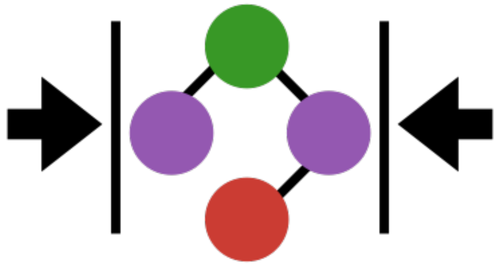
Analyzing Large Graphs with `QuasiStableColors.jl`



Accelerating Max-flow, Linear Programs and Centrality

Moe Kayali, Dan Suciu

University of Washington, Seattle

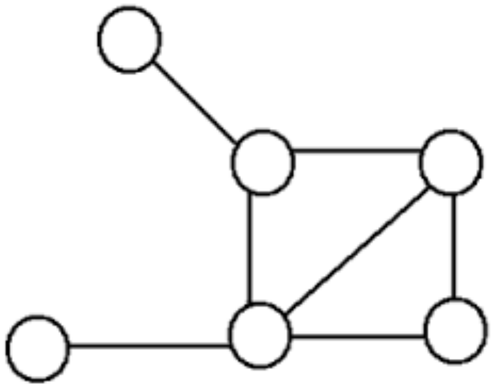
JuliaCon ’23 — July 27, 2023

Motivation

Graphs are:

Motivation

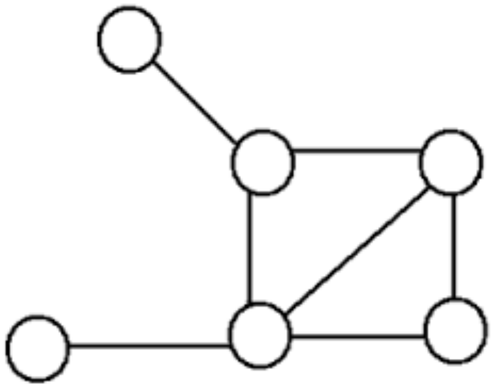
Graphs are:



A fundamental CS building block

Motivation

Graphs are:



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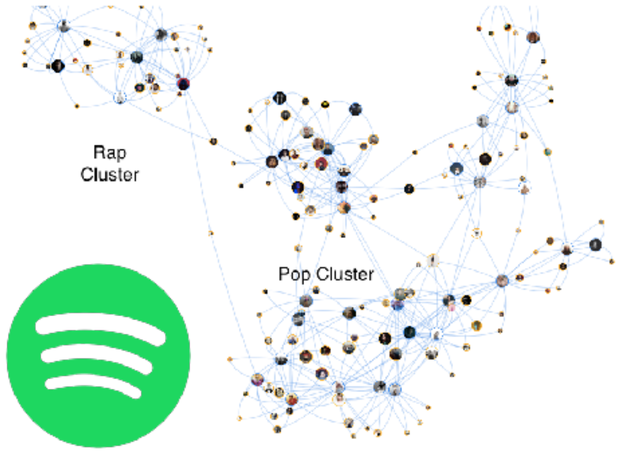
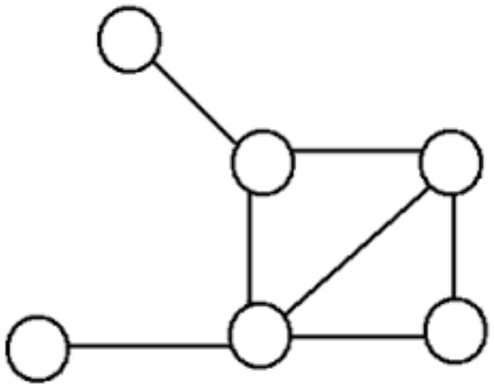


Spotify GNN-based Recommender

Increasingly applicable

Motivation

Graphs are:



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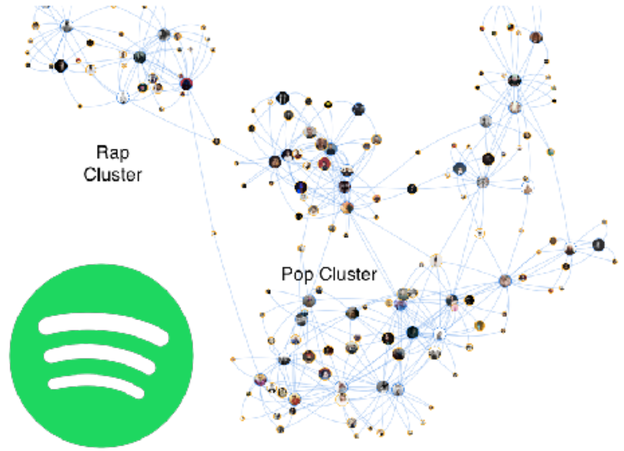
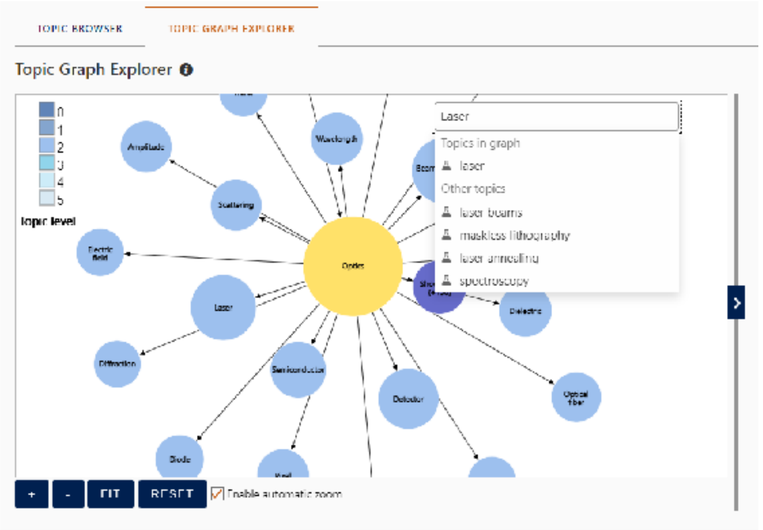


Spotify GNN-based Recommender

Increasingly applicable



Microsoft Academic Graph, >1B nodes

Increasingly large, complex

Motivation

Developed measures on graphs:

Motivation

Developed measures on graphs:

Maximum-flow/minimum-cut

Traffic Modeling

Motivation

Developed measures on graphs:

Maximum-flow/minimum-cut

Traffic Modeling

Centrality

Landmark, Fraud Detection

However…

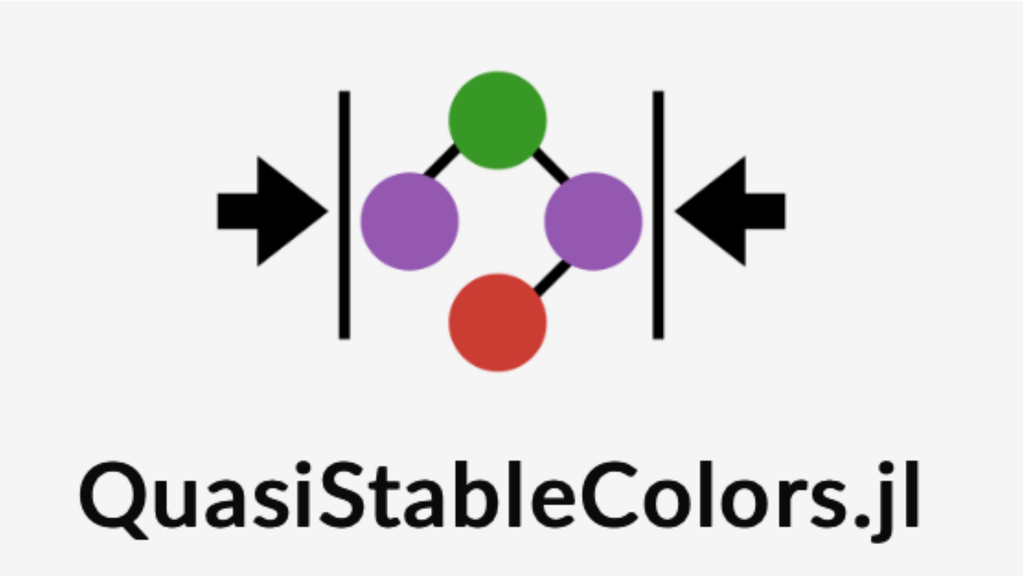
Despite the increasingly larger graphs practitioners encounter, **scalability of graph analysis methods remains poor**.

