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Engineering motif search for large graphs

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Simons Institute for the Theory of Computing
Thursday 5 November 2015

Tight results



Satisfiability Lower Bounds and Tight Results for Parameterized and Exponential-Time Algorithms

Nov. 2 – Nov. 6, 2015

Program: [Fine-Grained Complexity and Algorithm Design](#)

**Are tight algorithms useful,
in practice ?**

[here: practice ~ proof-of-concept algorithm engineering]

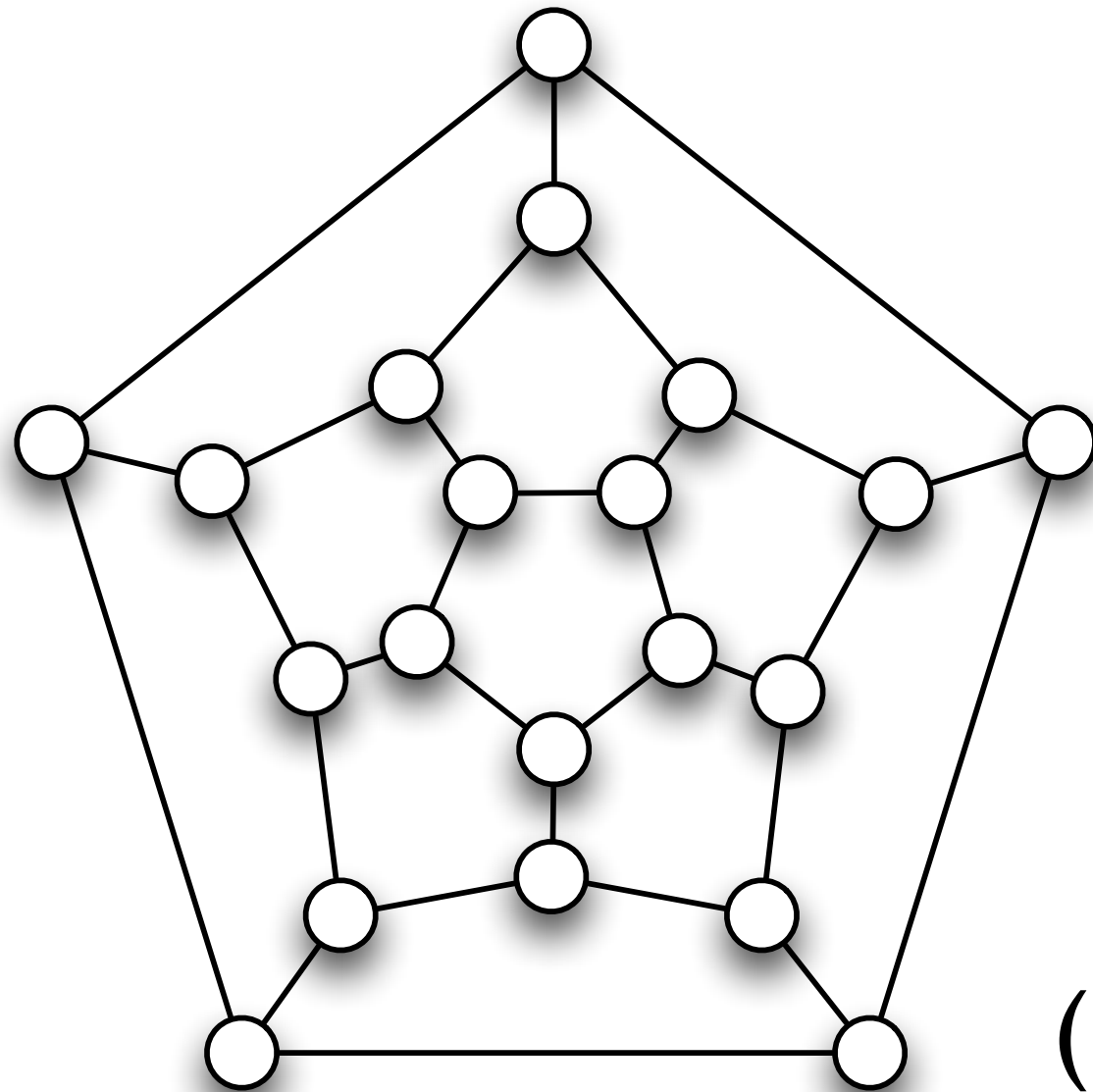
A coarse-grained view

- **Data**
 - “large” (e.g. large database)
- **Task**
 - “small” (e.g. search for a small *pattern* in data)
 - all too often NP-hard

We need a more *fine-grained* perspective

Graph search

Data

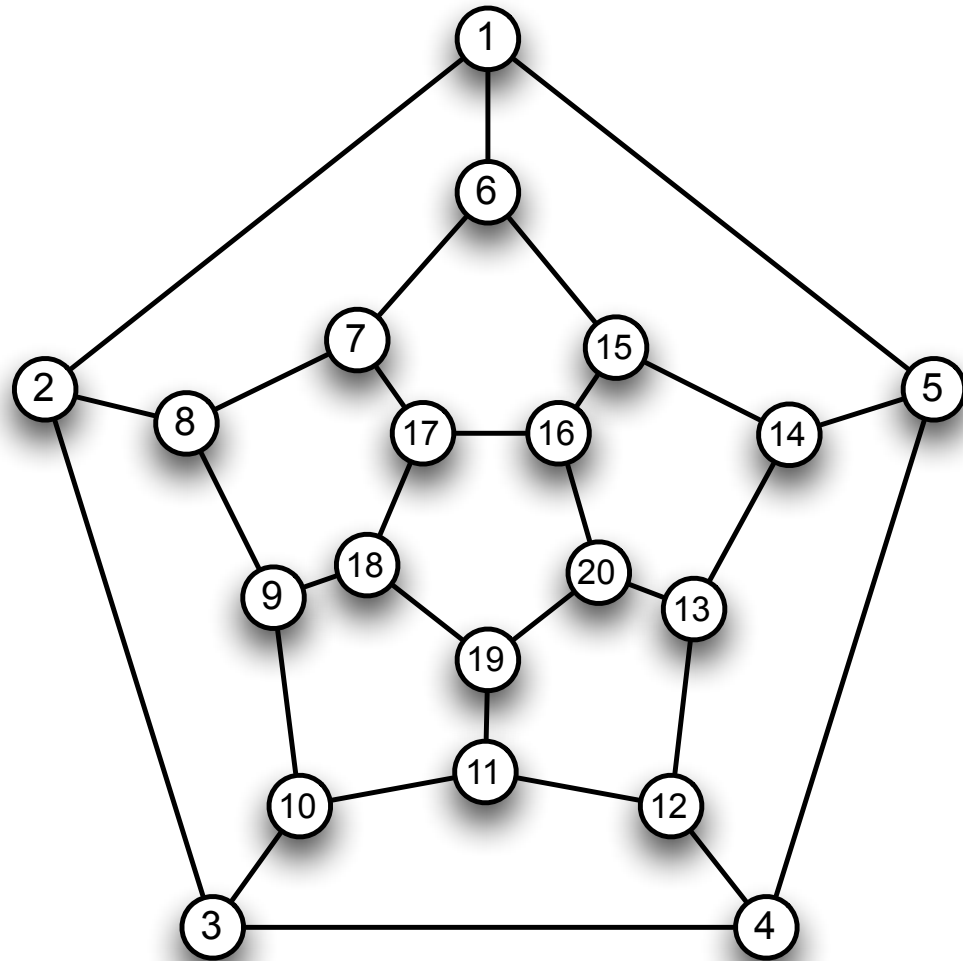


(+ annotation)

Pattern (query)

Task (search for *matches* to query)

Large data (large graph)



One edge
= two 64-bit integers
(2 x 8 = 16 bytes)

One terabyte
($= 10^{12}$ bytes)
stores about
60 billion edges

1, 2	2, 8	8, 9	14, 15	15, 16
2, 3	3, 10	9, 10	6, 15	16, 17
3, 4	4, 12	10, 11	7, 17	17, 18
4, 5	5, 14	11, 12	9, 18	18, 19
1, 5	6, 7	12, 13	11, 19	19, 20
1, 6	7, 8	13, 14	13, 20	16, 20

(edge list representation)

