-\varepsilon})$ for RNA Folding refutes SETH.

Quadratic Lower Bound?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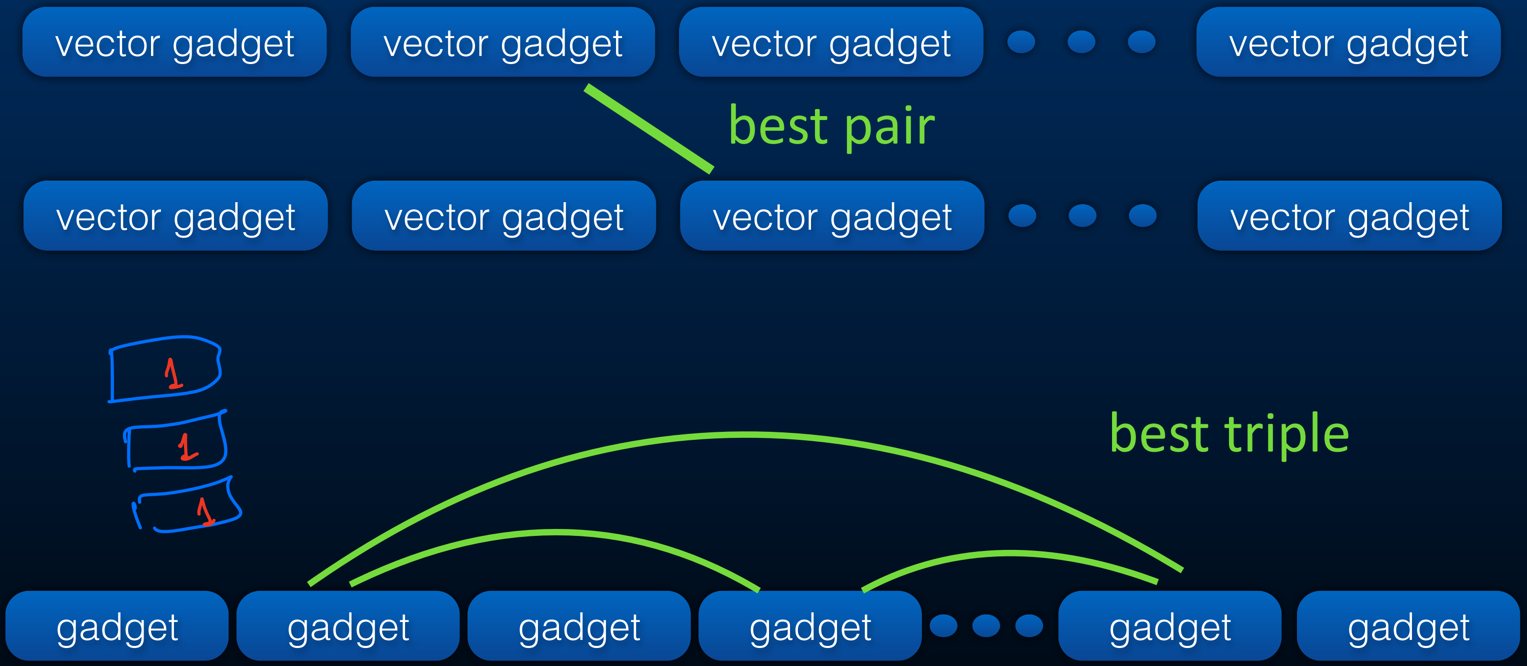
Higher Lower Bounds?



vector gadget vector gadget vector gadget • • • vector gadget

best pair

vector gadget vector gadget vector gadget • • • vector gadget

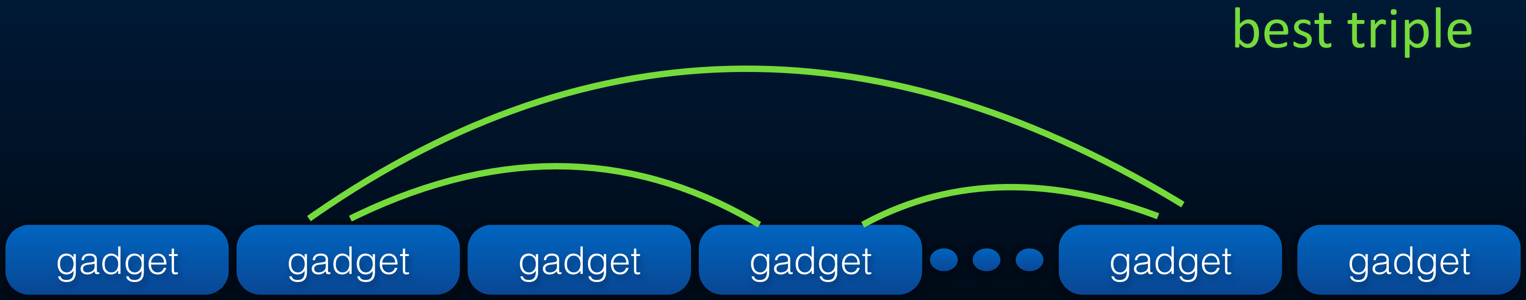
1
1
1

best triple

gadget gadget gadget gadget • • • gadget gadget

Higher Lower Bounds? $\Omega(n^{\omega})$?

Attempt: Reduce from Triangle detection.



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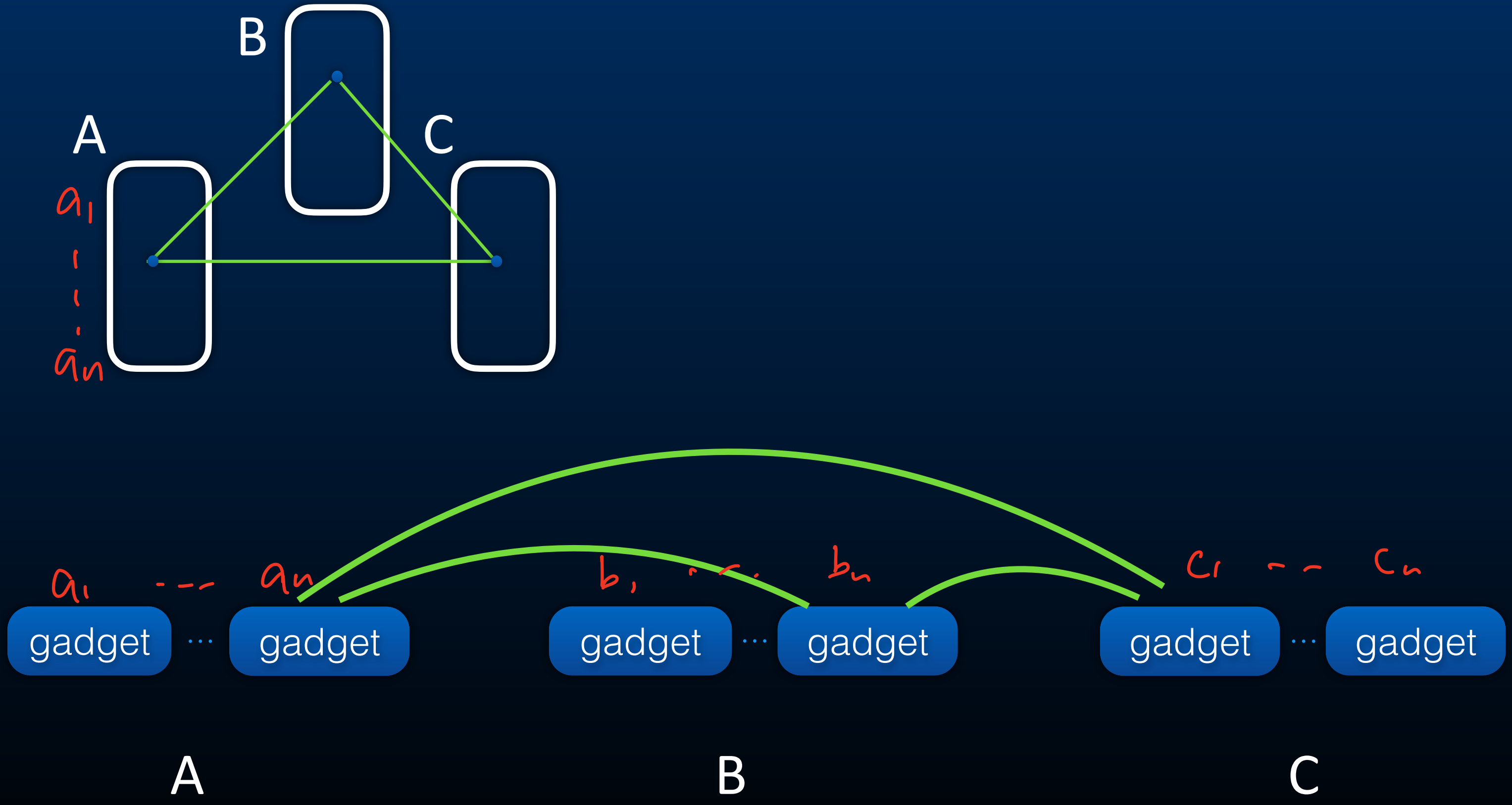


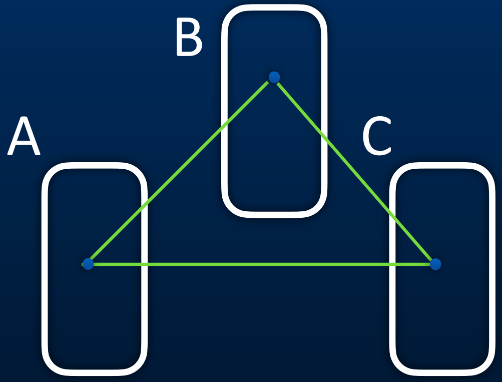
Higher Lower Bounds? $\Omega(n^{\omega})$?