Betweenness Centrality Performance

Node count	Runtime
100	5 milliseconds
1,000	270 milliseconds
10,000	4 minutes
100,000	42 minutes

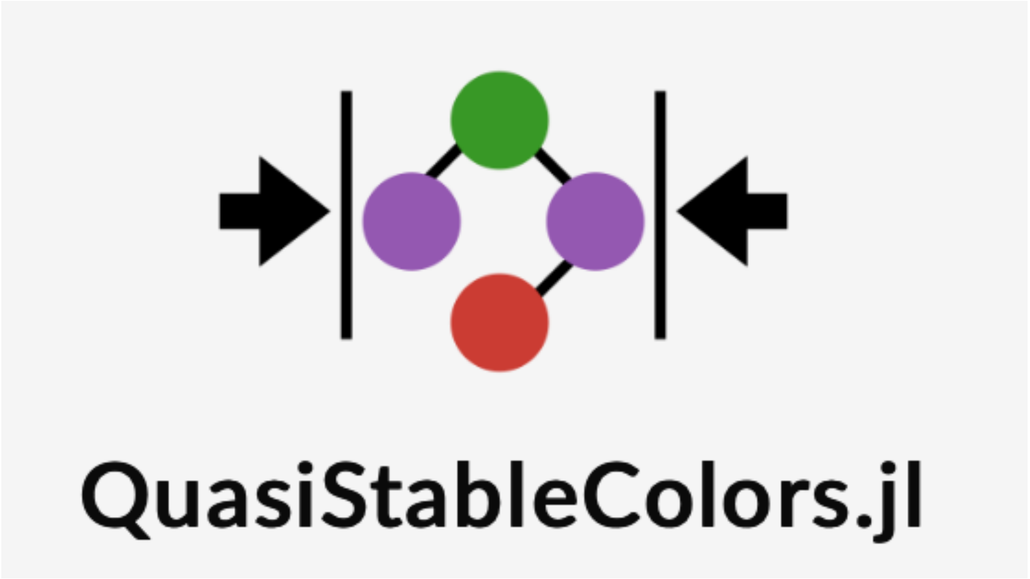
The Library

The Library



The Library

Implementation of a novel graph approximation approach, achieving average 10-100x speedup with less than <15% error



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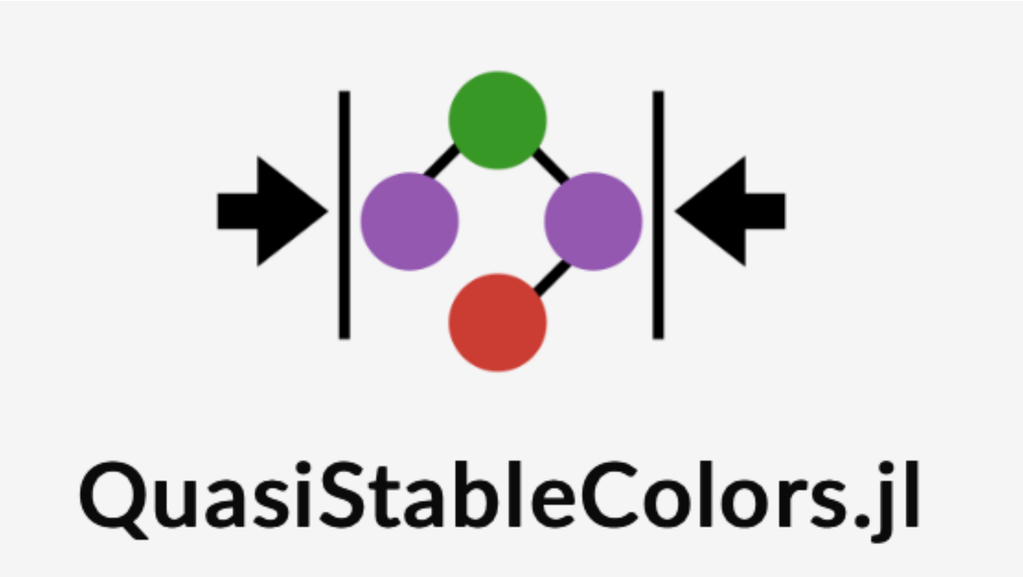
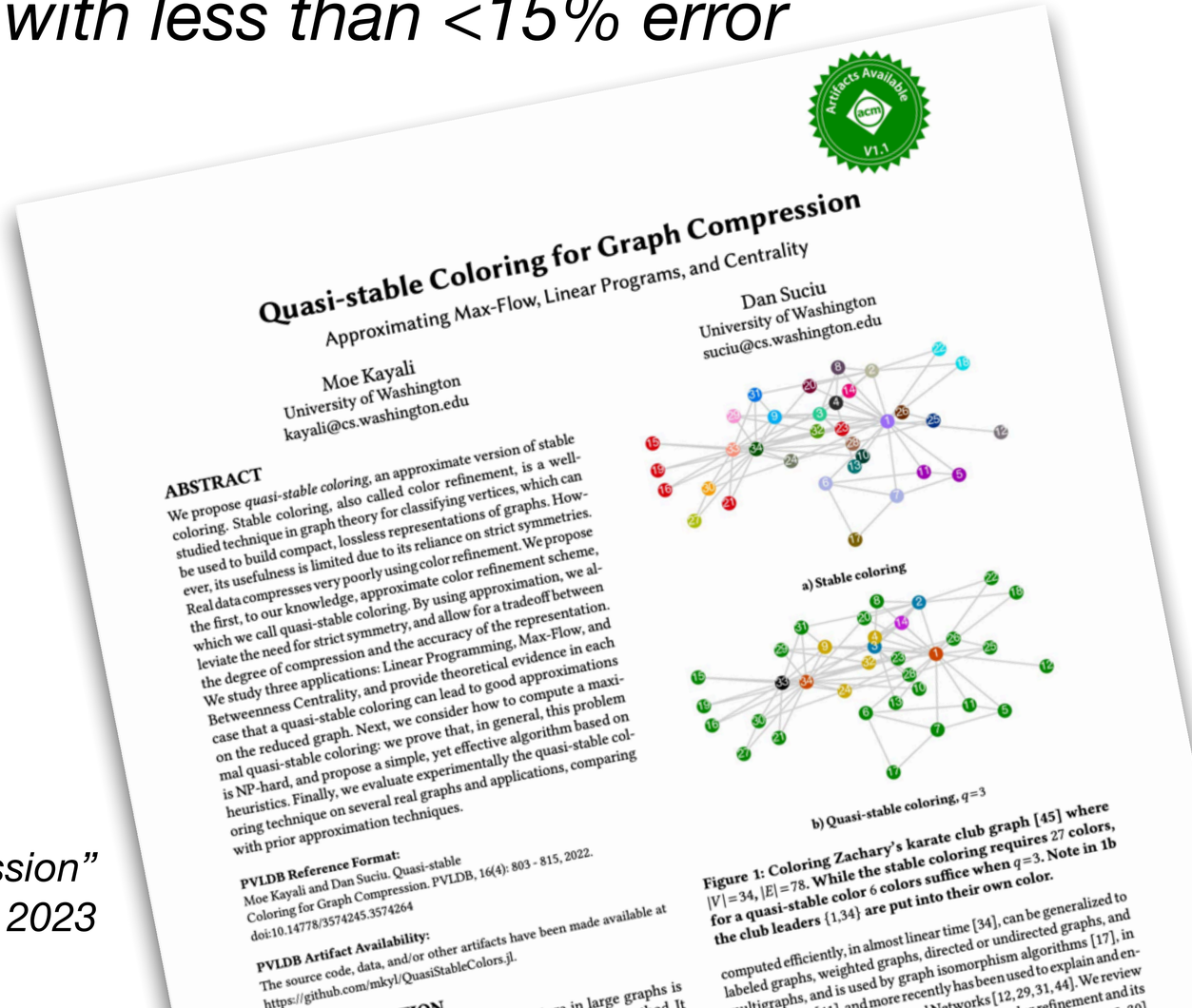