$\sim 10^{10}$ edges,
arbitrary topology

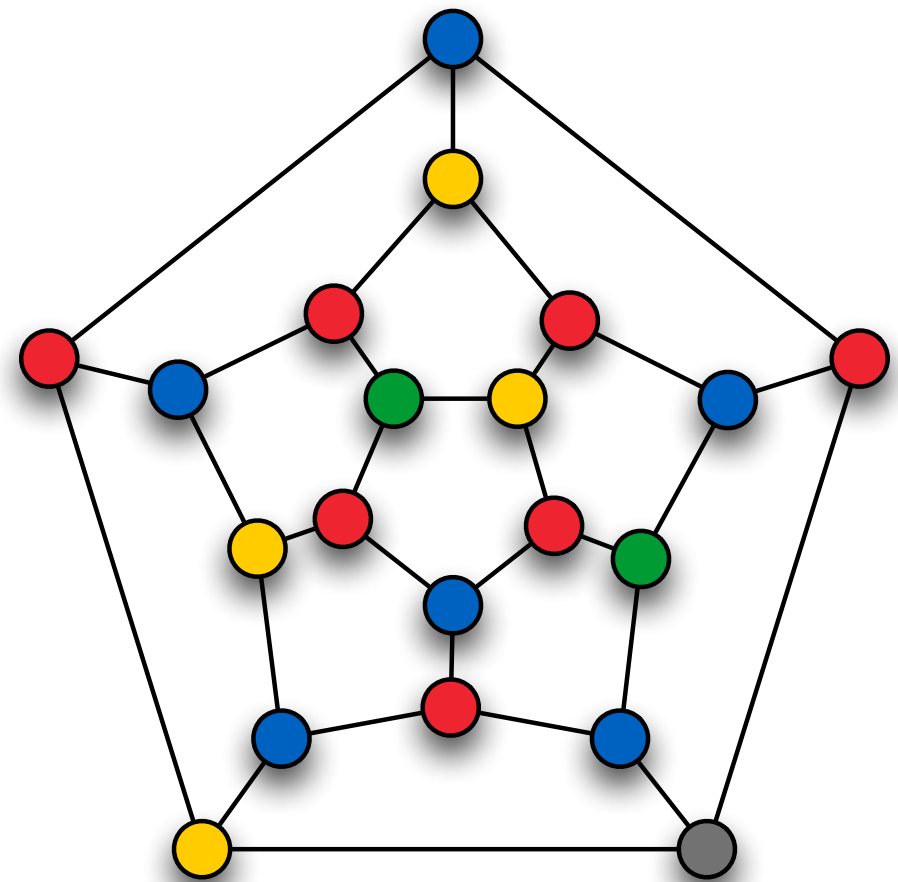
Motif search

Data

Vertex-colored graph H
(the host graph)

Query

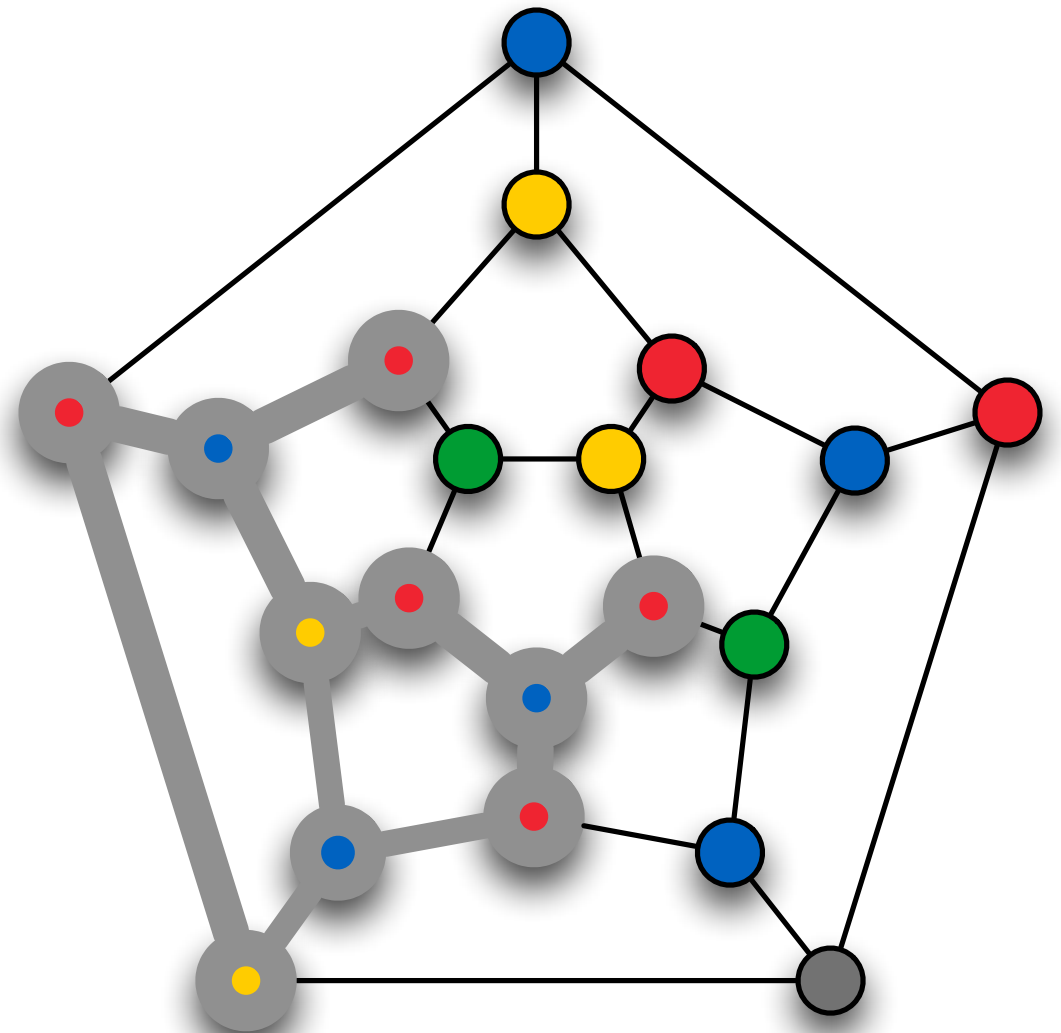
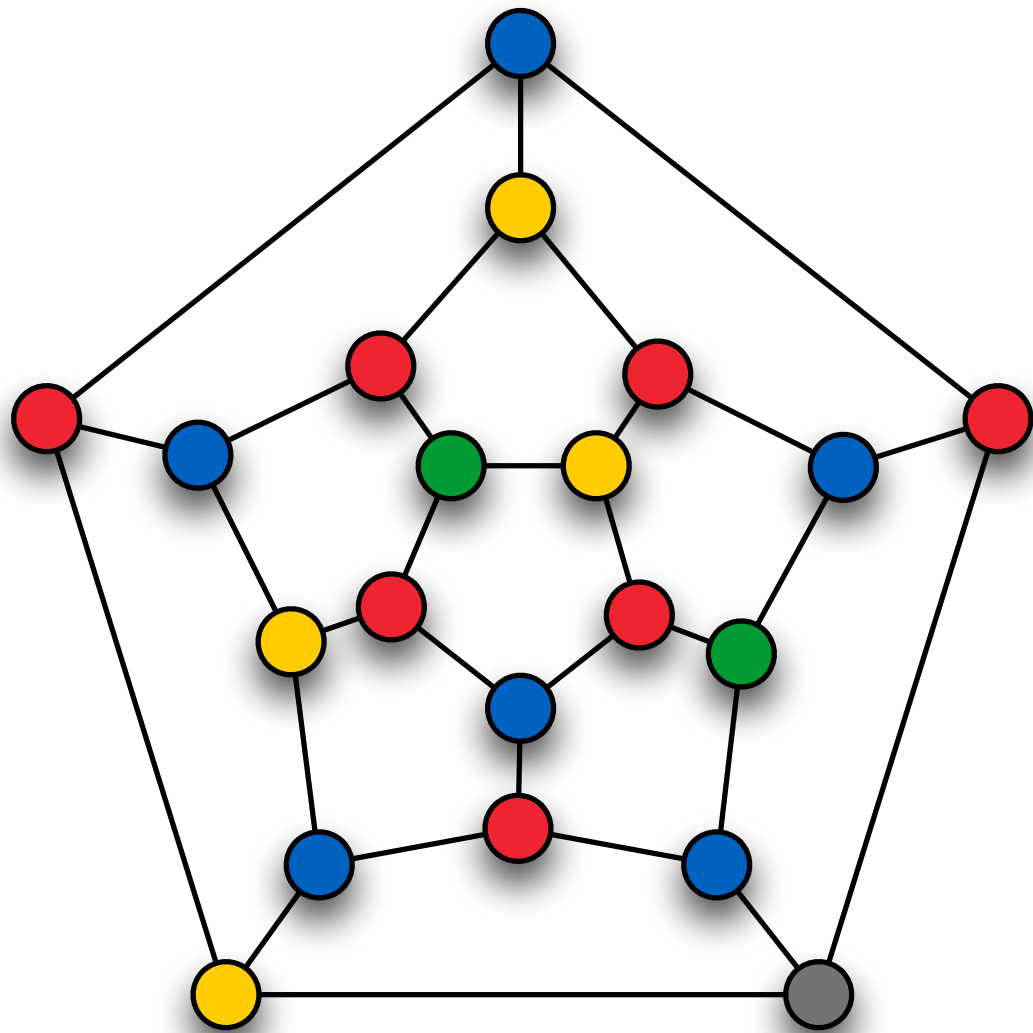
Multiset M
of colors (the motif)



Task (decision):

Is there a connected subgraph whose colors agree with M ?