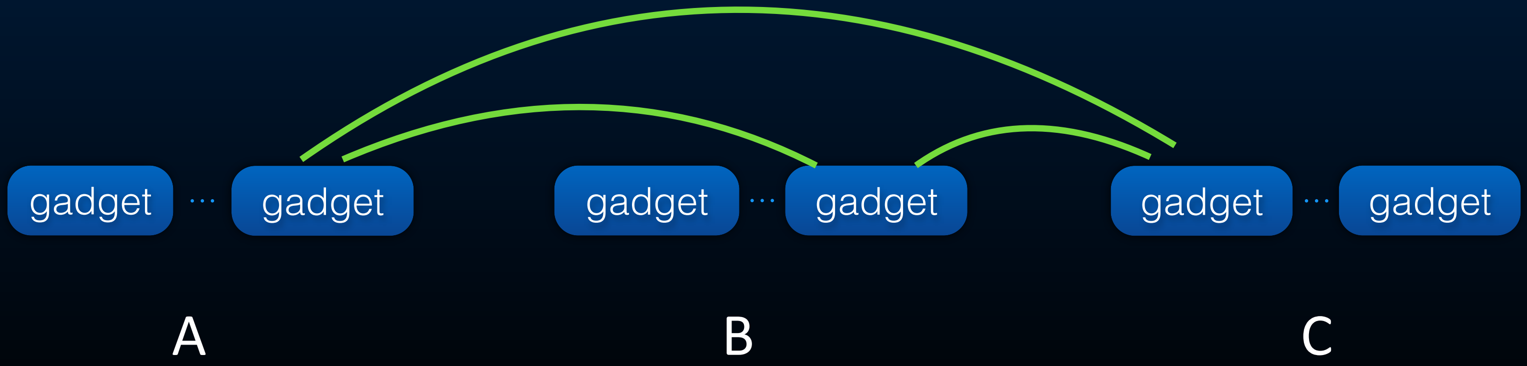
Want: Node gadgets such that:

$$OPT(\overset{\varepsilon}{\boxed{a}}\ \overset{\varepsilon'}{\boxed{b}}) > \tau$$

iff

$$(a,b) \in E$$





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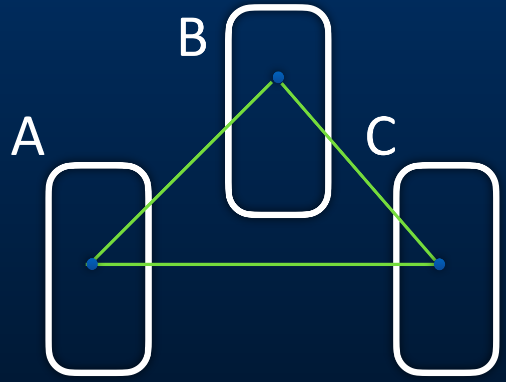
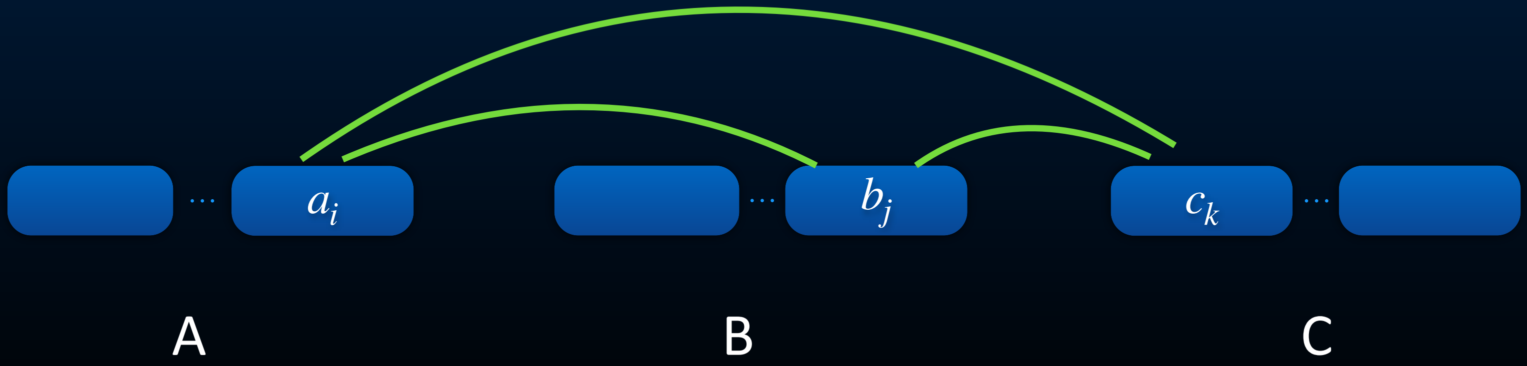


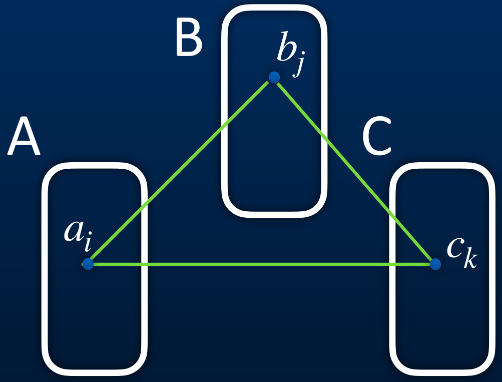


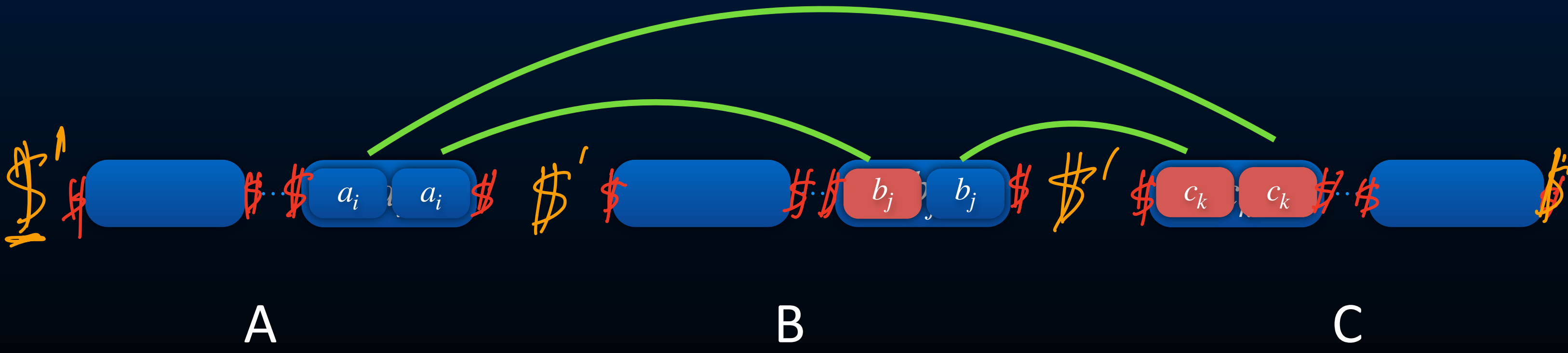
Higher Lower Bounds? $\Omega(n^{\omega})$?

Want: Node gadgets such that: $OPT($ a b $) > \tau$

iff

$(a, b) \in E$





Higher Lower Bounds? $\Omega(n^{\omega})?$

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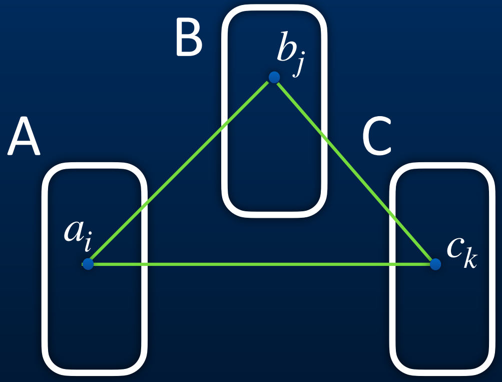

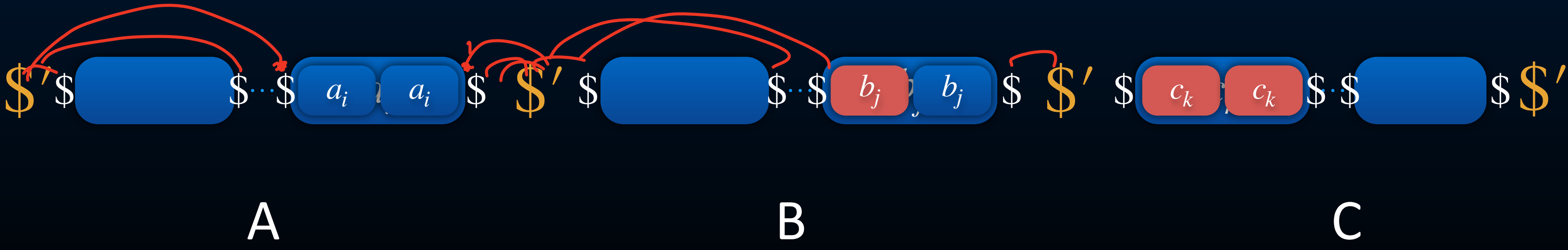

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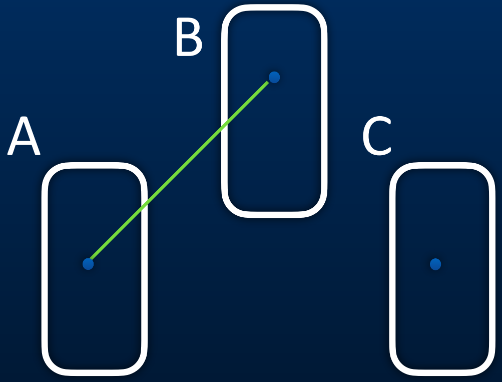
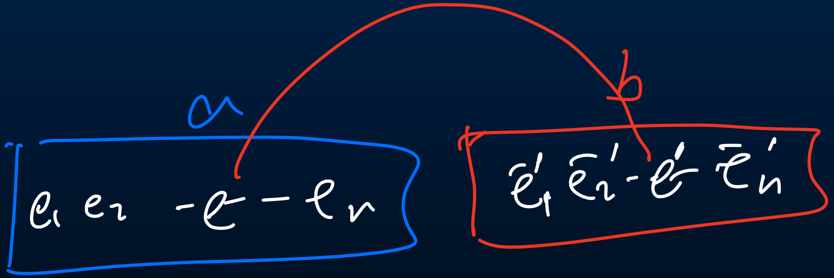


How?



1 if ∃ common edge

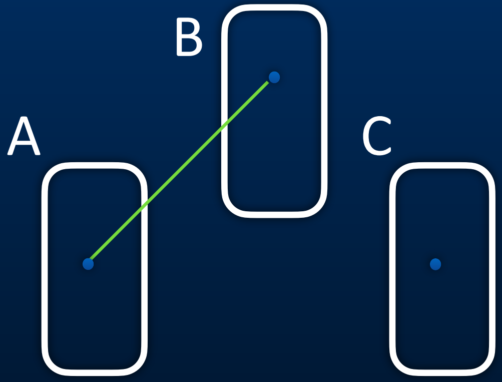
0 otherwise.

Higher Lower Bounds? $\Omega(n^{\omega})?$

Want: Node gadgets such that: $OPT(\boxed{a}\ \boxed{b}) > \tau$

iff

$(a, b) \in E$



How?

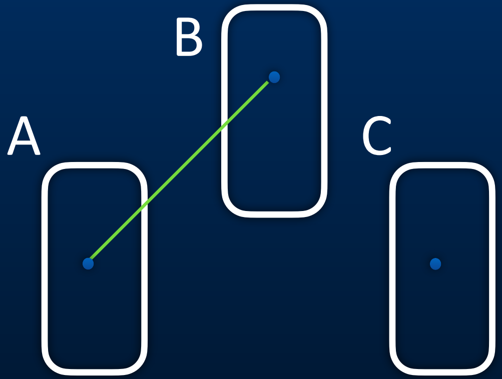
$\boxed{a}$ $\boxed{N_A(b) : a_3, a_7, a_{20}, \ldots}$

Just write a

List all $a \in N_A(b)$

Higher Lower Bounds? $\Omega(n^{\omega})?$

Want: Node gadgets such that:



$OPT(\boxed{a}\ \boxed{b}) > \tau$

iff

$(a,b) \in E$

How?