"Quasi-stable Coloring for Graph Compression"
appearing in Very Large Databases Conference (VLDB) 2023

API

`QuasiStableColors.Centrality.approx_betweenness_centrality` — Function

```
approx_betweenness_centrality(
    G::Graph,
    q::Number,
    n_colors::Int,
)
```

Approximate betweenness centrality using a q-stable coloring with maximum error `q` or size `n_colors`, whichever is smaller.

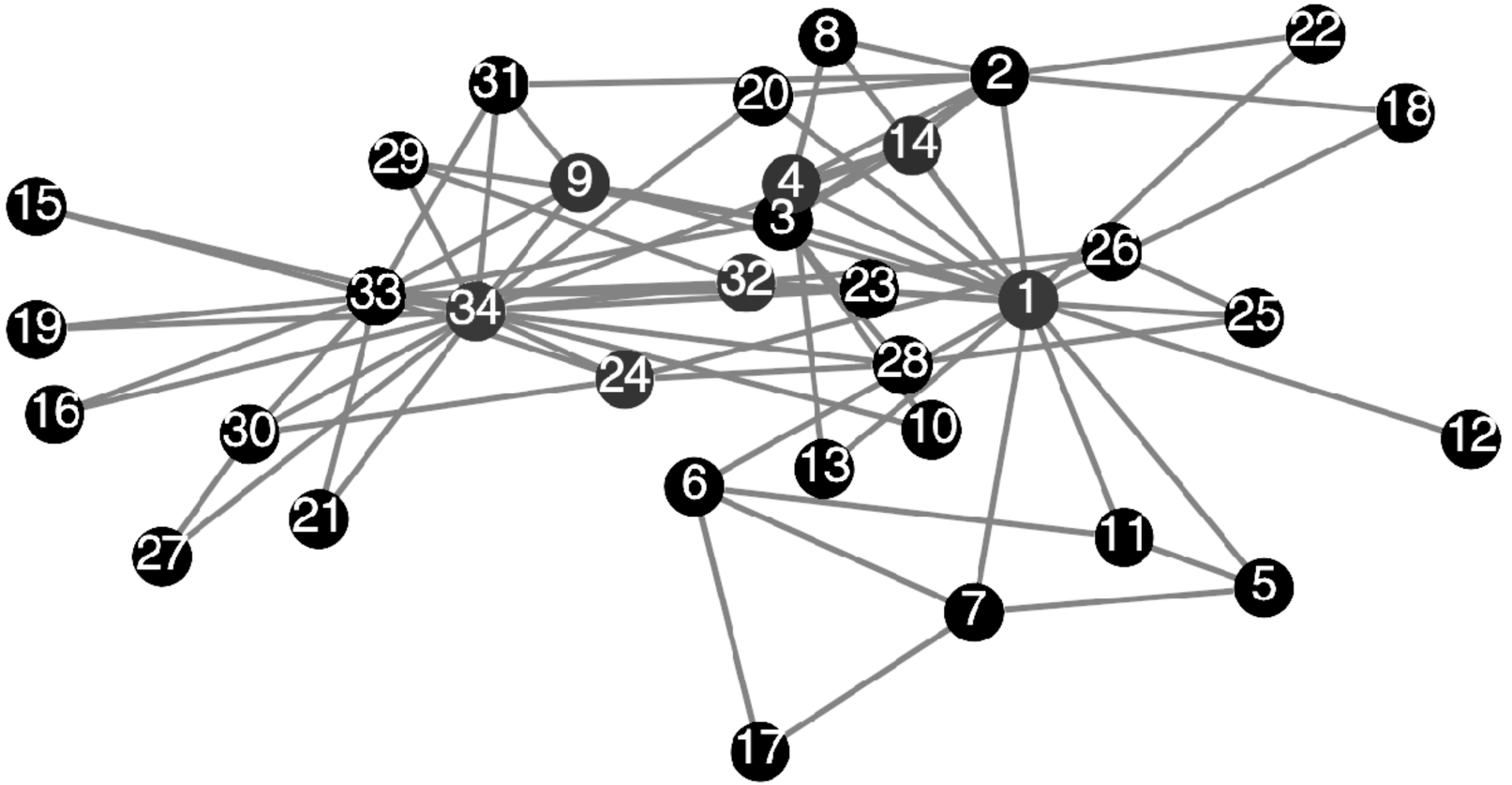
`QuasiStableColors.Optimize.lifted_minimize` — Function

```
lifted_minimize(
    A,
    b::Vector,
    c::Vector,
    q=0.0,
    n_colors=Inf,
)
```

Approximate the linear program $\min c^T x$ where $Ax \geq b, x \geq 0$.