Data, query, and one match



Limited background on motif search

- Extension of *jumbled pattern matching* on strings (=paths) and trees
- This variant introduced by Lacroix *et al.*
([IEEE/ACM Trans. Comput. Biology Bioinform. 2006](#))
- Many variants and extensions
 - Exact match
([Lacroix et al. 2006](#))
 - Match (large enough) multisubset
([Dondi et al. 2009](#))
 - Multiple color constraints, weights on edges, scoring by weight
([Bruckner et al. 2009](#))
 - Minimum-add / minimum-substitution distance
([Dondi et al. 2011](#))
 - Minimum weighted edit distance
([Björklund et al. 2013](#))
 -

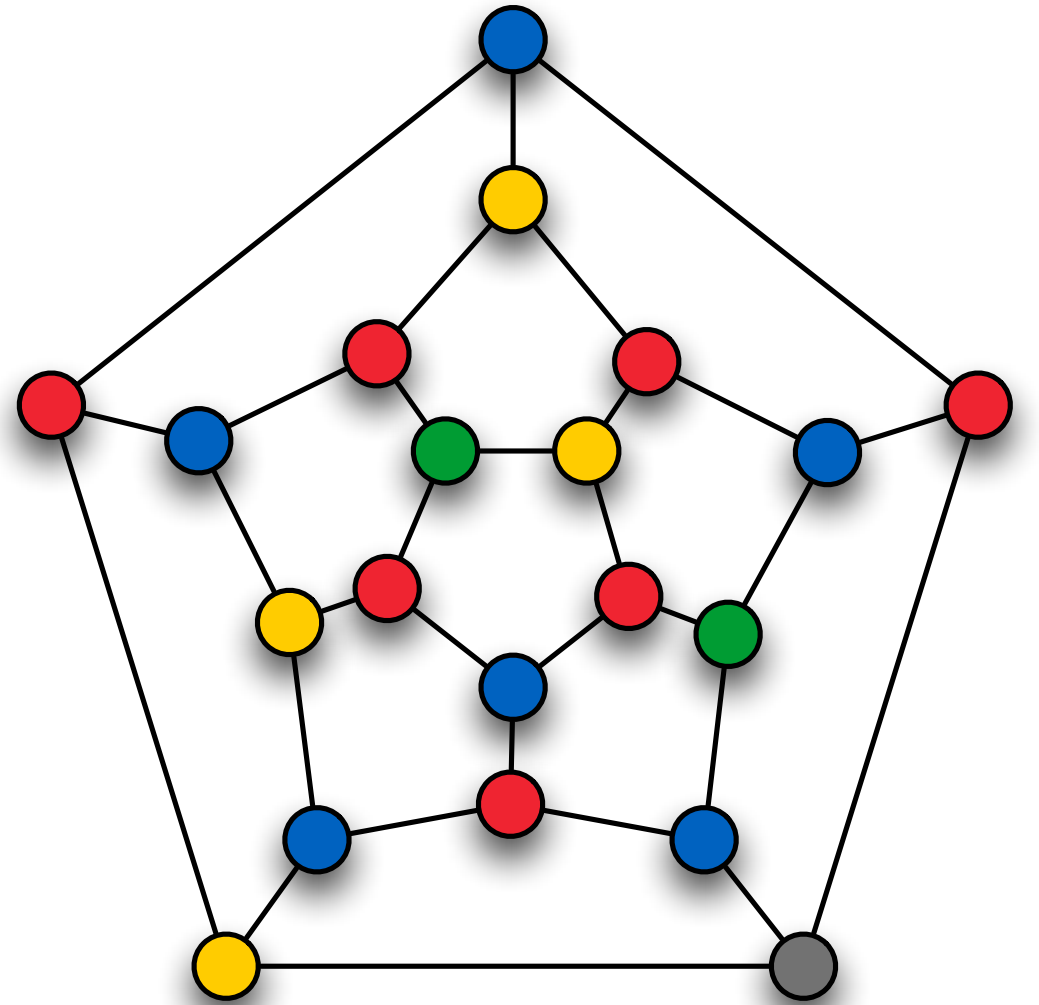
Complexity of motif search

NP-complete
if M has at least
two colors



(easy reduction from Steiner tree)

NP-complete on
trees with max. degree 3,
 M has distinct colors
(Fellows *et al.* 2007)



Solvable
in linear time
in the size of H

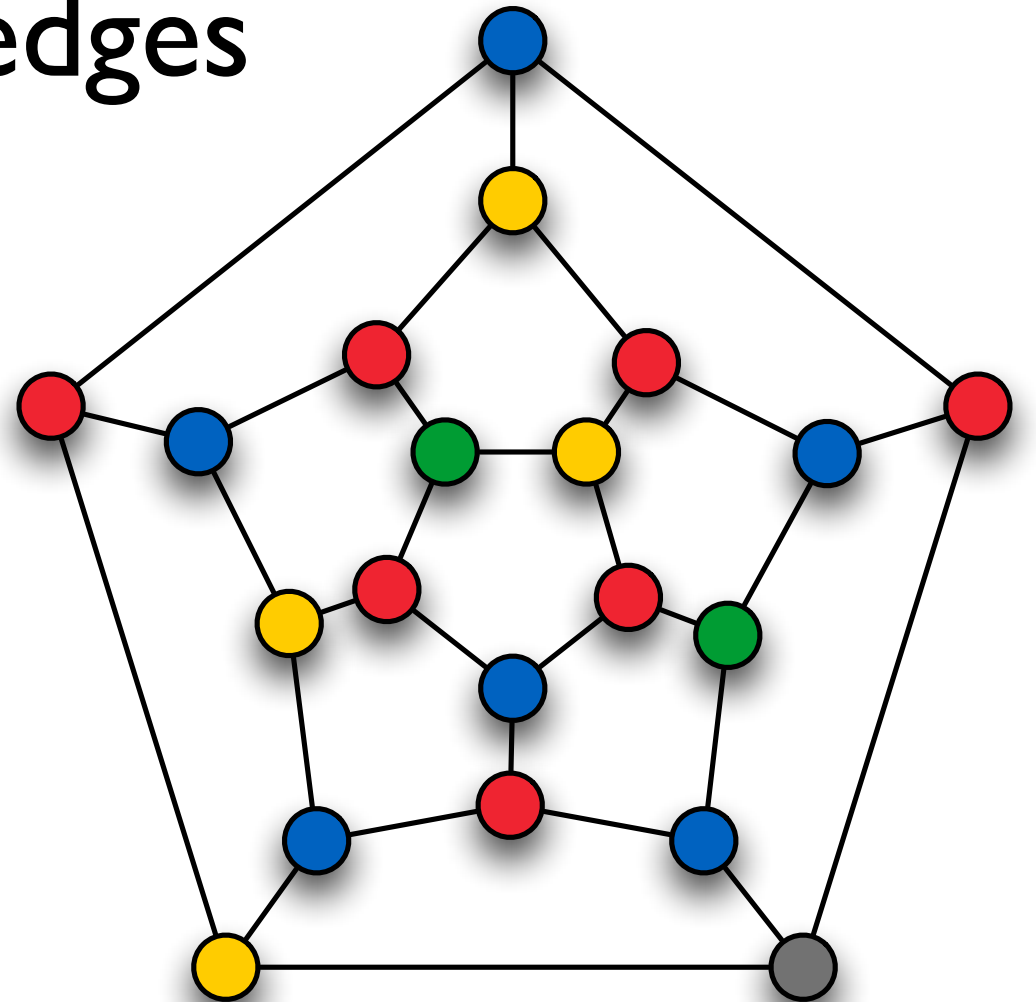
(and exponential in the size of M)

Parameterization

Let H have n vertices and m edges

Let M have size k

Worst-case running time
as a function of n, m, k ?



Dependence on k

<u>Authors</u>	<u>Time</u>		<u>Approach</u>
Fellows <i>et al.</i>	$O^*(\sim 87^k)$	2007	Color coding
Betzler <i>et al.</i>	$O^*(4.32^k)$	2008	Color coding
Guillemot & Sikora	$O^*(4^k)$	2010	Multilinear detection
Koutis	$O^*(2.54^k)$	2012	Constrained multilin.
<u>Björklund <i>et al.</i></u>	$O^*(2^k)$	2013	Constrained multilin.

“FPT race”

tight
(unless there is
a breakthrough for
SET COVER)

Tightness (conditional)

SET COVER

Input: Sets $S_1, S_2, \dots, S_m \subseteq \{1, 2, \dots, n\}$

Budget $t \in \mathbb{Z}$

Question:

Do there exist sets $S_{i_1}, S_{i_2}, \dots, S_{i_t}$ with $S_{i_1} \cup S_{i_2} \cup \dots \cup S_{i_t} = \{1, 2, \dots, n\}$?