$\boxed{a}$

$\boxed{N_A(b) : a_3, a_7, a_{20}, \ldots}$

Just write a

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$OPT = 1$ iff $(a,b) \in E$

Higher Lower Bounds? $\Omega(n^{\omega})?$

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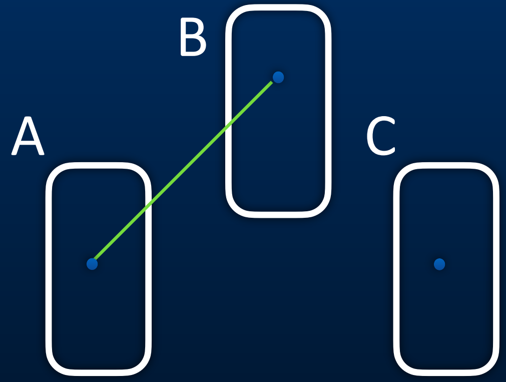

$OPT(\boxed{a}\ \boxed{b}) > \tau$

iff

$(a, b) \in E$

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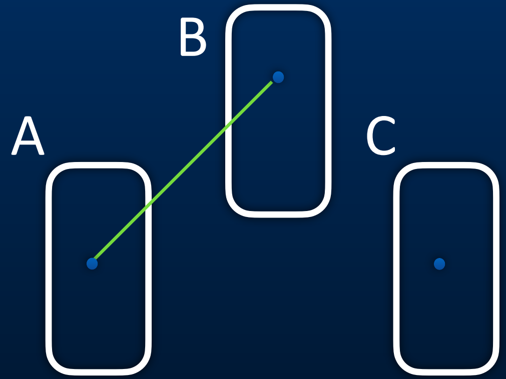
Issue: Gadget size is $\Theta(n)$… Total length is $\Theta(n^2)$.

Higher Lower Bounds? $\Omega(n^{\omega})$?

Want: Node gadgets such that:



$OPT(\; a \;\; b \;) > \tau$

iff

$(a,b) \in E$

How?

a $\qquad$ $N_A(b) : a_3, a_7, a_{20}, \ldots$

Just write a $\qquad$ List all $a \in N_A(b)$

$OPT = 1$ iff $(a,b) \in E$

$N = n^2$

$N^{\omega/2-\varepsilon} \underset{\text{for RNA}}{\Longrightarrow} n^{\omega-\varepsilon'}$ for Δ.

Issue: Gadget size is $\Theta(n)$... Total length is $\Theta(n^2)$.

Thm: $O(n^{\omega/2-\varepsilon})$ for RNA Folding, breaks the Triangle bound.

Higher Lower Bounds? $\Omega(n^{\omega})$?

Want: Node gadgets such that: $OPT($ a b $) > \tau$

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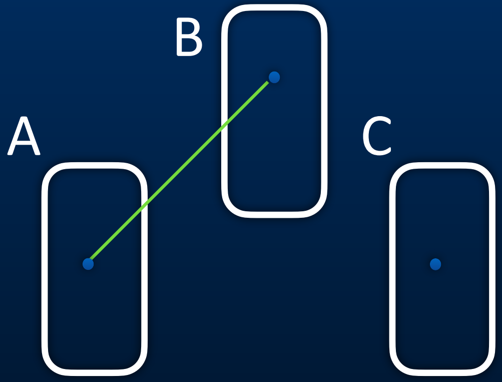
$(a, b) \in E$



a

$N_A(b) : a_3, a_7, a_{20}, \ldots$

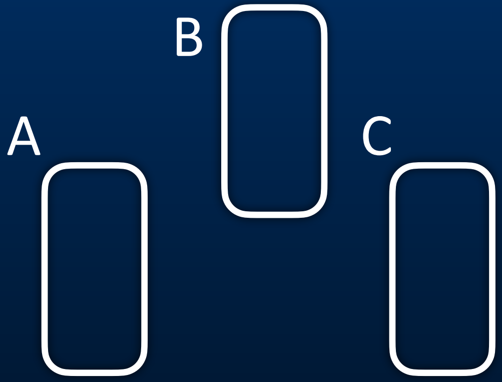
Just write a

List all $a \in N_A(b)$

Want: Shorter node gadgets… $\tilde{O}(1)$ bits.

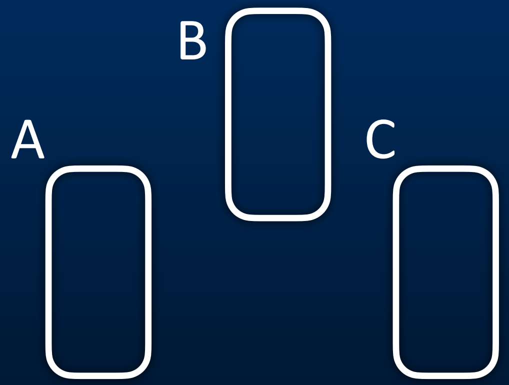
Issue: Impossible… need $\Omega(n^2)$ bits to represent a graph!

Is Triangle hard on “compressible” graphs?



Can the edges be encoded with $o(n^2)$ bits?

Is Triangle hard on "compressible" graphs?



Can the edges be encoded with $o(n^2)$ bits?

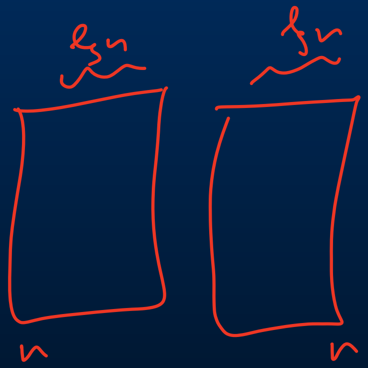
k-SAT

n^k bits → OV

$N = 2^{n/2}$

$(\lg N)^k$

Is OV hard on "compressible" inputs?

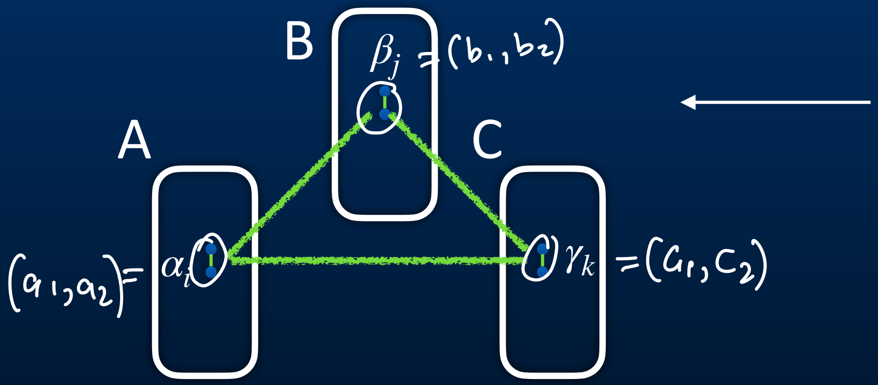


$\tilde{\Theta}(n)$ bits in general

SETH ⇒ $\Omega(n^2)$ even when the instance can be represented in $\tilde{O}(1)$ bits.

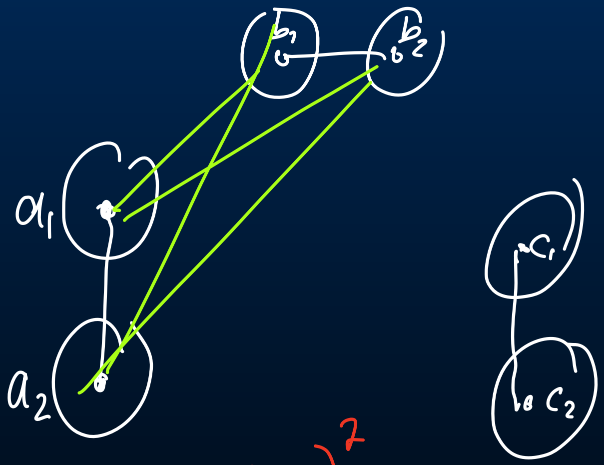
Is Triangle hard on "compressible" graphs?

3-Clique



6-Clique

$O(n^{2\omega})$ time



$N = O(n^2)$ nodes,

$O(N^2) = O(n^4)$ edges,

But only $O(N) = O(n^2)$ bits!

$\Omega(n^\omega)$

$(6\cdot n)^2$

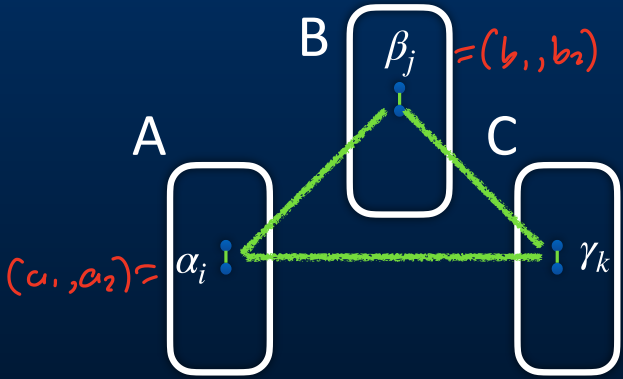
k-Clique Conjecture: "yes"

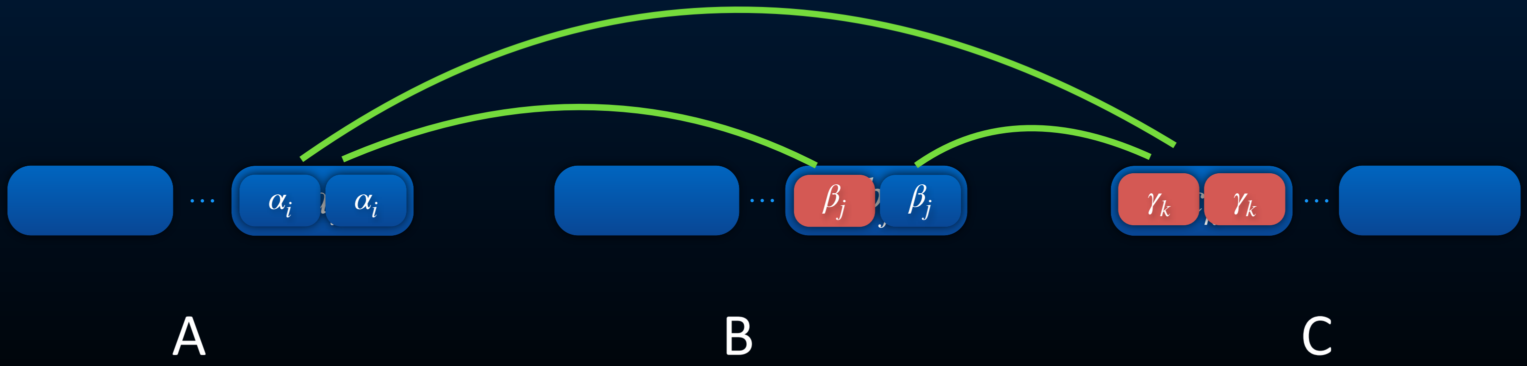
Higher Lower Bounds? $\Omega(n^{\omega})$?

Want: "Node" gadgets such that: $OPT(\boxed{\alpha = a_1, a_2}\ \boxed{\beta = b_1, b_2}) > \tau$

iff

$(a_1, b_1), (a_1, b_2), (a_2, b_1), (a_2, b_2) \in E$





Higher Lower Bounds? $\Omega(n^{\omega})$?