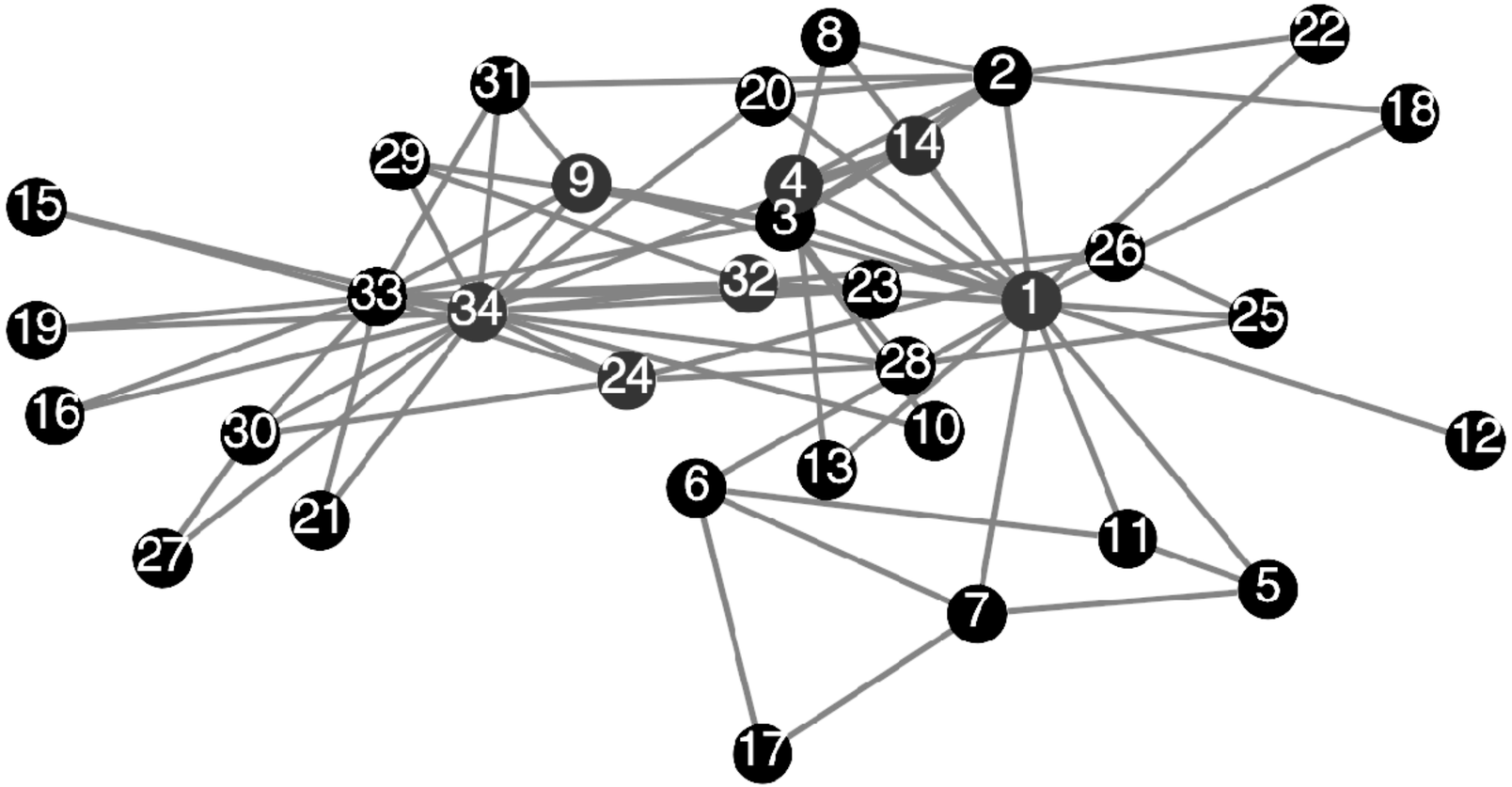
Uses a quasi-stable coloring with maximum error `q` or `n_colors` colors, whichever is smaller.

`QuasiStableColors.Flow.lifted_maxflow` — Function



Karate Club

W. W. Zachary. An information flow model for conflict and fission in small groups. Journal of anthropological research, 33(4):452–473, 1977.



Karate Club

$$|V| = 34, |E| = 78$$

`QuasiStableColors.q_color` — Method

```
q_color(
    G::AbstractGraph{T},
    q = 0.0,
    n_colors = Inf,
    weights::SparseMatrixCSC{<:Number,Int} = nothing,
    special =  Set{T}(),
    warm_start = Vector{Vector{T}}(),
)
```

Compute a quasi-stable coloring for the graph `G`. Typically, you should set one of:

- **`q`**: maximum q-error allowed
- **`n_colors`**: number of colors to use

Advanced, optional parameters:

- **`weights`**: edge weights to use
- **`weighting`**: whether to prioritize larger colors (i.e. with more members).

`false` to prioritize colors with the largest error, regardless of color size.

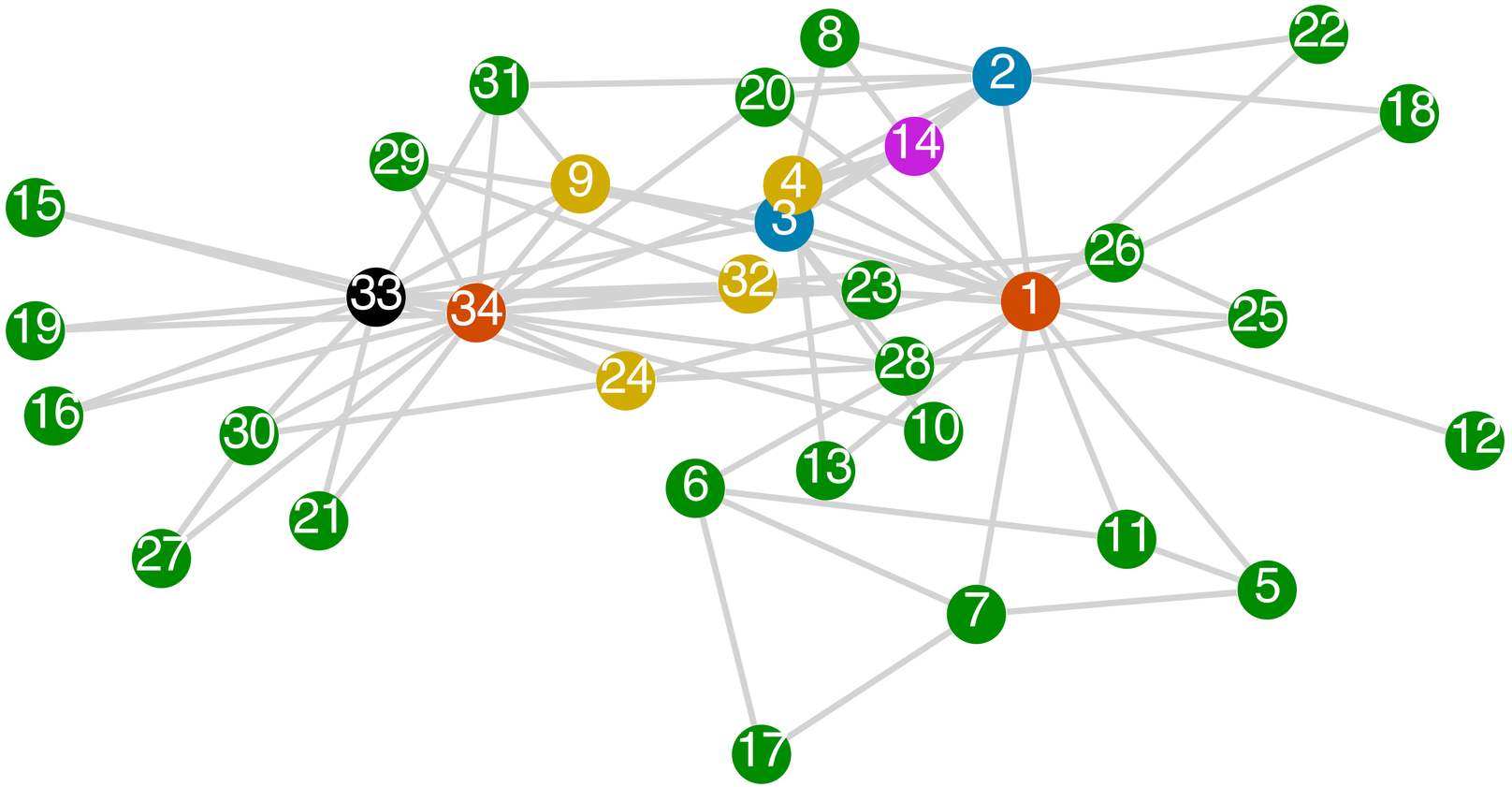
- **`warm_start`**: coloring to refine. If not provided, starts using coarsest

(single color) partitioning.