Theorem [Björklund, K., Kowalik 2013]

If GRAPH MOTIF can be solved in $O^*((2-\varepsilon)^k)$ time,
then SET COVER can be solved in $O^*((2-\varepsilon')^n)$ time

Key lemma [implicit in Cygan et. al 2012]:

If SET COVER can be solved in $O^*((2-\varepsilon)^{n+t})$ time,
then it can also be solved in $O^*((2-\varepsilon')^n)$ time

Tight results



Satisfiability Lower Bounds and Tight Results for Parameterized and Exponential-Time Algorithms

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**Are tight algorithms useful,
in practice ?**

Tight results

**Are tight algorithms useful,
in practice ?**

**For GRAPH MOTIF,
can we engineer an implementation
that scales to *large* graphs?
(as long as the motif size *k* is small)**

Starting point (theory): $\tilde{O}(2^k k^2 m)$ -time randomized algorithm
(decides *existence* of match)

Theory background for tight algorithm

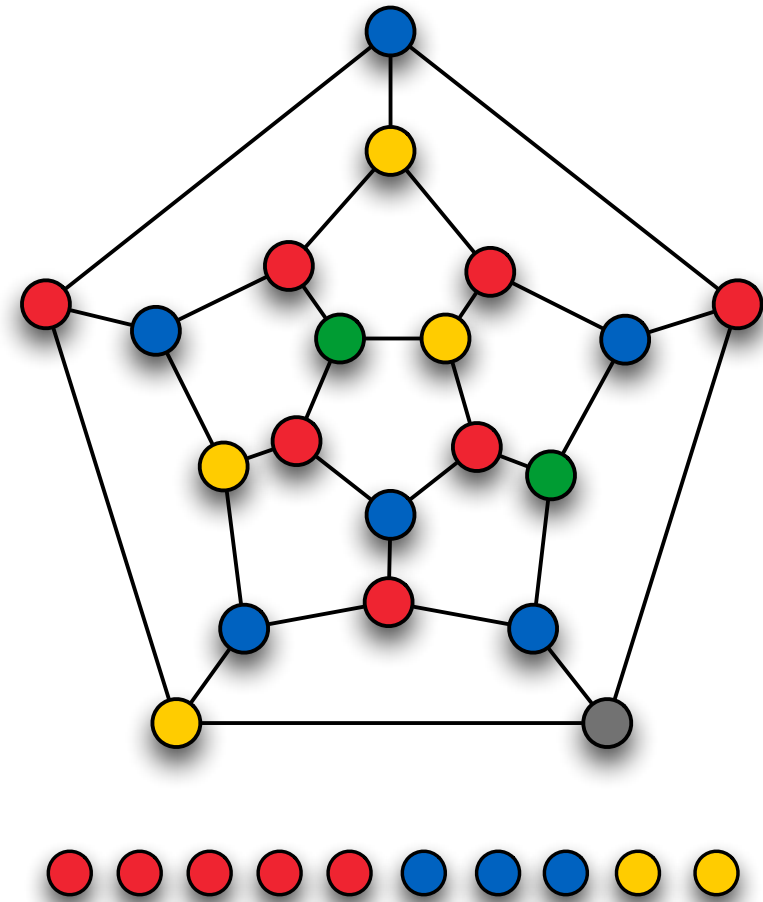
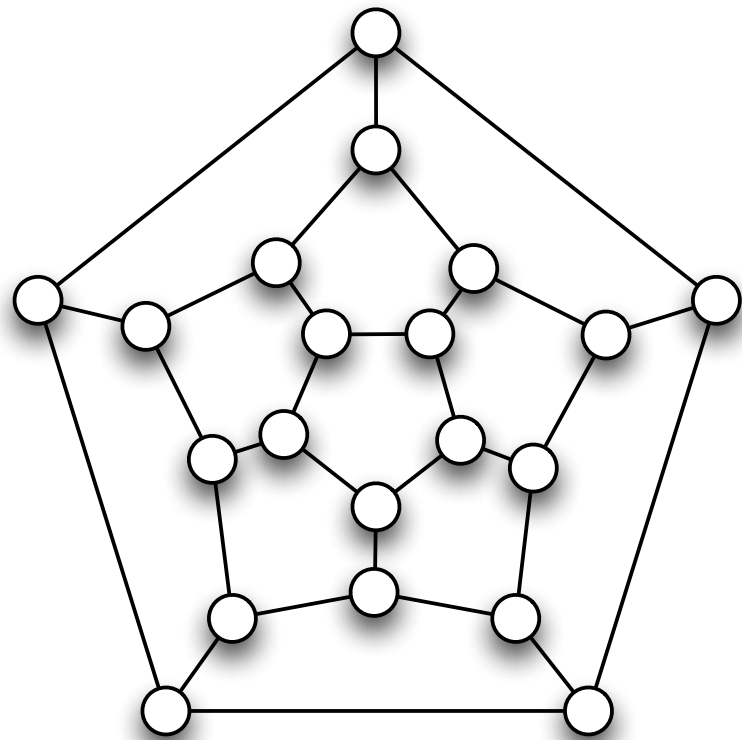
- Key idea: **algebrize** the combinatorial problem
— here: use *constrained multilinear detection*
- Pioneered in the context of group algebras

Koutis (2008), Williams (2009),
Koutis and Williams (2009),
Koutis (2010), Koutis (2012)

- Here we use generating polynomials
and substitution sieving in characteristic 2

Björklund (2010),
Björklund *et al.* (2010, 2013)

The algebraic view



1) connected subgraphs

... are witnessed by *multilinear monomials* in a generating polynomial $P_{H,k}(\mathbf{x}, \mathbf{y})$

fast evaluation algorithm for $P_{H,k}(\mathbf{x}, \mathbf{y})$

2) match colors with motif

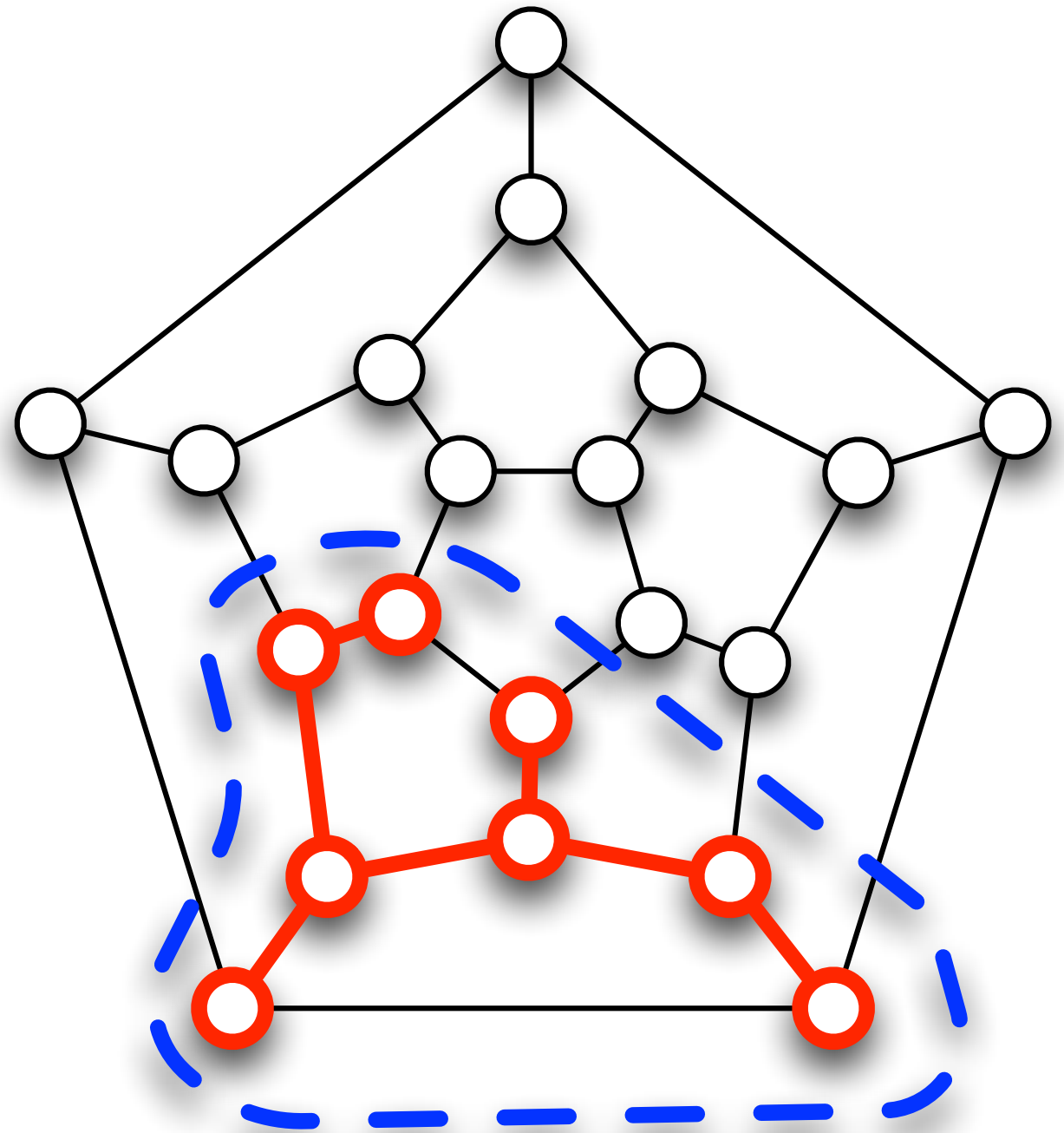
... *multilinear monomials* whose colors match motif