Want: "Node" gadgets such that: $OPT(\ \alpha = a_1, a_2 \quad \beta = b_1, b_2\ ) > \tau$

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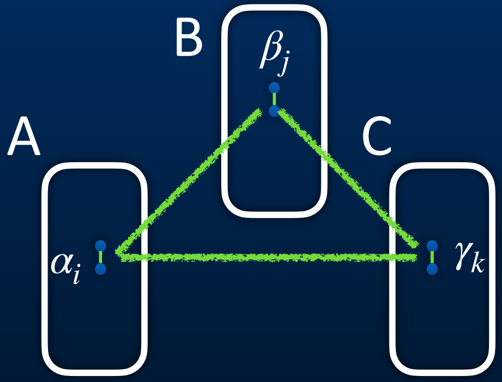


$a_1 \quad a_2 \ a_2 a_1$

$N(b_1) \quad N(b_2) \quad Nb_1 \, Nb_2$

$\# a_1 \# a_2 \# a_1 \# a_2 \#$

$\#' \underset{A_2}{N(b_1)} \#' \underset{A_1}{N(b_1)} \#' N(b_2) \#' N(b_2) \#'$

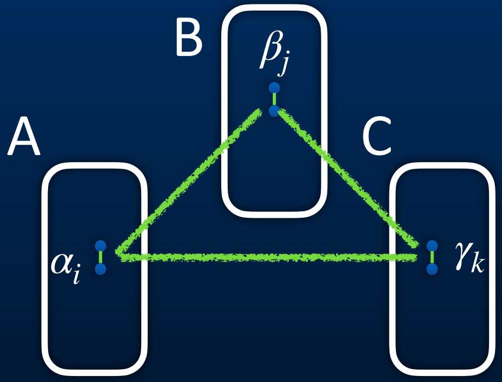
$OPT = 4$ iff (α, β) is a 2x2-biclique.

k-Clique Lower Bounds $\Omega(n^{\omega})$

Want: "Node" gadgets such that: $OPT(\alpha = a_1, a_2 \quad \beta = b_1, b_2) > \tau$

iff

$(a_1, b_1), (a_1, b_2), (a_2, b_1), (a_2, b_2) \in E$



6-Clique

$N = n^3 \longleftarrow \Omega(n^{2\omega})$

$\Omega(N^{\omega \cdot \frac{2}{3} - \varepsilon})$

Total length is $O(n^2) \cdot O(n) = \underline{O(n^3)}$.

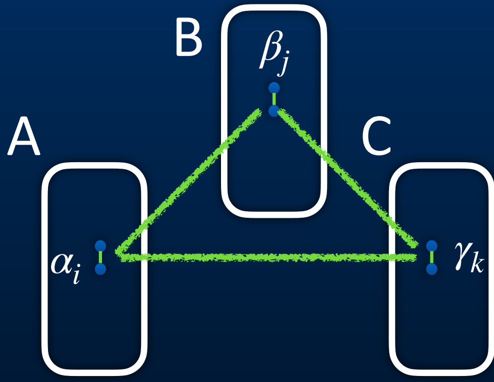
Thm: $O(n^{2\omega/3-\varepsilon})$ for RNA Folding, breaks the 6-Clique bound.

k-Clique Lower Bounds $\Omega(n^{\omega})$

Want: "Node" gadgets such that: $OPT(\boxed{\alpha = a_1, a_2}\ \boxed{\beta = b_1, b_2}) > \tau$

iff

$(a_1, b_1), (a_1, b_2), (a_2, b_1), (a_2, b_2) \in E$



3k-Clique

$N = n^k \cdot n \cdot \cancel{2}$
$= n^{k+1}$

$\leftarrow \Omega(n^{\omega k})$

Total length is $O(n^2) \cdot O(n) = O(n^3)$.

$\Omega(N^{\frac{k}{k+1} \cdot \omega - \varepsilon})$

Thm: $O(n^{2\omega/3-\varepsilon})$ for RNA Folding, breaks the 6-Clique bound.

Start from 3k-Clique: total length is $O(n^{k+1})$.

Thm: $O(n^{\frac{k}{k+1}\omega-\varepsilon})$ for RNA Folding, breaks the 3k-Clique bound.

k-Clique Conjecture(s)

Weighted k-Clique Conjecture:

No $O(n^{(1-\varepsilon)\cdot k})$ *time alg for Min-Weight k-Clique.*

Combinatorial k-Clique Conjecture:

No $O(n^{(1-\varepsilon)\cdot k})$ *time alg for k-Clique, combinatorially.*

Unweighted k-Clique Conjecture:

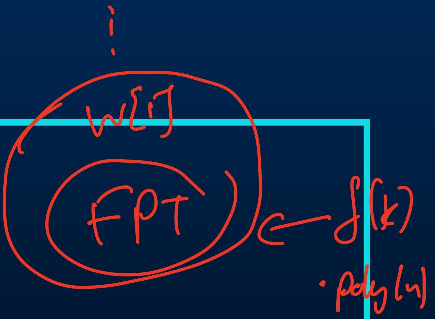
No $O(n^{(\omega/3-\varepsilon)\cdot k})$ *time alg for k-Clique.*

k-Clique

Longstanding Open Questions:

- Faster, $O(n^{(\omega/3-\varepsilon)\cdot k})$ *for k-Clique*?
- $O(n^{(1-\varepsilon)\cdot k})$ *without matrix mult.?*
- $O(n^{(1-\varepsilon)\cdot k})$ *for Min-Weight-k-Clique?*

Some Known Hardness for k-Clique:



The canonical W[1]-complete problem.

$n^{\sqrt{k}}$

$n^{o(k)}$ refutes ETH. [Chen et al. 05]

$O(n^{k/2-\varepsilon})$ implies faster k-SUM. [A.- Lewi -Williams 14]

Faster alg implies faster MAX-CUT. [Williams 04]

etc…

MAX-2SAT 1.21^n

RNA Folding

Upper bounds:

k-Clique lower bounds:

	Upper bounds:	k-Clique lower bounds:
Dynamic Programming	$O(n^3)$	$\Omega(n^{3-\varepsilon})$ (Combinatorial)
		$\Omega(n^{\omega-\varepsilon})$

RNA Folding

Upper bounds:

k-Clique lower bounds:

Dynamic Programming $O(n^3)$

$\Omega(n^{3-\varepsilon})$ (Combinatorial)

$O(n^{2.99})$ *via MM?*

$\Omega(n^{\omega-\varepsilon})$

[ABV FOCS '15]

RNA Folding

	Upper bounds:	k-Clique lower bounds:
Dynamic Programming	$O(n^3)$	$\Omega(n^{3-\varepsilon})$ (Combinatorial)
$O(n^{2.99})$ via MM?		$\Omega(n^{\omega-\varepsilon})$ [ABV FOCS '15]

CFG Parsing

CYK Parser (60's) *(Combinatorial)*	$O(n^3)$	$\Omega(n^{3-\varepsilon})$ (Combinatorial)
Valiant's Parser ('75) *(via MM)*	$O(n^\omega)$	$\Omega(n^{\omega-\varepsilon})$

RNA Folding

Upper bounds:

k-Clique lower bounds:

Dynamic Programming $O(n^3)$ $\Omega(n^{3-\varepsilon})$ (Combinatorial)

$O(n^{2.99})$ via MM? $O(n^{2+\omega/3})$ $\Omega(n^{\omega-\varepsilon})$

[BGSV FOCS'16, CDX SODA'22]

[ABV FOCS '15]

CFG Parsing

CYK Parser (60's)
(Combinatorial)

$O(n^3)$

$\Omega(n^{3-\varepsilon})$ (Combinatorial)

Valiant's Parser ('75)
(via MM)

$O(n^{\omega})$

$\Omega(n^{\omega-\varepsilon})$

Tight lower bounds under the **k-Clique conjectures**

[A. - Backurs - Vassilevska W FOCS'15]

- CFG Parsing
- RNA Folding
- Dyck Language Edit Distance

[Backurs - Dikkala - Tzamos ICALP'16]

- Max Weight Rectangle

[Backurs - Tzamos ICML'17]

- Improving Viterbi's Algorithm

[Bringmann - Gronlund - Larsen FOCS'17]

- Word Break

[Bringmann - Gawrychowski - Mozes - Weimann SODA'18]

- Tree Edit Distance

[Lincoln - Vassilevska W - Williams SODA'18]

- Shortest Cycle in Sparse Graphs

Formal Languages.

Computational Biology.

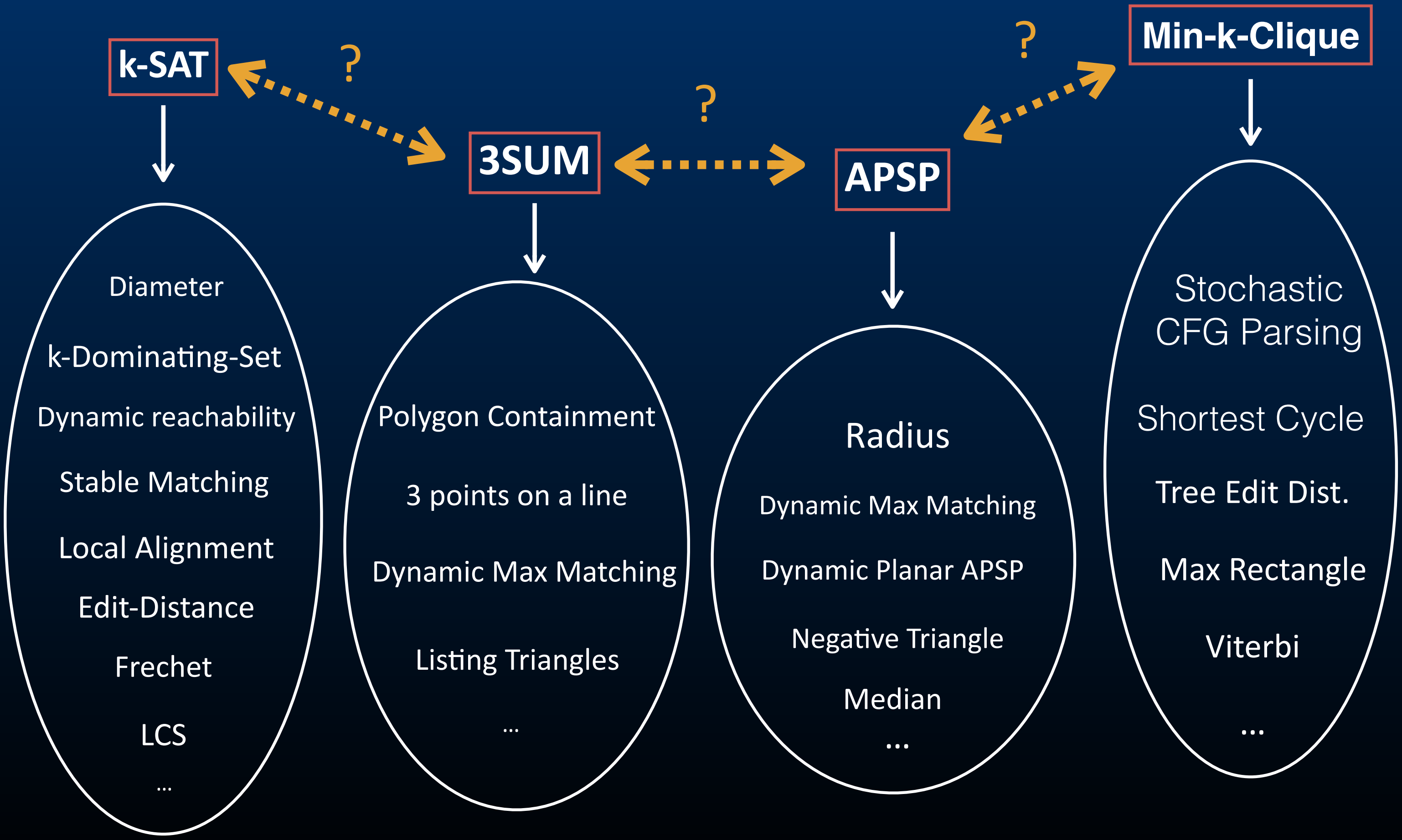
Comp Geometry.