- **`special`**: node IDs which will always get tl

```
C = QSC.q_color(g, q=1.0)
```

```
Quasi-stable coloring(color count=4, max q-error=1.0)
```



Karate Club

$$|V| = 34, |E| = 78,\ q = 3.0, |P| = 6$$

Quasi-Stable Coloring

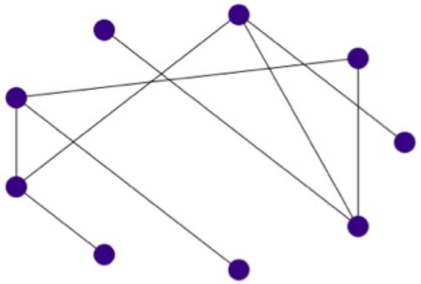
A generalization of stable coloring.

DEFINITION. (*Quasi-stable Coloring*) Call a coloring $P = \{P_1, \ldots, P_k\}$ quasi-stable if, for some $q \geq 0$:

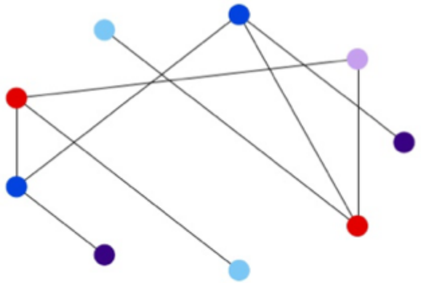
$$\forall i, j, \forall x, y \in P_i : \quad -q \leq |N(x) \cap P_j| - |N(y) \cap P_j| \leq q$$

where $N(v)$ denotes the neighbors of vertex v.

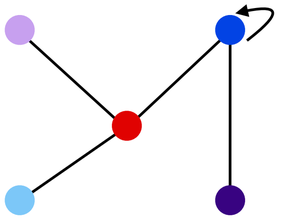
Compression



Initial Graph

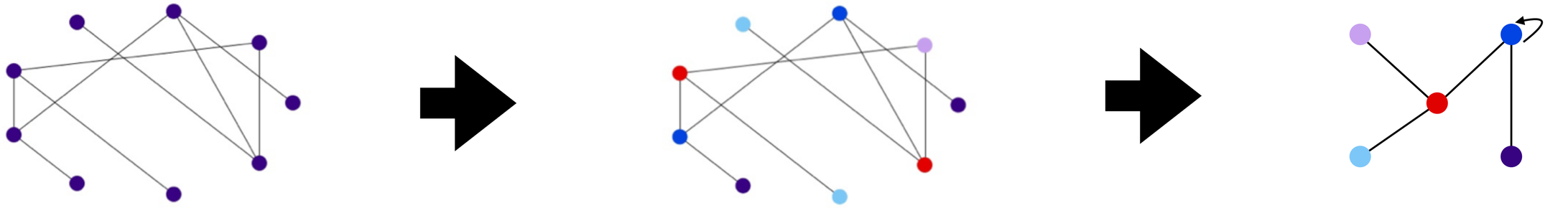


Quasi-Stable Coloring



Lifted Graph,
Quotient Graph

Compression



Initial Graph

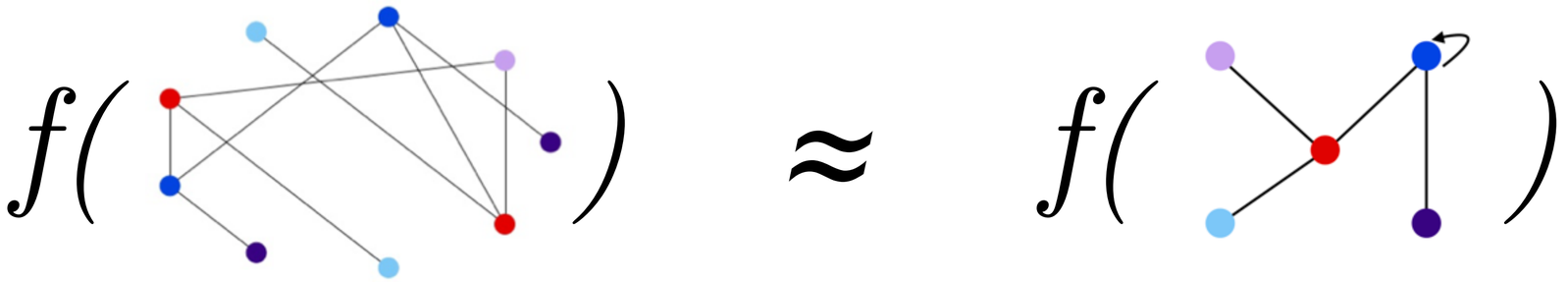
Quasi-Stable Coloring

Lifted Graph,
Quotient Graph

Adapted from
M. Grohe. word2vec, node2vec, graph2vec, x2vec: Towards a theory of vector embeddings of structured data. PODS 2020, Portland, OR, USA, June 14-19, 2020, pages 1–16. ACM, 2020.

Applications

(1) Max-flow/Min-cut (2) Linear Optimization (3) Betweenness Centrality



The Catch

Theorem: Computing a *maximal* quasi-stable coloring is NP-complete, and similarly for any ε-stable coloring.

Experiments

Datasets and Setup

Table 2: Summary of graphs used for evaluation

Name	Vertices	Edges	Real/ Sim.	Source
General evaluation				
Karate	34	75	R	[10]
OpenFlights	3 425	38 513	R	[35]
DBLP	317 080	1 049 866	R	[7]
Centrality				
Astrophysics	18 772	198 110	R	[23]
Facebook	22 470	171 002	R	[26]
Deezer	28 281	92 752	R	[38]
Enron	36 692	183 831	R	[21]
Epinions	75 879	508 837	R	[36]
Maximum-flow				
Tsukuba0	110 594	506 546	R	[32]
Tsukuba2	110 594	500 544	R	[32]
Venus0	166 224	787 946	R	[39]
Venus1	166 224	787 716	R	[39]
Sawtooth0	164 922	790 296	R	[39]
Sawtooth1	164 922	789 014	R	[39]
SimCells	903 962	6 738 294	S	[18]
Cells	3 582 102	31 537 228	R	[18]

Table 3: Summary of the linear programs used for evaluation. All instances are from real problems.

Name	Rows	Cols.	Non-zeros	Sol. time	Source
qap15	6 331	22 275	110 700	22 min	[27]
nug08-3rd	19 728	20 448	139 008	100 min	[27]
supportcase10	10 713	1 429 098	4 287 094	31 min	[27]
ex10	69 609	17 680	1 179 680	24 min	[27]

Experiments

Speed-Accuracy Tradeoff

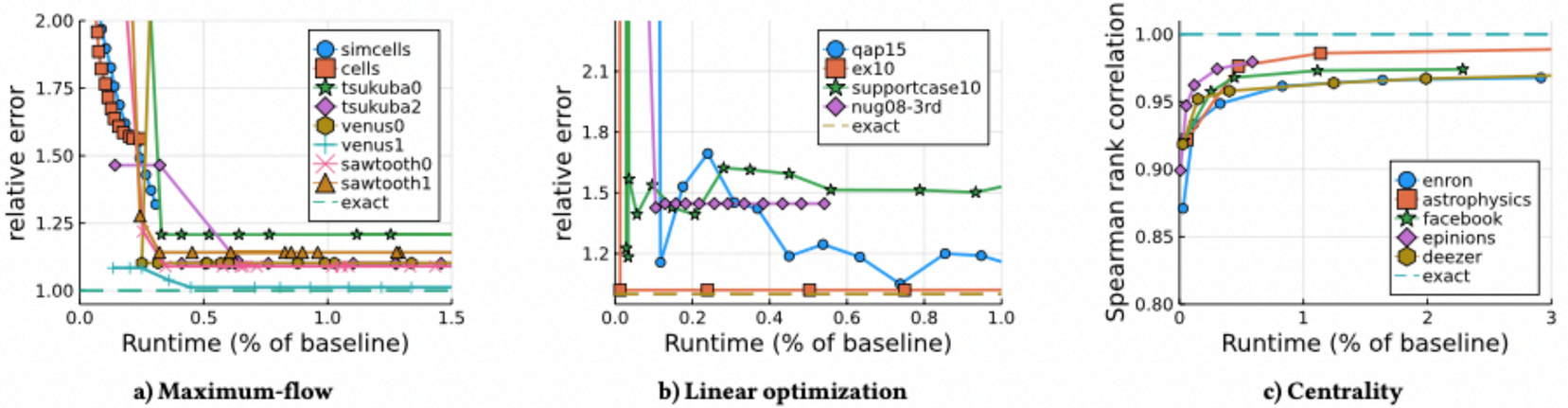


Figure 7: Speed-accuracy trade-offs for three task types and 20 datasets. Runtime reported is end-to-end, including the time taken for graph coloring, building an approximate instance of the problem and solving it.