randomized detection with 2^k evaluations of $P_{H,k}(\mathbf{x}, \mathbf{y})$

Connected sets to multilinearity

Intuition:
Use spanning trees to
witness connected sets

Every connected
set of vertices
has at least one
spanning tree



Connected sets to multilinearity

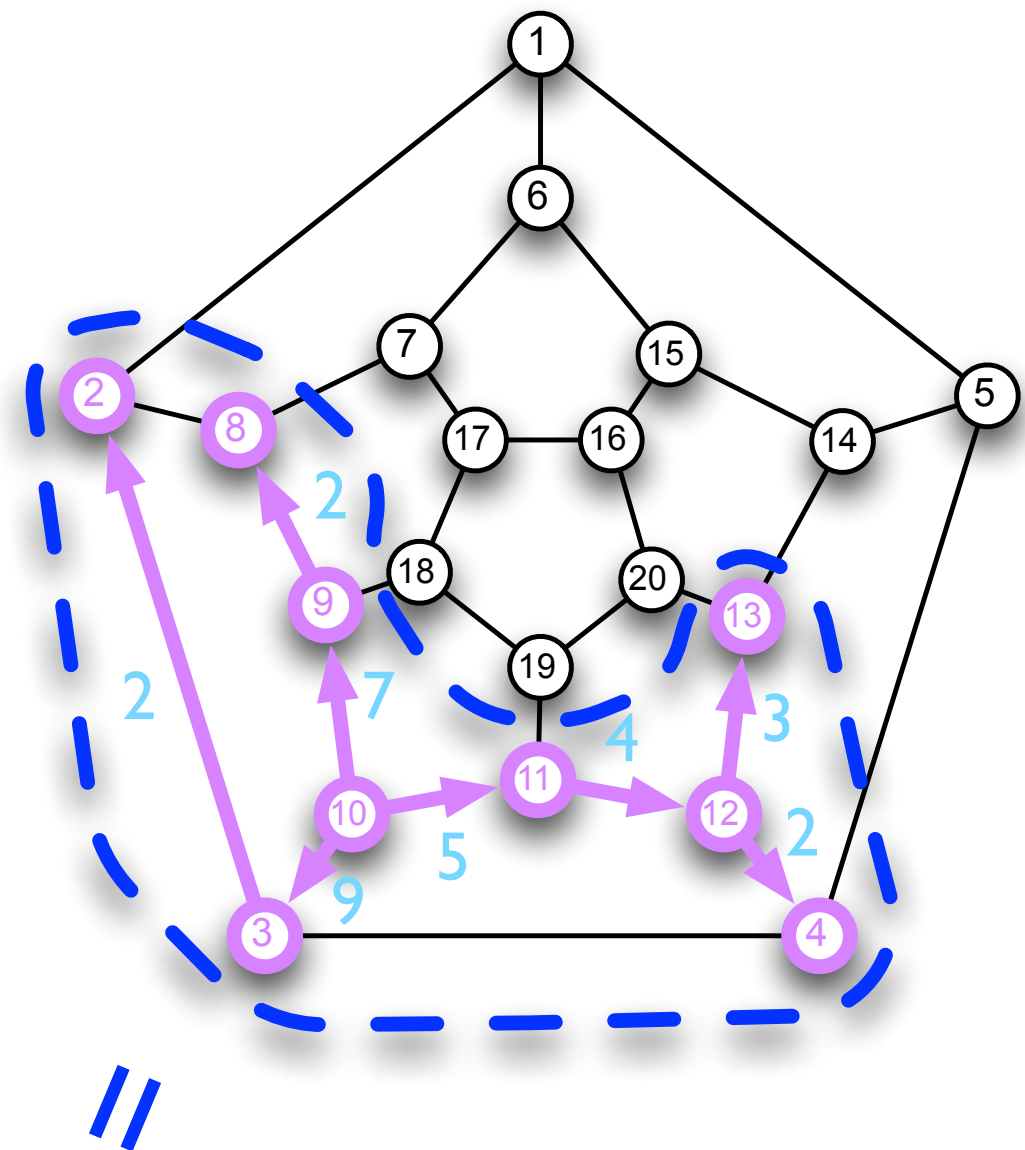
- Key idea:
Branching walks (Nederlof 2008)
[introduced in the context of inclusion-exclusion algorithms for Steiner tree]
- Transported to multivariate polynomial algebrizations of connected sets
(Guillemot and Sikora 2010)
- A multivariate polynomial with edge-linear time, vertex-linear working memory evaluation algorithm
(Björklund, K., Kowalik 2013 & 2015)

The polynomial $P_{H,k}(x,y)$

Each “*rooted spanning tree*” of size k in H occurs as a unique *multilinear monomial* in $P_{H,k}(x,y)$

There are no other *multilinear* monomials in $P_{H,k}(x,y)$

Given values to the variables x,y , the value $P_{H,k}(x,y)$ can be computed fast



$x_2 x_3 x_4 x_8 x_9 x_{10} x_{11} x_{12} x_{13} y_{2,(3,2)} y_{2,(9,8)} y_{9,(10,3)} y_{7,(10,9)} y_{5,(10,11)} y_{4,(11,12)} y_{2,(12,4)} y_{3,(12,13)}$

Evaluation algorithm at point $(\mathbf{x}, \mathbf{y})$

Base case, for all $u \in V(H)$

$$P_{1,u}(\mathbf{x}, \mathbf{y}) = x_u$$

Dynamic programming

– edge-linear $\tilde{O}(k^2m)$ time

– vertex-linear $\tilde{O}(kn)$ working memory

Iteration, for all $\ell = 2, 3, \dots, k$ and all $u \in V(H)$

$$P_{\ell,u}(\mathbf{x}, \mathbf{y}) = \sum_{v \in N_H(u)} y_{\ell,(u,v)} \sum_{\substack{\ell_1 + \ell_2 = \ell \\ \ell_1, \ell_2 \geq 1}} P_{\ell_1,u}(\mathbf{x}, \mathbf{y}) P_{\ell_2,v}(\mathbf{x}, \mathbf{y})$$

Finally, take the sum over all root vertices

$$P(\mathbf{x}, \mathbf{y}) = \sum_{u \in V(H)} P_{k,u}(\mathbf{x}, \mathbf{y})$$

Rand. algorithm for motif search (decision)

- Ideas: 1) polynomial $P_{H,k}(\mathbf{x}, \mathbf{y})$
2) constrained multilinearity sieve
3) DeMillo–Lipton–Schwartz–Zippel lemma
- Requires 2^k evaluations of $P_{H,k}(\mathbf{x}, \mathbf{y})$, which leads to running time $\tilde{O}(2^k k^2 m)$ and working memory $\tilde{O}(kn)$
- Algorithm is (essentially) just a big sum:
The 2^k evaluations can be executed *in parallel*

No false positives

False negatives with probability at most $k \cdot 2^{-b+1}$
(arithmetic over $\text{GF}(2^b)$, $b = O(\log k)$)

Tight results

**Are tight algorithms useful,
in practice ?**

Starting point (theory): $\tilde{O}(2^k k^2 m)$ -time randomized algorithm
for graph motif
(decides *existence* of match)

Engineering aspects

- Here focus on:
Shared-memory multiprocessors (CPU-based)
- Two key subsystems
 - Memory (DDR3/DDR4-SDRAM)
 - CPUs (Intel x86–64 with ISA extensions)
(e.g. Haswell/Broadwell microarchitecture with AVX2, PCLMULQDQ)

Engineering an implementation

the new generating polynomial $P_{H,k}(x,y)$
and **parallel** evaluation algorithm

- **Capacity**

- $O(kn)$ working memory
- use ISA extensions (AVX2 + PCLMULQDQ), if available, for arithmetic in $GF(2^b)$

- **Bandwidth**

- use memory one 512-bit cache line at a time
- use all CPUs, all cores, all (vector) ports
multithreading **vectorization**

- **Latency**

- hardware *and* software prefetching
- hide latency with enough instructions “in flight”