Machine Learning.

Pattern Matching.

Distance computations.

How are these conjectures related?



k-SAT

Diameter

k-Dominating-Set

Dynamic reachability

Stable Matching

Local Alignment

Edit-Distance

Frechet

LCS

...

3SUM

Polygon Containment

3 points on a line

Dynamic Max Matching

Listing Triangles

...

APSP

Radius

Dynamic Max Matching

Dynamic Planar APSP

Negative Triangle

Median

...

Min-k-Clique

Stochastic CFG Parsing

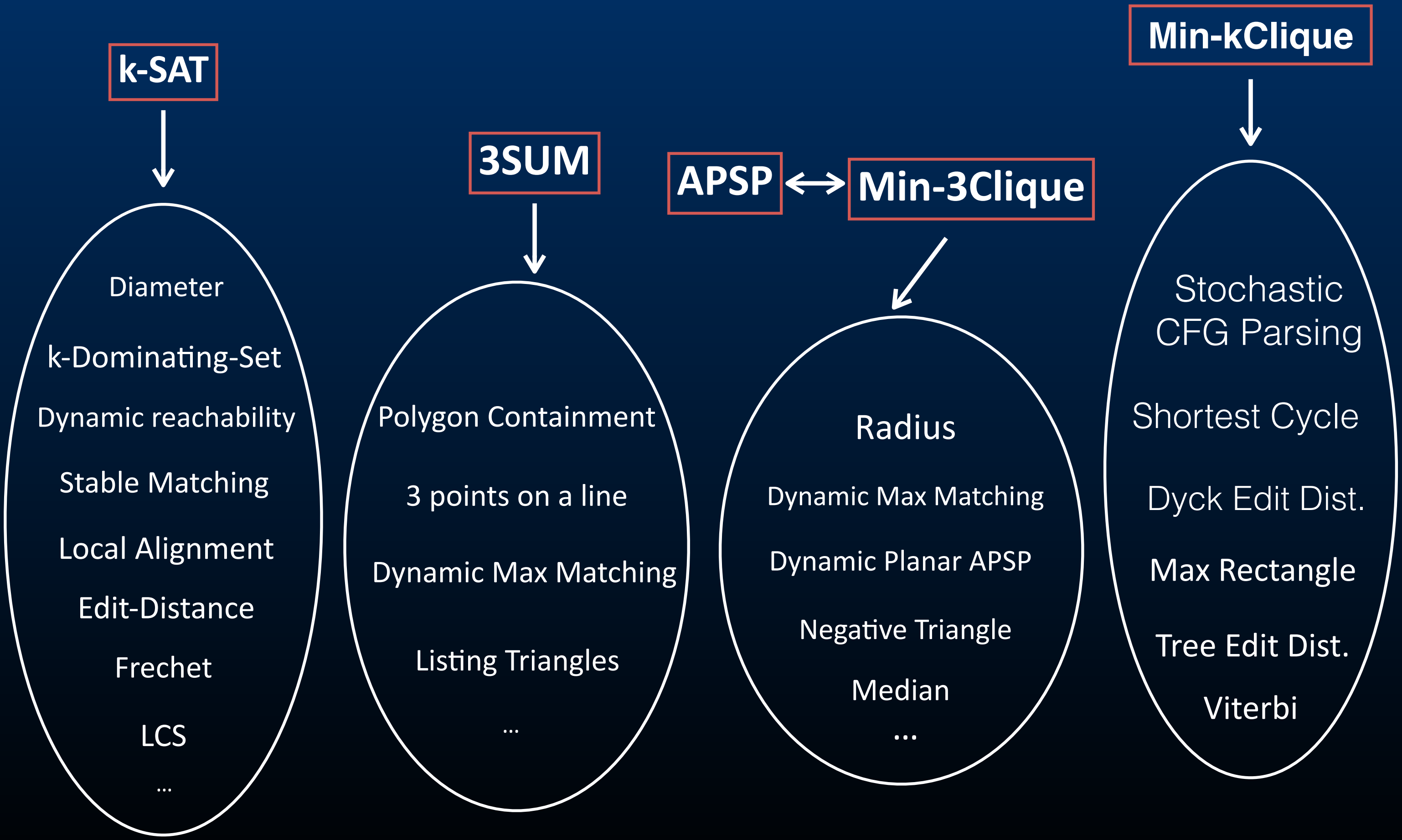
Shortest Cycle

Tree Edit Dist.

Max Rectangle

Viterbi

...



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APSP ↔ **Min-3Clique**

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Min-kClique

Stochastic CFG Parsing

Shortest Cycle

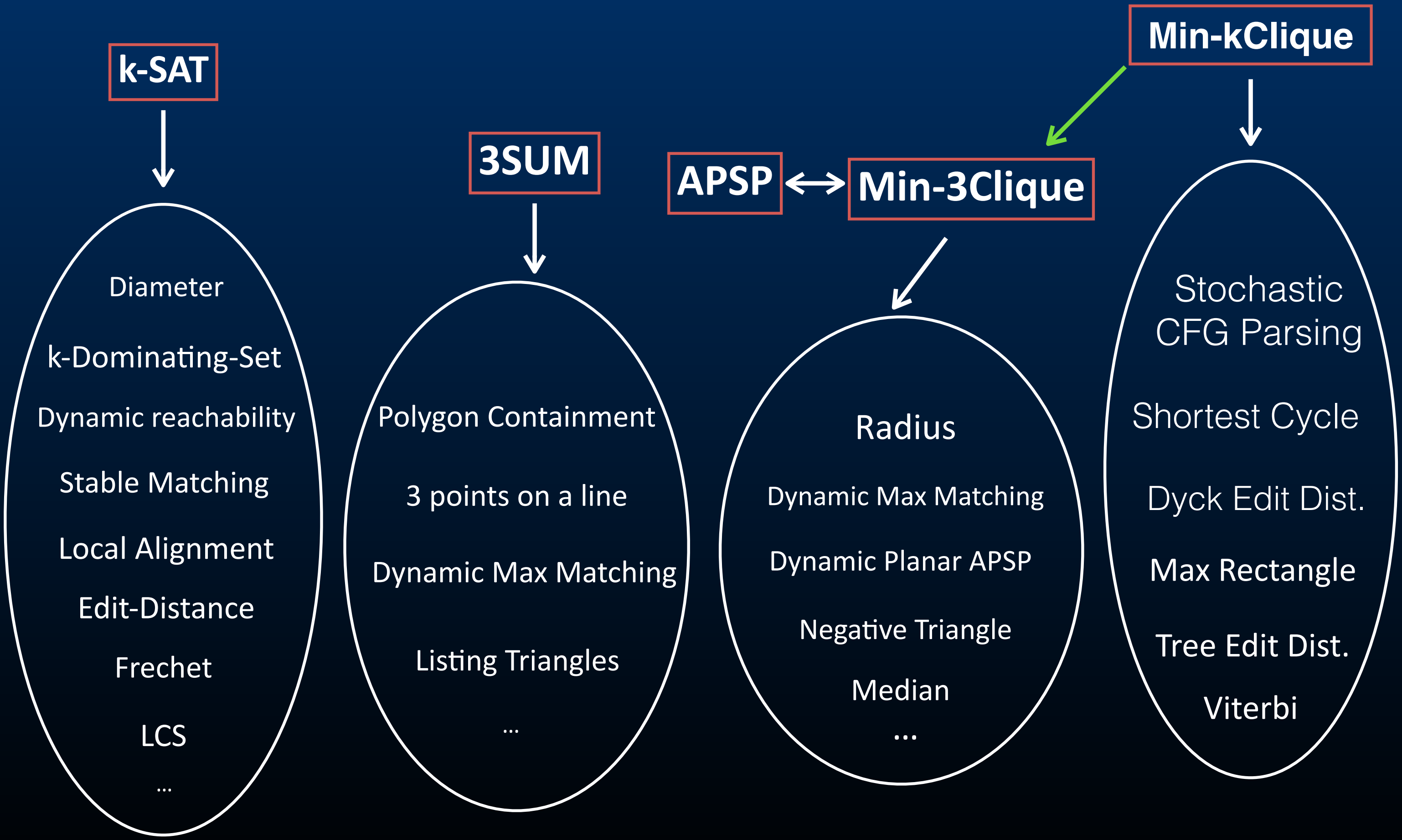
Dyck Edit Dist.

Max Rectangle

Tree Edit Dist.