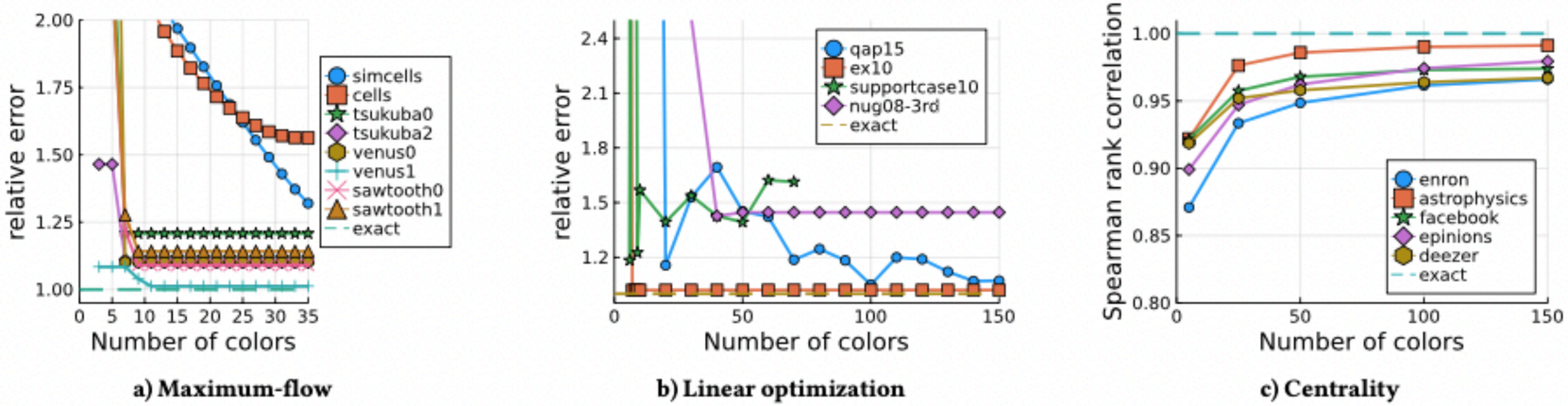


Figure 8: Accuracy as a function of the number of colors, across the same three tasks.

Experiments

Runtime and compression ratios

Table 4: Runtime and compression ratios of quasi-stable coloring *vs.* prior work (stable coloring [4, 22]) for selected datasets.

Dataset	Max q	Mean q	Colors	Compression	Time
OpenFlights	stable ($q=0$)		2 637	1.29:1	150ms
	q = 64	15.8	9	380:1	10ms
	q = 32	6.96	17	200:1	20ms
	q = 16	2.22	39	87:1	60ms
	q = 8	0.52	106	32:1	350ms
Epinions	stable ($q=0$)		53 068	1.42:1	49s
	q = 64	4.42	71	1 000:1	2.39s
	q = 32	1.17	144	526:1	8.95s
	q = 16	0.79	316	240:1	40.5s
	q = 8	0.22	869	87:1	5m19s
DBLP	stable ($q=0$)		233 466	1.35:1	14m52s
	q = 64	11.94	21	15 000:1	2.28s
	q = 32	2.22	89	3 500:1	22.6s
	q = 16	0.39	373	850:1	6m39s
	q = 8	0.06	1513	210:1	2h38m

Experiments

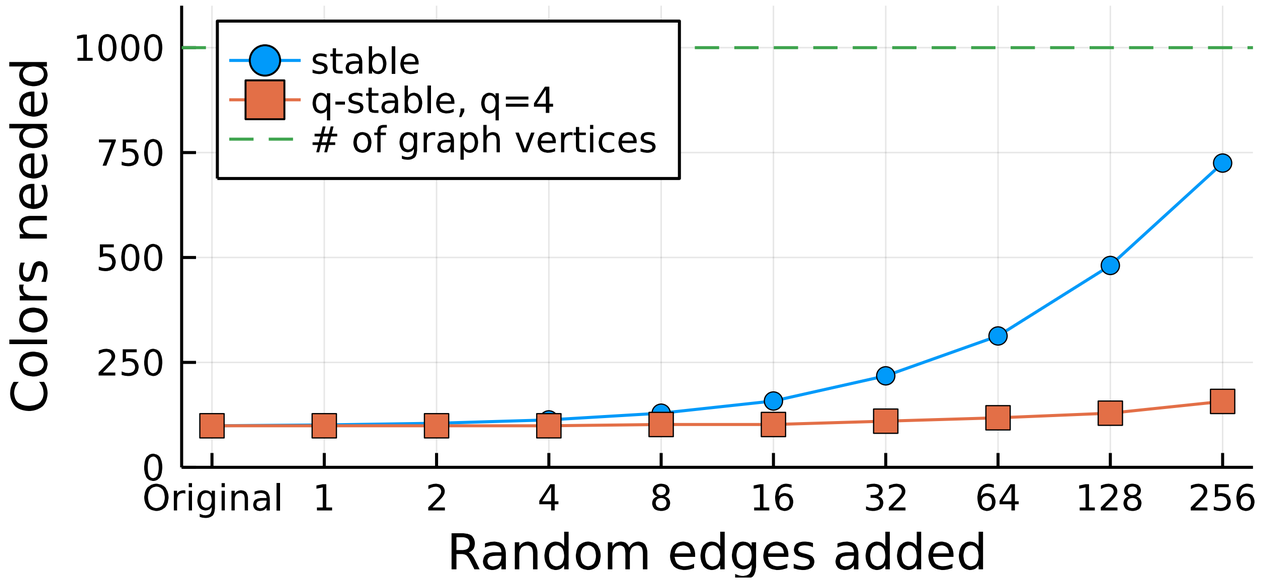
Q-Stable Coloring *vs.* Prior Approximations

Table 1: Runtime comparison of q-stable colors vs. prior approximations (Riondato-Kornaropoulos [37] and early-stopping [33]) and exact algorithms (Brandes [5] and interior-point solver [43]). Runtime to achieve a target approximation quality is measured; target is correlation (ρ) with ground truth values for centrality and relative error for linear optimization. "×" is 20-minute timeout. Units in seconds, lower is better.