Evaluating $P_{H,k}(\mathbf{x}, \mathbf{y})$

Base case, for all $u \in V(H)$

$$P_{1,u}(\mathbf{x}, \mathbf{y}) = x_u$$

**Vectorization over
several independent
points $(\mathbf{x}^{(j)}, \mathbf{y}^{(j)})$ at once**

Iteration, for all $\ell = 2, 3, \dots, k$ and all $u \in V(H)$

$$P_{\ell,u}(\mathbf{x}, \mathbf{y}) = \sum_{v \in N_H(u)} y_{\ell,(u,v)} \sum_{\substack{\ell_1 + \ell_2 = \ell \\ \ell_1, \ell_2 \geq 1}} P_{\ell_1,u}(\mathbf{x}, \mathbf{y}) P_{\ell_2,v}(\mathbf{x}, \mathbf{y})$$

Finally, take the sum over all root vertices

$$P(\mathbf{x}, \mathbf{y}) = \sum_{u \in V(H)} P_{k,u}(\mathbf{x}, \mathbf{y})$$

**Multithreading over
vertices u
(layer ℓ fixed)**

Inner loop in C

Iteration, for all $\ell = 2, 3, \dots, k$ and all $u \in V(H)$

$$P_{\ell,u}(\mathbf{x}, \mathbf{y}) = \sum_{v \in N_H(u)} y_{\ell,(u,v)} \sum_{\substack{\ell_1 + \ell_2 = \ell \\ \ell_1, \ell_2 \geq 1}} P_{\ell_1,u}(\mathbf{x}, \mathbf{y}) P_{\ell_2,v}(\mathbf{x}, \mathbf{y})$$

```
for(index_t l1 = 1; l1 < l; l1++) {
    line_t p1, p2;
    index_t l2 = l-l1;
    index_t i_v_l2 = ARB_LINE_IDX(b, k, l2, v);
    LINE_LOAD(p2, d_s, i_v_l2);           // data-dependent load
    index_t i_u_l1 = ARB_LINE_IDX(b, k, l1, u);
    LINE_LOAD(p1, d_s, i_u_l1);
    index_t i_nv_l2 = ARB_LINE_IDX(b, k, l2, nv);
    LINE_PREFETCH(d_s, i_nv_l2);          // user prefetch data-dependent
                                          // load (for next vertex v)
    line_t p;
    LINE_MUL(p, p1, p2);
    LINE_ADD(s, s, p);
}
```

Compiled inner loop (w/ AVX2 +PCLMULQDQ)

```
.L610:
    movq    %r9,    %rcx
    movq    %rdi,   %rsi
    imulq   %r8,    %rcx
    subq    %rax,   %rsi
    leaq    -1(%rsi,%rcx), %rcx
    salq    $6,     %rcx
    vmovdqu (%rdx,%rcx), %ymm6
    vmovdqu 32(%rdx,%rcx), %ymm5
    movq    %rbx,   %rcx
    imulq   (%r15), %rcx
    vmovdqa %xmm6, %xmm0
    vextracti128 $0x1, %ymm6, %xmm6
    leaq    -1(%rax,%rcx), %rcx
    addq    $1,     %rax
    salq    $6,     %rcx
    vmovdqu (%rdx,%rcx), %ymm1
    vmovdqu 32(%rdx,%rcx), %ymm4
    leaq    -1(%rsi,%r10), %rcx
    vmovdqa %xmm1, %xmm7
    vextracti128 $0x1, %ymm1, %xmm1
    vpclmulqdq $0, %xmm6, %xmm1, %xmm2
    vpclmulqdq $0, %xmm0, %xmm7, %xmm3
    vpclmulqdq $17, %xmm6, %xmm1, %xmm1
    vmovdqa %xmm4, %xmm6
    vinserti128 $0x1, %xmm2, %ymm3, %ymm3
    vpclmulqdq $17, %xmm0, %xmm7, %xmm0
    vinserti128 $0x1, %xmm1, %ymm0, %ymm0
    vpunpcklqdq %ymm0, %ymm3, %ymm1
    vpunpckhqdq %ymm0, %ymm3, %ymm3
    vmovdqa %xmm5, %xmm7
    vpsrlq    $60, %ymm3, %ymm0
    vextracti128 $0x1, %ymm4, %xmm4
    vextracti128 $0x1, %ymm5, %xmm5
    vpsrlq    $61, %ymm3, %ymm2
    salq      $6, %rcx
    cmpq      %rax, %rdi
    vpxor     %ymm0, %ymm2, %ymm2
    vpsrlq    $63, %ymm3, %ymm0

    prefetcht0 (%rdx,%rcx)
    vpxor     %ymm2, %ymm0, %ymm2
    vpxor     %ymm2, %ymm3, %ymm2
    vpsllq    $1, %ymm2, %ymm0
    vpxor     %ymm1, %ymm0, %ymm0
    vpsllq    $3, %ymm2, %ymm1
    vpclmulqdq $0, %xmm7, %xmm6, %xmm3
    vpxor     %ymm0, %ymm1, %ymm0
    vpsllq    $4, %ymm2, %ymm1
    vpxor     %ymm0, %ymm1, %ymm0
    vpclmulqdq $17, %xmm7, %xmm6, %xmm1
    vpxor     %ymm0, %ymm2, %ymm2
    vpclmulqdq $0, %xmm5, %xmm4, %xmm0
    vpclmulqdq $17, %xmm5, %xmm4, %xmm4
    vinserti128 $0x1, %xmm0, %ymm3, %ymm3
    vinserti128 $0x1, %xmm4, %ymm1, %ymm1
    vpunpcklqdq %ymm1, %ymm3, %ymm4
    vpunpckhqdq %ymm1, %ymm3, %ymm1
    vpsrlq    $61, %ymm1, %ymm3
    vpxor     %ymm2, %ymm8, %ymm8
    vmovdqa   %ymm8, 80(%rsp)
    vpsrlq    $60, %ymm1, %ymm0
    vpxor     %ymm0, %ymm3, %ymm0
    vpsrlq    $63, %ymm1, %ymm3
    vpxor     %ymm0, %ymm3, %ymm0
    vpxor     %ymm0, %ymm1, %ymm0
    vpsllq    $3, %ymm0, %ymm3
    vpsllq    $1, %ymm0, %ymm1
    vpxor     %ymm4, %ymm1, %ymm1
    vpxor     %ymm1, %ymm3, %ymm1
    vpsllq    $4, %ymm0, %ymm3
    vpxor     %ymm1, %ymm3, %ymm1
    vpxor     %ymm1, %ymm0, %ymm0
    vpxor     %ymm0, %ymm9, %ymm9
    vmovdqa   %ymm9, 112(%rsp)
    jg        .L610
```

4 x GF(2⁶⁴) vectorization (4 independent points)

Open source

<https://github.com/pkaski/motif-search>

Experiments

**For GRAPH MOTIF,
can we engineer an implementation
that scales to *large* graphs?
(as long as the motif size k is small)**