Viterbi

An easy connection



k-SAT

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APSP ⟷ **Min-3Clique**

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Min-kClique

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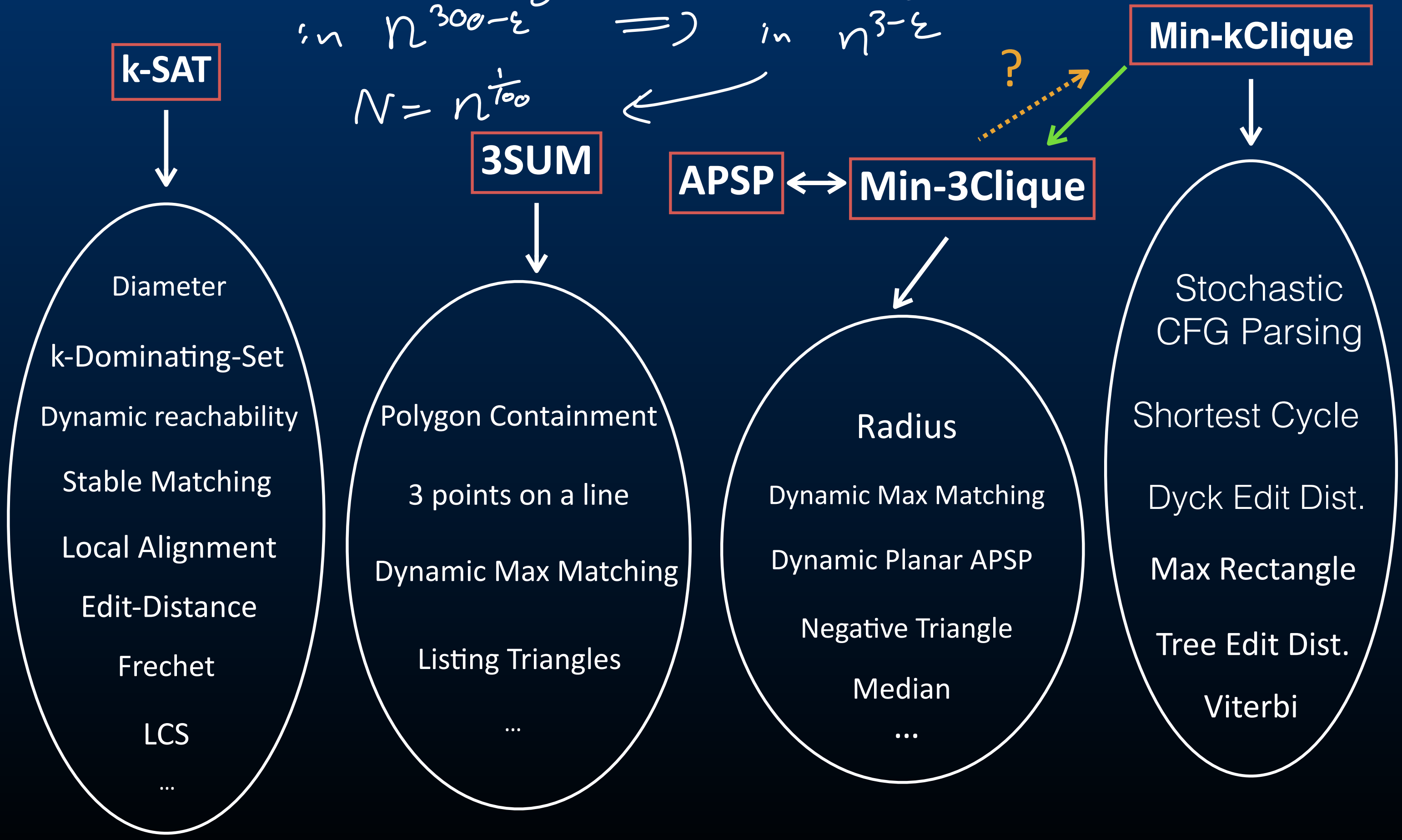
Barrier: low complexity to high complexity

300-Clique in $n^{300-\varepsilon}$ $\Rightarrow$ 3-Clique in $n^{3-\varepsilon}$

$N = n^{\frac{1}{100}}$



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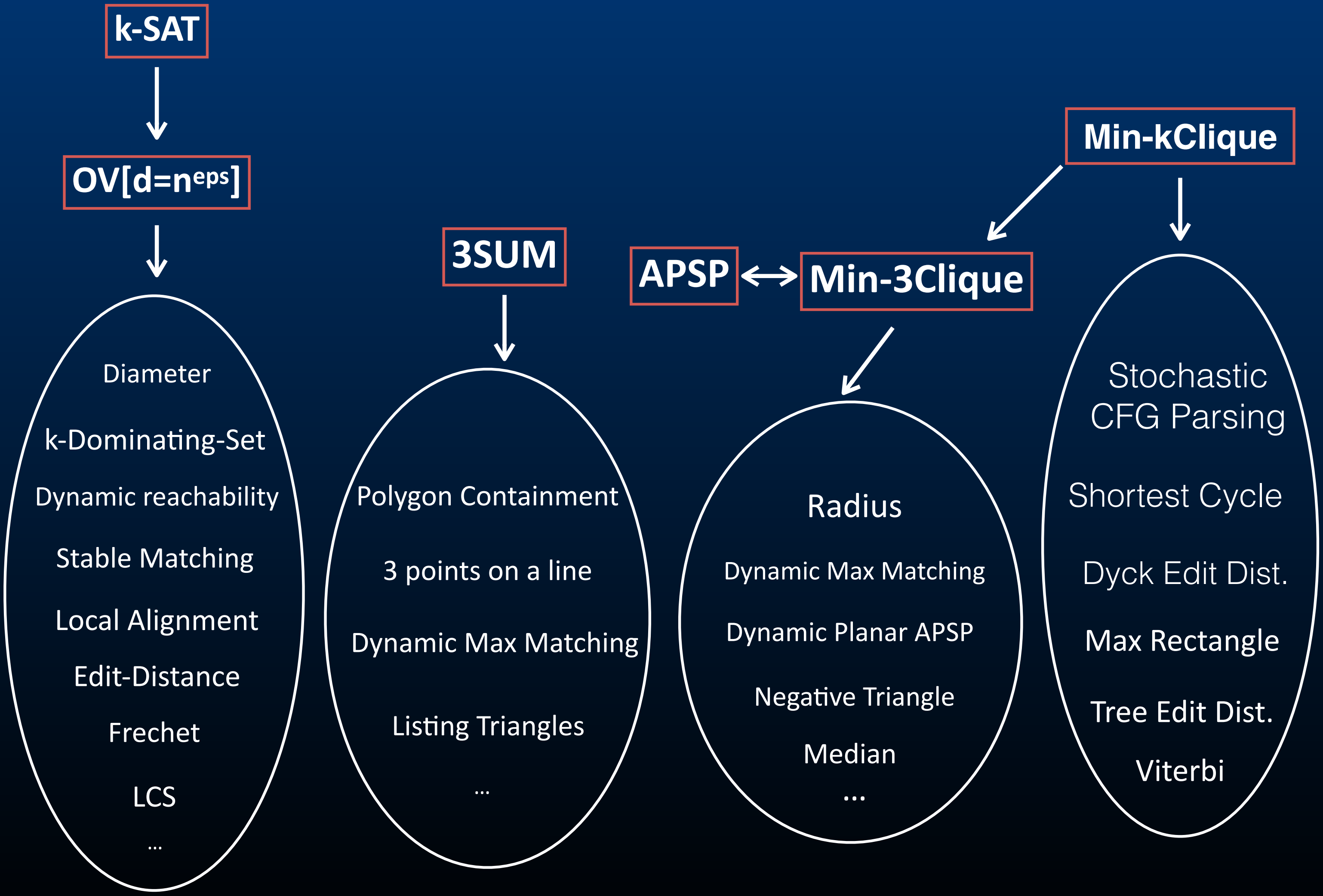

k-SAT

OV[d=n^{eps}]

Diameter

k-Dominating-Set

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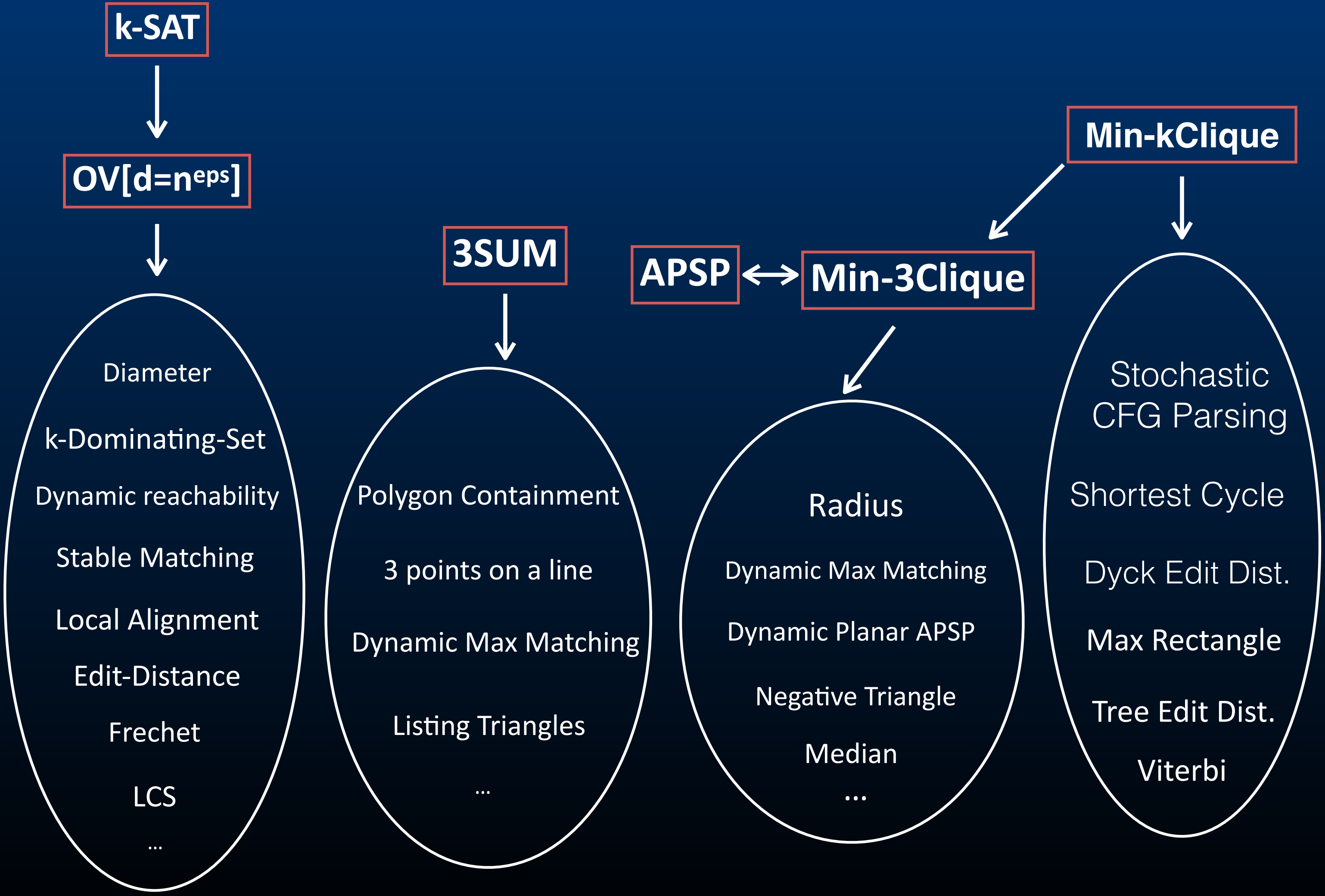
More connections?