	Betweenness centrality: ours, [37], and [5]						
	$\rho = 0.90$		$\rho = 0.95$		$\rho = 0.97$		Exact
	Ours	Prior	Ours	Prior	Ours	Prior	
Astroph.	**0.13**	15.2	**1.03**	41.4	**2.49**	61.1	223
Facebook	**0.07**	3.2	**0.53**	7.1	**2.23**	12.6	221
Deezer	**0.05**	3.6	**1.11**	7.2	**8.56**	14.8	295
Enron	**0.41**	2.6	**3.06**	5.6	10.8	**8.7**	380
Epinions	**0.18**	17.1	**3.15**	36.5	**7.95**	58.2	2552
	Linear optimization: ours, [33], and [43]						
	rel. err. = 3.0		rel. err. = 2.0		rel err. = 1.5		Exact
	Ours	Prior	Ours	Prior	Ours	Prior	
qap15	**3.20**	112.	**4.91**	524.	**11.4**	×	1 320
nug08.	**5.40**	1 027.	**6.65**	×	**6.65**	×	6 000
support.	**0.51**	143.	**4.98**	143.	×	×	1 860
ex10	**0.247**	795.	**14.0**	795.	**14.0**	795.	1 440

Quasi-Stable Colors

Robust against perturbations



Aside: Julia for Academic Research

The Good

- Excellent fit with academic work patterns: rapid development cycle when testing ideas

- Progressive improvement for performance-critical components

- Ecosystem tooling allows for easily distribution, replication of work

The Bad

- Decision paralysis: ambiguity in library choice confusing for newcomers

- Limitations in tooling (CPU and memory profiling) make performance issues opaque

- Language conventions, software design patterns still developing (risk of anti-patterns)

Recap

Reference implementation at
`https://github.com/mkyl/QuasiStableColors.jl`

Install the package:

```
moe@MacBook-Pro ~> julia
(@v1.8) pkg> add QuasiStableColors
```

Got potential applications? Reach out!

kayali@cs.washington.edu
@moe_kayali

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Questions?

Algorithm

Color refinement algorithm is not practical for q-coloring.

For stable coloring, all refinement orders are equivalent and arrive at the unique such color.

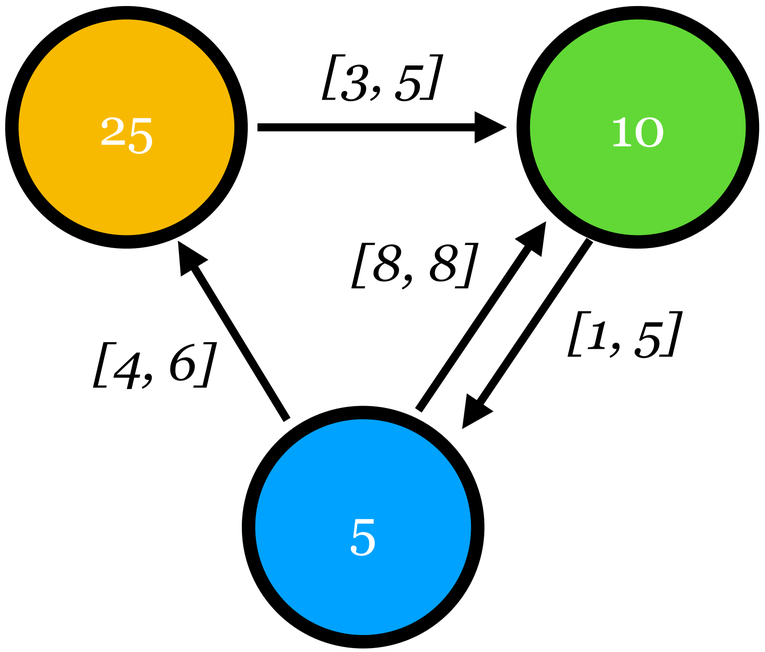
Not so for q-colors: choice of partitions to refine decides quality of coloring. Generally, many distinct colors for a fixed value of q.

Algorithm 1: Computing an approximate partition over weighted graph G, with n colors or ε maximum error

Data: $G = (V, E), W : V \times V \to \mathbb{R}^+$
Parameters: $n \in \mathbb{Z}^+, \varepsilon \in \mathbb{R}_{\geq 0}$
Result: $P \subset \mathcal{P}(V)$

$P \leftarrow \{V\}$;
while $|P| < n$ **do**
  $U_{ij}, L_{ij} \leftarrow \max_{v \in P_i} \deg(v, P_j), \min_{v \in P_i} \deg(v, P_j)$;
  $Err \leftarrow U - L$;
  if $\max Err \leq \varepsilon$ **then**
    break;
  $C_{ij} \leftarrow |E \cap (P_i \times P_j)|$; // count edges
  $Err_{\text{weighted}} \leftarrow Err \odot C$; // element-wise product
  $i, j \leftarrow \text{argmax}_{i,j} Err_{\text{weighted}}$; // witness
  threshold $\leftarrow \sqrt{U_{ij} \times L_{ij}}$;
  // Split P_i at threshold
  $P_{\text{retain}} \leftarrow \{v \in P_i \mid \deg(v, P_j) \leq \text{threshold}\}$;
  $P_{\text{eject}} \leftarrow P_i \setminus P_{\text{retain}}$;
  $P \leftarrow P \setminus \{P_i\} \cup \{P_{\text{retain}}, P_{\text{eject}}\}$;

Algorithm



Quotient Graph

[min, max] degree

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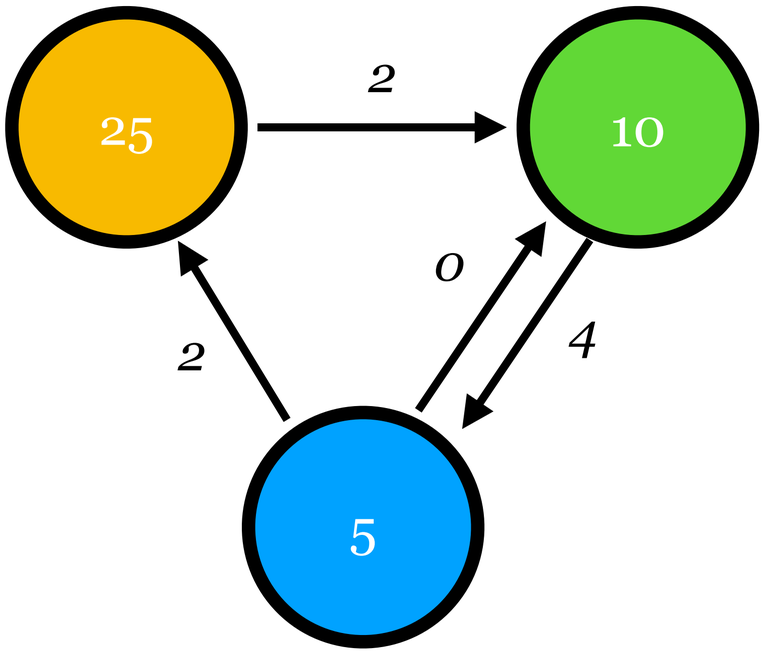
Algorithm



Quotient Graph

degree range

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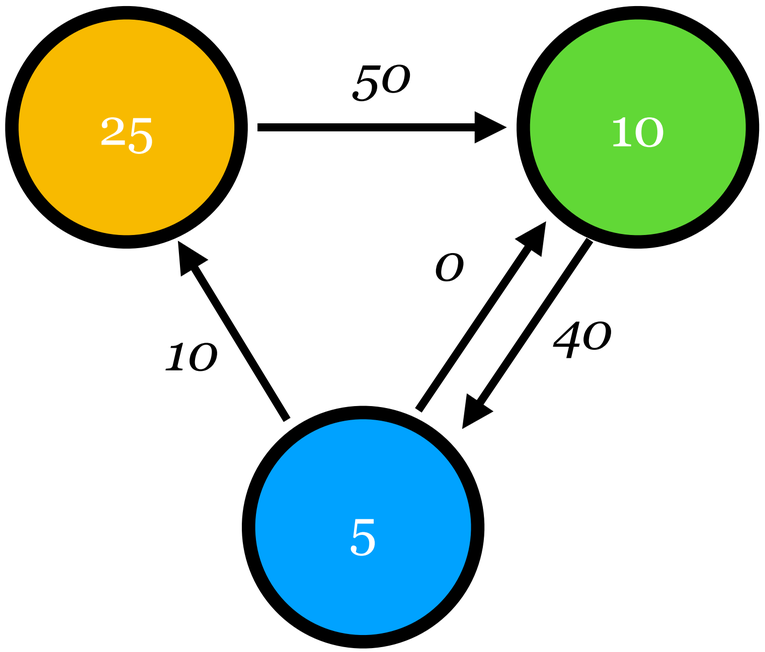
Algorithm