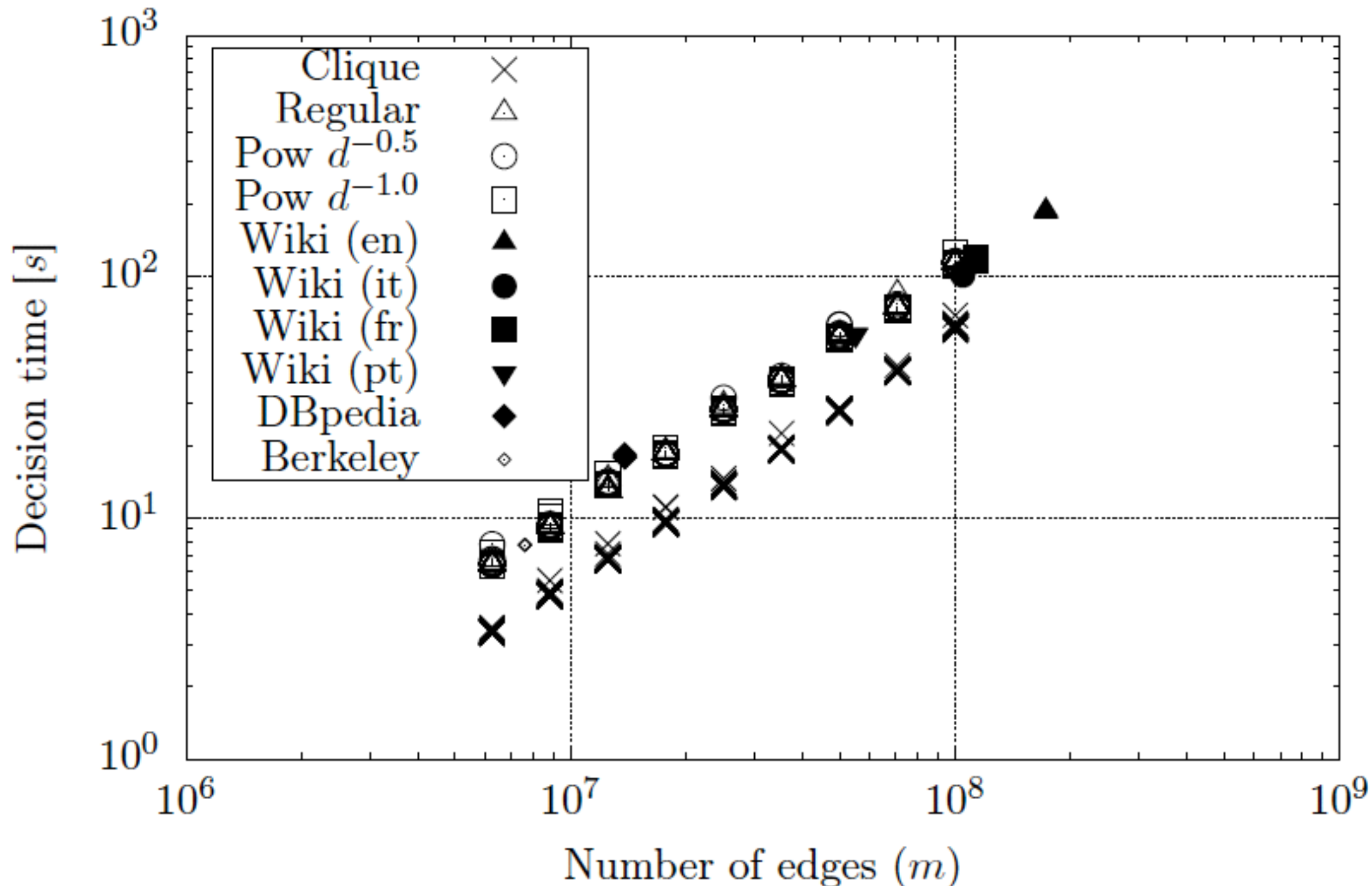
Hardware configurations

- **Small-memory node (1 CPU, total 4 cores)**
 - 1 x 3.20-GHz Intel Core i5-4570 CPU
(Haswell muarch, 4 cores, 6 MiB LLC, 2 channels to main mem.)
 - 16 GiB main memory (4 x 4 GiB DDR3-1600)
- **Large-memory node (2 CPU, total 20 cores)**
 - 2 x 2.80-GHz Intel Xeon E5-2680 v2 CPU
(Ivy Bridge muarch, 10 cores, 25 MiB LLC, 4 channels to main mem.)
 - 256 GiB main memory (16 x 16 GiB DDR3-1866)
- **Fat-memory node (4 CPU, total 24 cores)**
 - 4 x 2.67-GHz Intel Xeon X7542 CPU
(Nehalem muarch, 6 cores, 18 MiB LLC, 1 channel to main mem.)
 - 1 TiB main memory (64 x 16 GiB DDR3-1066)

Edge-linear scaling

[Natural graphs from the Koblenz network collection]