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$OV[d=n^{eps}]$

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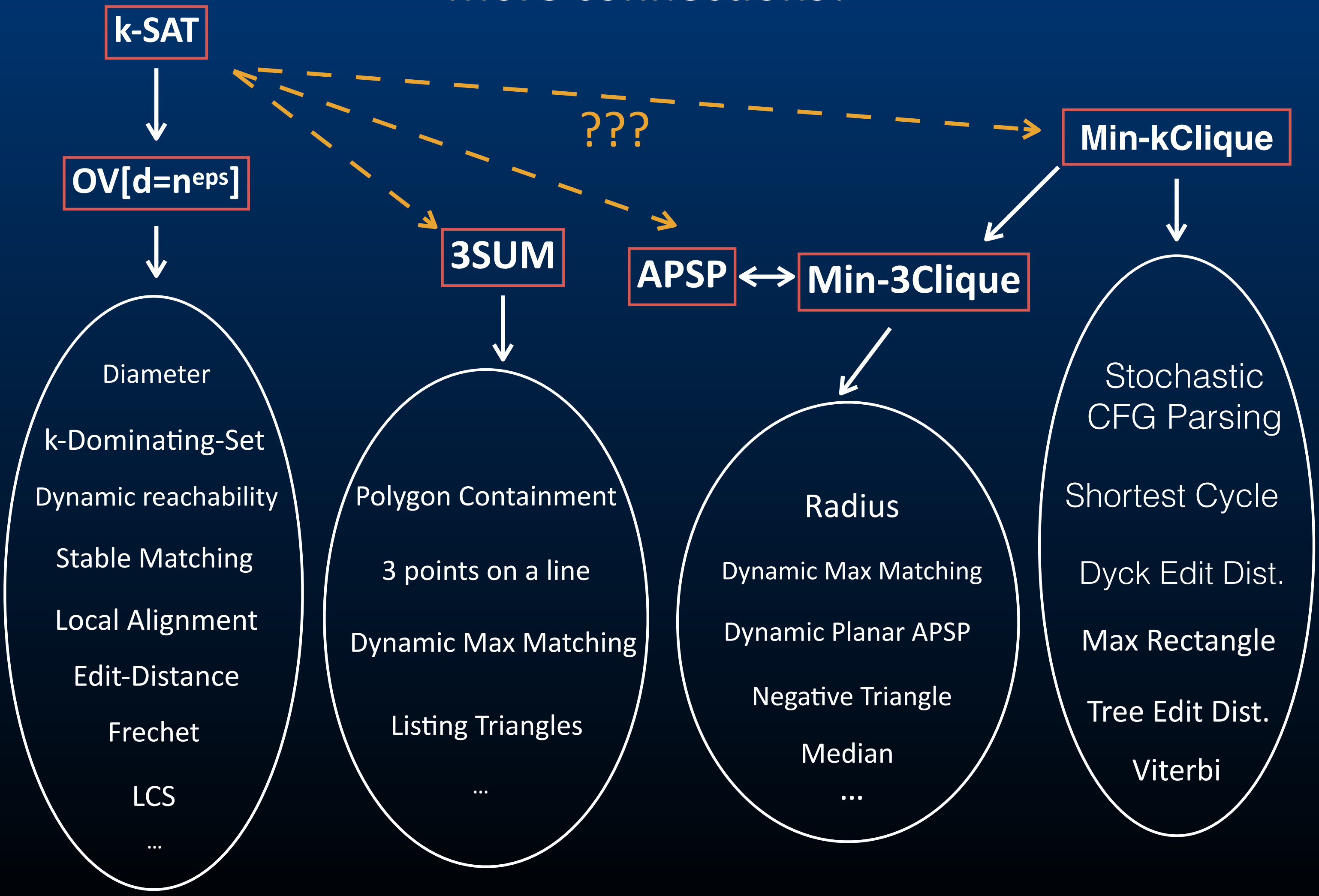

k-SAT

OV[$d=n^{eps}$]

???

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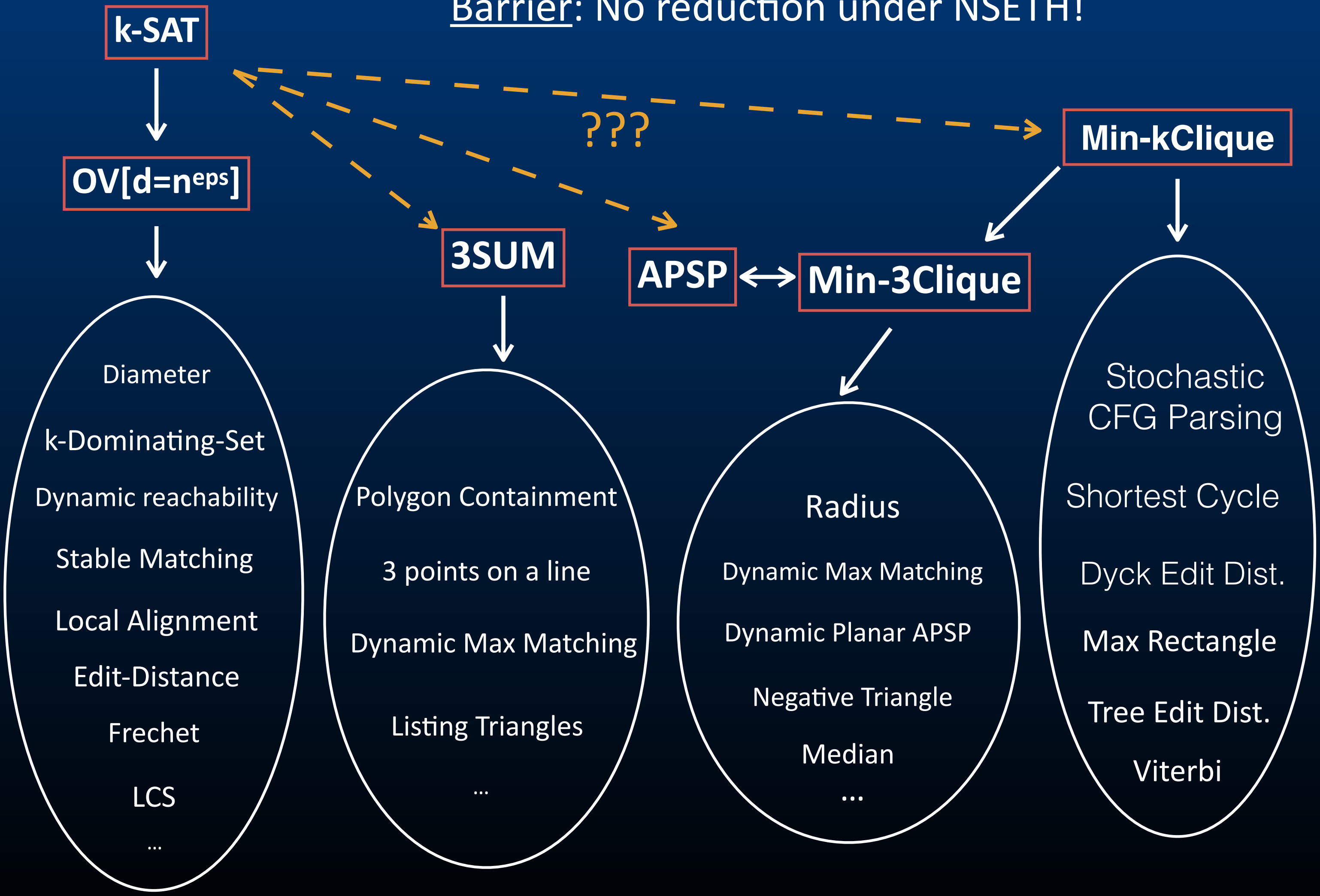
[Carmosino - Gao - Impagliazzo - Mikhailin - Paturi - Schneider ’16]

Barrier: No reduction under NSETH!



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$OV[d=n^{eps}]$

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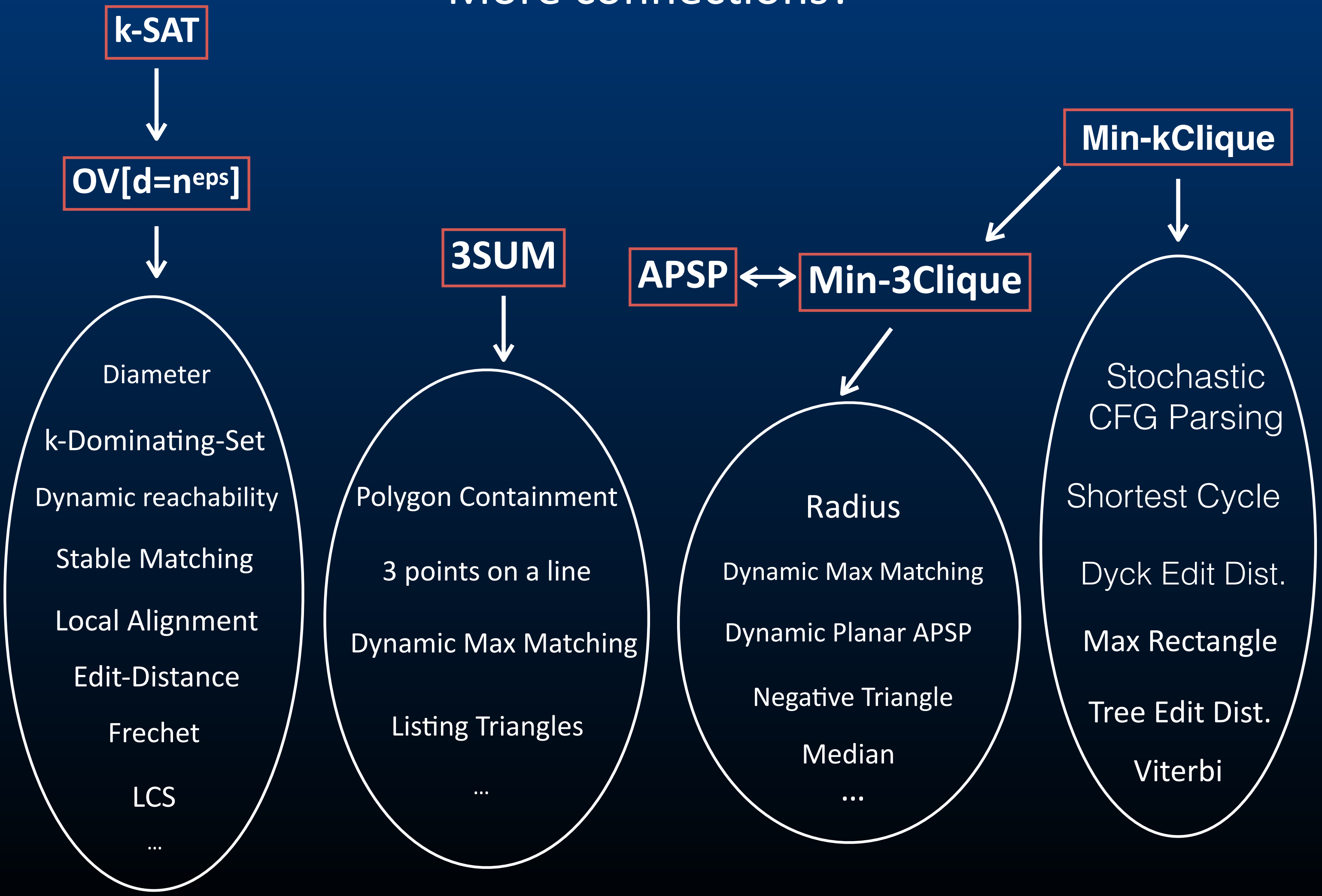