Quotient Graph

(weighted) degree range

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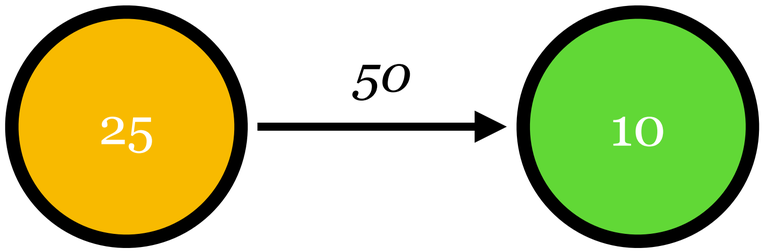
Algorithm



Quotient Graph

witness selection

Algorithm 1: Computing an approximate partition over weighted graph G, with n colors or ε maximum error

Data: $G = (V, E), W : V \times V \to \mathbb{R}^+$
Parameters: $n \in \mathbb{Z}^+, \varepsilon \in \mathbb{R}_{\geq 0}$
Result: $P \subset \mathcal{P}(V)$

$P \leftarrow \{V\}$;
while $|P| < n$ **do**
  $U_{ij}, L_{ij} \leftarrow \max_{v \in P_i} \deg(v, P_j), \min_{v \in P_i} \deg(v, P_j)$;
  $Err \leftarrow U - L$;
  if $\max Err \leq \varepsilon$ **then**
    break;
  $C_{ij} \leftarrow |E \cap (P_i \times P_j)|$; // count edges
  $Err_{\text{weighted}} \leftarrow Err \odot C$; // element-wise product
  $i, j \leftarrow \text{argmax}_{i,j} Err_{\text{weighted}}$; // witness
  threshold $\leftarrow \sqrt{U_{ij} \times L_{ij}}$;
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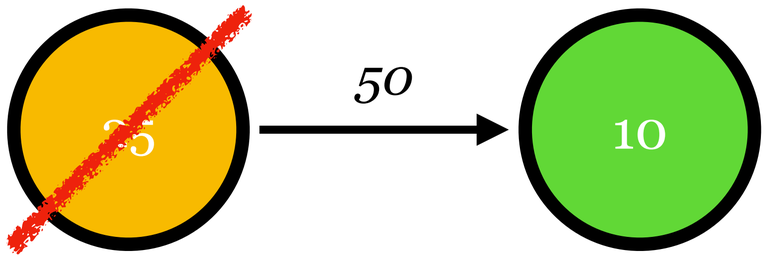

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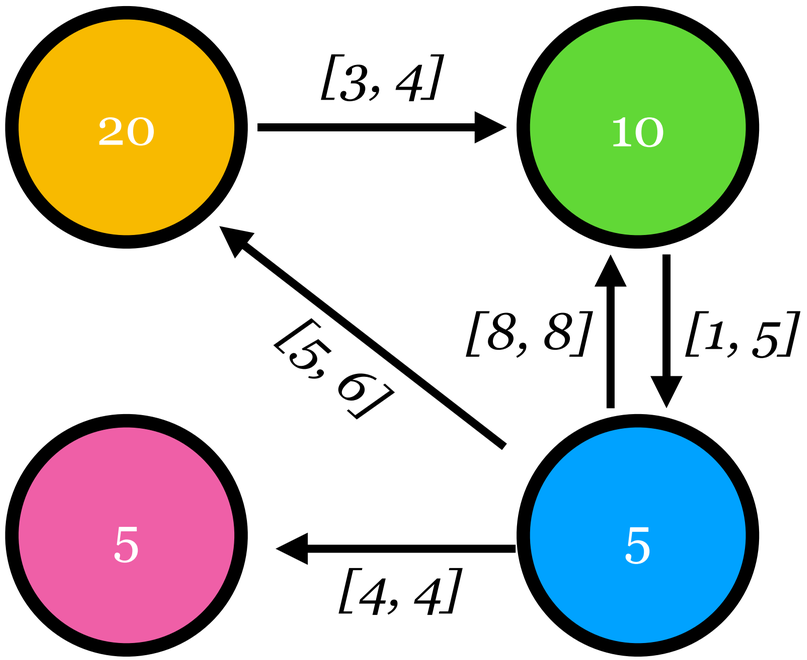
Algorithm



Quotient Graph

iteration complete

Algorithm 1: Computing an approximate partition over weighted graph G, with n colors or ε maximum error

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Color Refinement

aka *1-dimensional Weisfeiler-Leman*

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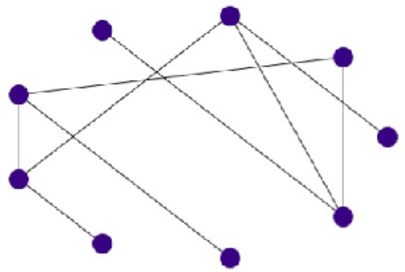
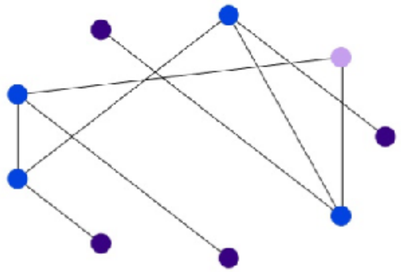
***Note**: Distinct from proper vertex coloring, chromatic number, etc.*

Color Refinement

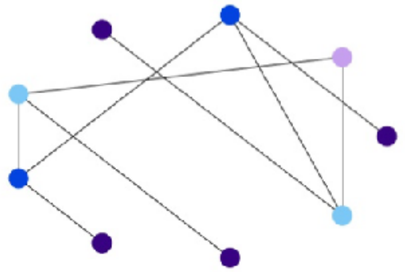
aka *1-dimensional Weisfeiler-Leman*



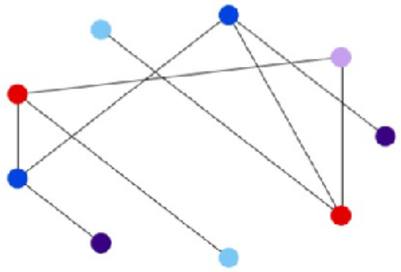
initial graph



colouring after round 1



colouring after round 2



stable colouring after round 3

***Note**: Distinct from proper vertex coloring, chromatic number, etc.*

M. Grohe. word2vec, node2vec, graph2vec, x2vec: Towards a theory of vector embeddings of structured data. PODS 2020, Portland, OR, USA, June 14-19, 2020, pages 1–16. ACM, 2020.

Color Refinement

DEFINITION. (*Stable Coloring*) Call a coloring $P = \{P_1, \ldots, P_k\}$ stable if

$$\forall i, j, \forall x, y \in P_i : \quad |N(x) \cap P_j| = |N(y) \cap P_j|$$

where $N(v)$ denotes the neighbors of vertex v.