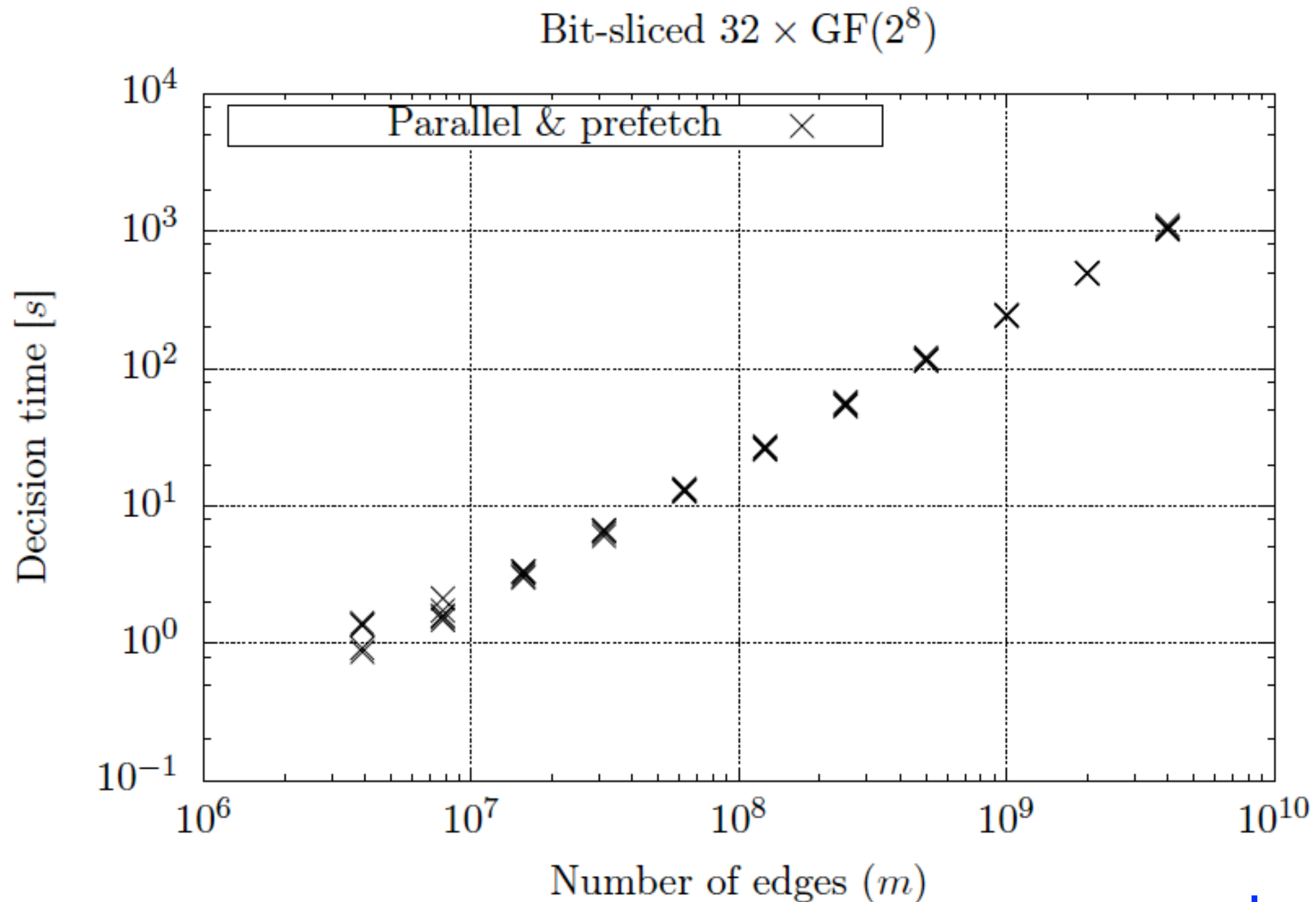
Bit-packed $8 \times \text{GF}(2^{64})$



Small-memory node

$k = 5$

Edge-linear scaling

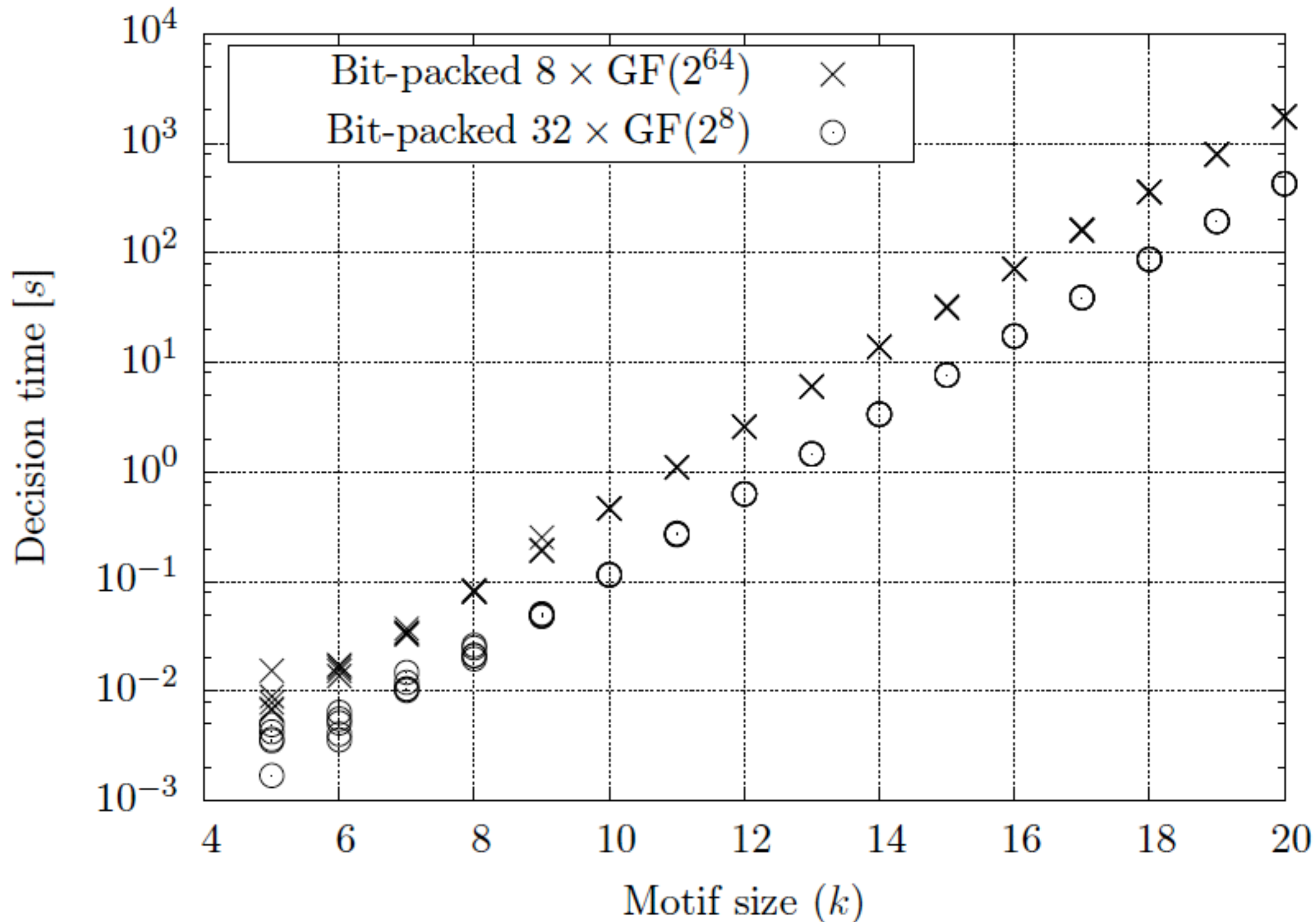


Large-memory node

$k = 5$ fixed

5 independent random 20-regular graphs for each value of m

Exponential scaling in k

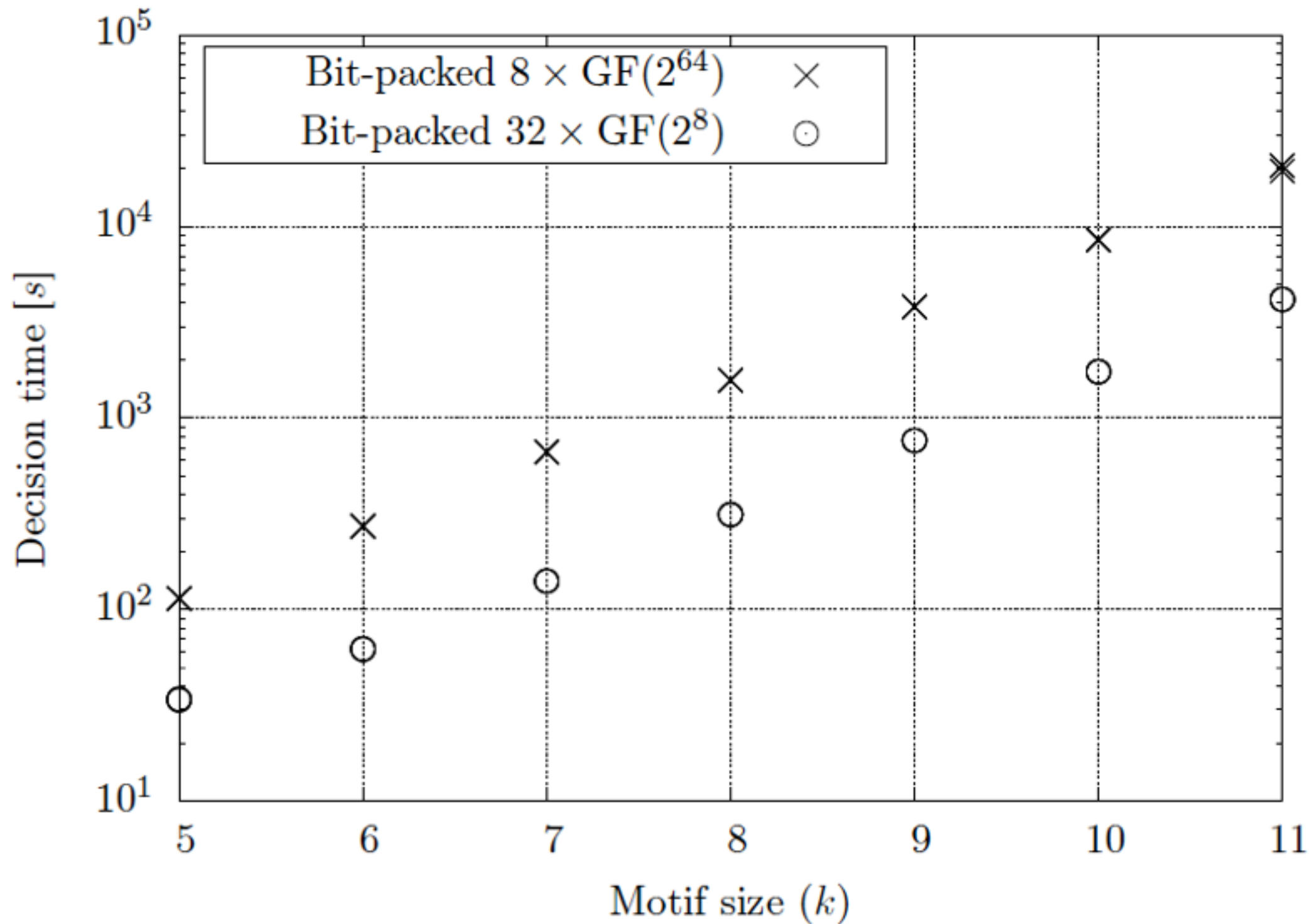


Small-memory node

$n = 1000, m = 10000$

5 independent random 20-regular graphs for each value of k

Exponential scaling in k



Small-memory node

$n = 10$ million, $m = 100$ million
5 independent random 20-regular graphs for each value of k

Large graphs

Vertices	Edges	Input	Preprocess	Decision	Total	Peak memory
2 000 000 000	20 000 000 004	2330 s	1937 s	3163 s	7452 s	693 GiB
1 000 000 000	10 000 000 004	1057 s	987 s	1545 s	3599 s	347 GiB
500 000 000	5 000 000 004	492 s	407 s	770 s	1673 s	174 GiB
250 000 000	2 500 000 004	237 s	183 s	376 s	799 s	87 GiB
125 000 000	1 250 000 004	112 s	90 s	182 s	386 s	44 GiB
62 500 000	625 000 004	55 s	43 s	88 s	187 s	22 GiB
1 000 000 000	20 000 000 004	2040 s	1830 s	2915 s	6805 s	623 GiB
500 000 000	10 000 000 004	939 s	816 s	1430 s	3196 s	312 GiB
250 000 000	5 000 000 004	467 s	409 s	704 s	1586 s	156 GiB
125 000 000	2 500 000 004	221 s	182 s	343 s	749 s	78 GiB
62 500 000	1 250 000 004	109 s	88 s	165 s	363 s	39 GiB

generate random regular input
(in edge list format)

convert from edge list to adjacency list

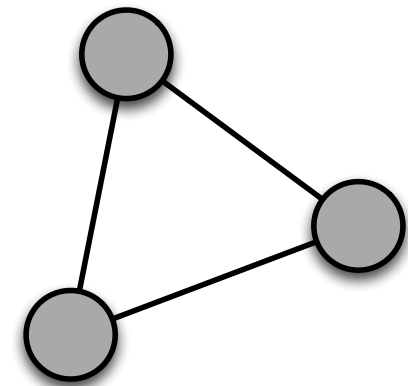
decision algorithm runtime

Fat-memory node

$k = 5$

Summary (engineering)

- A proof-of-concept practical algorithm for small k , large m
- NP-hard problem, yet in practice (for small k) can process inputs with hundreds of millions of edges — many polynomial-time algorithms do worse than this!



- Algorithm is “just a big sum” — the same polynomial evaluated at different points — easy SIMD parallelization

Summary (engineering)

- Some implementation details to get performance:
 - Vectorized finite-field arithmetic (low-level implementation)
 - Using memory one 512-bit cache line at a time
 - Coping with latency:
memory layout to enable *hardware prefetching*,
software-prefetch indirect reads ahead of time
- Not covered in this presentation:
how to upgrade decision algorithm to list all solutions
- See paper (ALENEX'15) and source code (~6000 lines of C):

<http://dx.doi.org/10.1137/1.9781611973754.10>

<https://github.com/pkaski/motif-search>

Summary (theory)

- **Theory work supports engineering**
(here: generating polynomial, multilinear sieves,
polynomial identity testing, ...)
- Derandomization?
Indexing (preprocessing) the data to enable fast search?
- Coping with increasing latencies?
- *Yet tighter (yet more fine-grained) algorithms?*
 - E.g. from *multiplicative* to **additive** dependency
in the size of the data?

$$O(2^k \text{ poly}(k) m) \rightarrow O(2^k \text{ poly}(k) + \text{poly}(k) m)$$

Thank you!

<http://dx.doi.org/10.1137/1.9781611973754.10>

<https://github.com/pkaski/motif-search>