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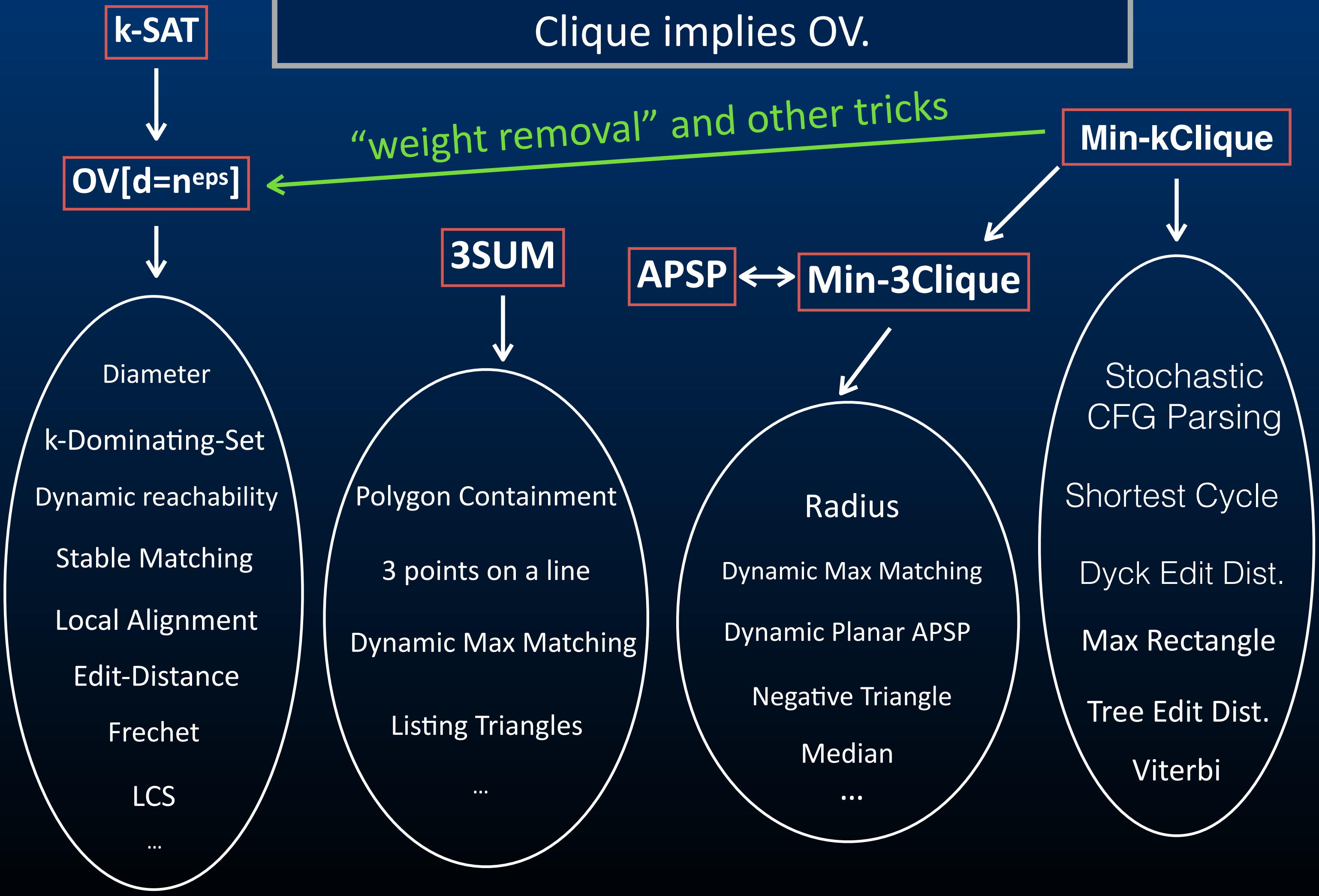
[A.-Bringmann-Dell-Nederlof ’18]
Clique implies OV.



k-SAT

OV[$d=n^{eps}$]

“weight removal” and other tricks

Min-kClique

3SUM

APSP

Min-3Clique

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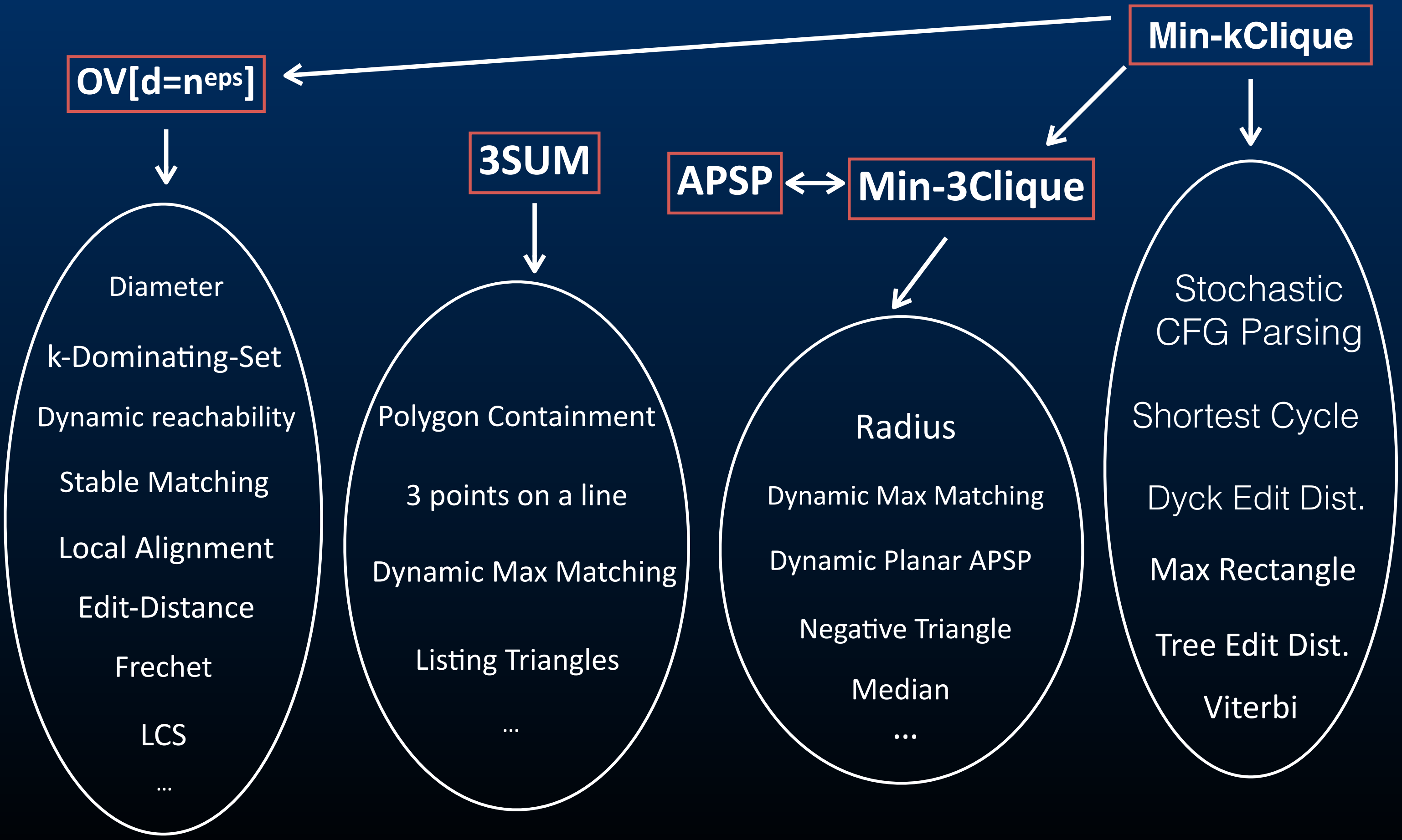
The source of all lower bounds in P?



Min-kClique

OV[d=n^{eps}]

3SUM

APSP

Min-3Clique

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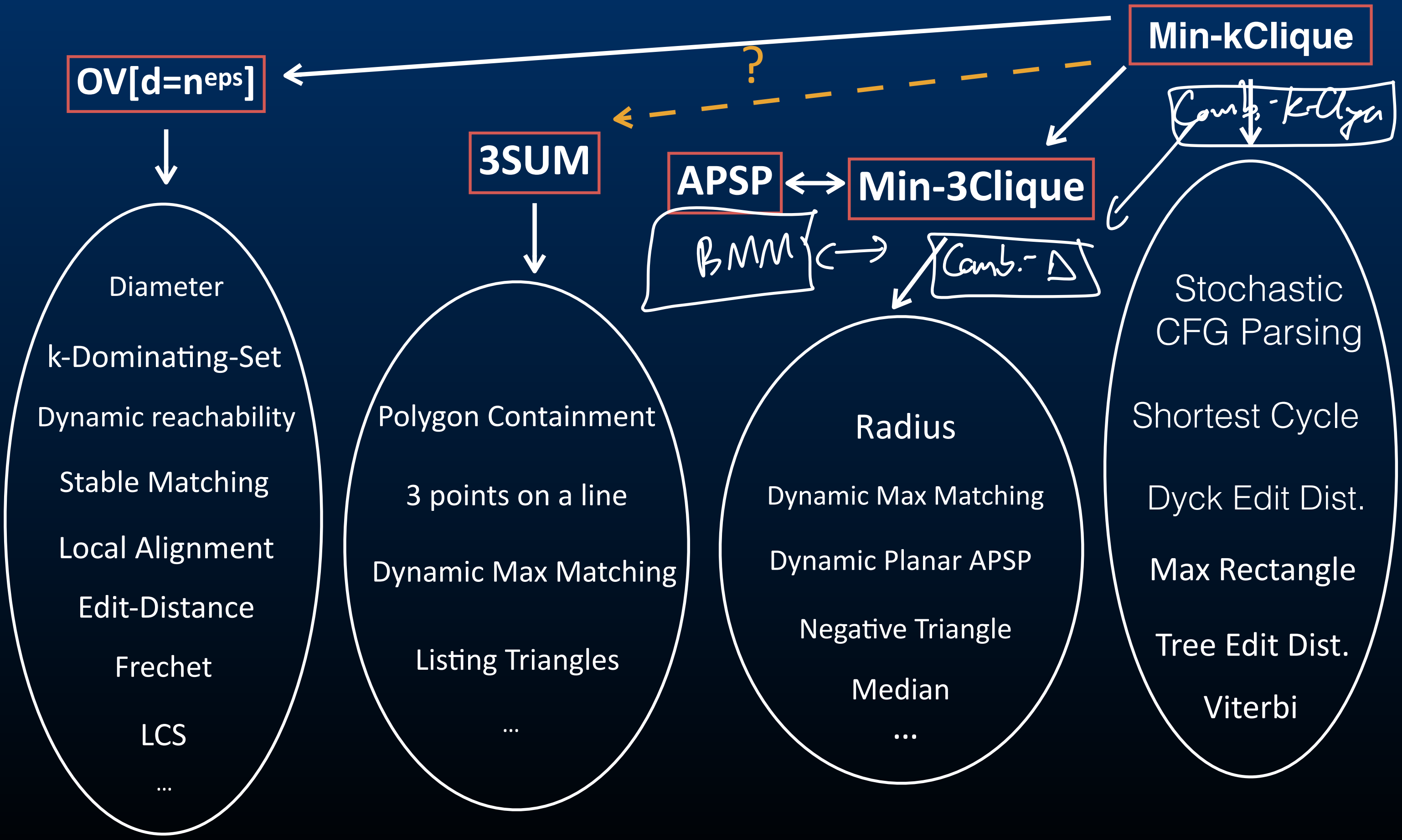

Min-kClique

Comb.-k-Clique

?

OV[d=n^{eps}]

3SUM

APSP ↔ **Min-3Clique**

BMM ↔ Comb.-Δ

Diameter

k-Dominating-Set

Dynamic reachability

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…

Polygon Containment

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…

Stochastic CFG Parsing

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Tree Edit Dist.

Viterbi