Graphs in Machine Learning

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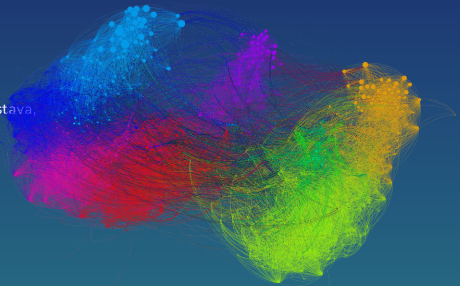
TA: Pierre Perrault

Partially based on material by: Daniele Calandriello, Nikhil Srivastava, Yiannis Koutis, Joshua Batson, Daniel Spielman



Last Lecture

- Examples of applications of online SSL
- Analysis of online SSL
- SSL Learnability
- When does graph-based SSL provably help?
- Scaling harmonic functions to millions of samples

This Lecture

- Large-scale graph construction and processing (in class)
- Scalable algorithms:
  - Graph sparsification (presented in class)
  - Online face recognizer (to code in Matlab)
  - Iterative label propagation (to code in Matlab)

This Lecture/Lab Session

- AR: record a video with faces

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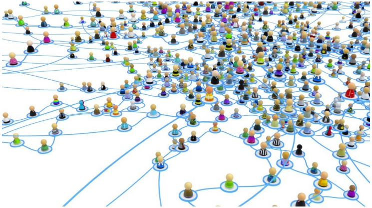
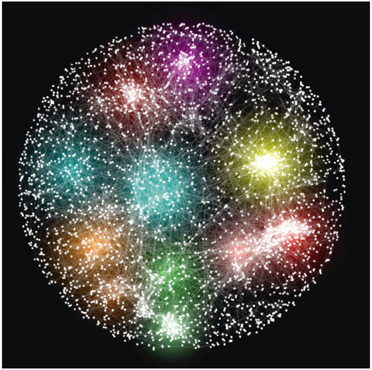
- *Deadline:* 11. 12. 2017

Large scale Machine Learning on Graphs

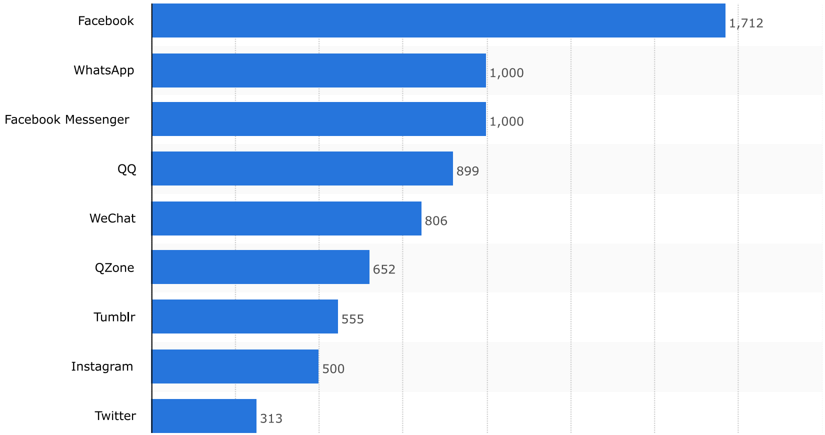


http://blog.carsten-eickhoff.com



Botstein et al.

Are we large yet?



"One **trillion** edges: graph processing at Facebook-scale."
Ching et al., VLDB 2015

Computational bottlenecks

In theory:

Space

$[\mathcal{O}(m), \mathcal{O}(n^2)]$ to store

Time

$\mathcal{O}(n^2)$ to construct

$\mathcal{O}(n^3)$ to run algorithms

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- Pagerank on Facebook Graph:

  3 minutes per iteration, hundreds of iterations, tens of hours on 200 machines, run once per day

Two phases

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2 Run your algorithm on the graph

Large scale graph construction

Main bottleneck: **time**

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Can we find close neighbours without checking all distances?

Distance Approximation

Split your data in small subset of close points

Can find efficiently some (not all) of the neighbours.

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More general problem: learning good codeword representation

Storing graph in memory

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As a Fermi (back-of-the-envelope) problem

- Storing a graph with m edges require to store m tuples $(i, j, w_{i,j})$ of 64 bit (8 bytes) doubles or int.

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- For standard cloud providers, the largest compute-optimized instances has 36 cores, but only 60 GB of memory.
- We can store $60 * 1024^3/(3 * 8) \sim 2.6 \times 10^9$ (2.6 billion) edges in a single machine memory.

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    What if it needs nonlocal data? Iterative algorithms?

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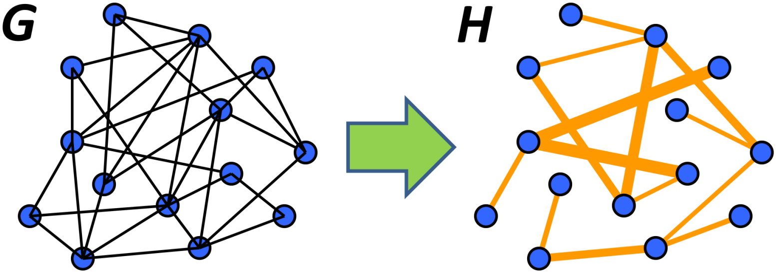
    More on this later

Graph Sparsification

Goal: Get graph G and find sparse H



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in a tree — sure, in a dense graph perhaps not

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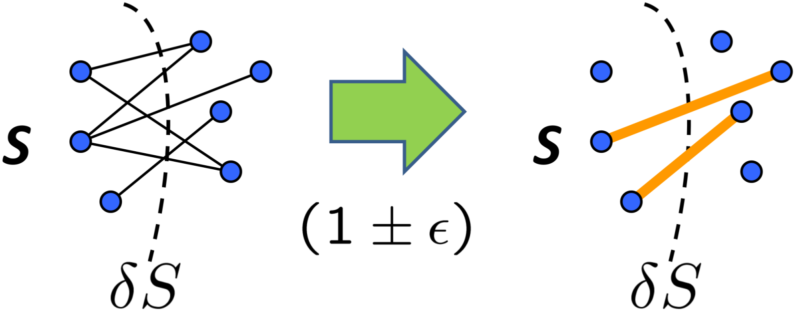

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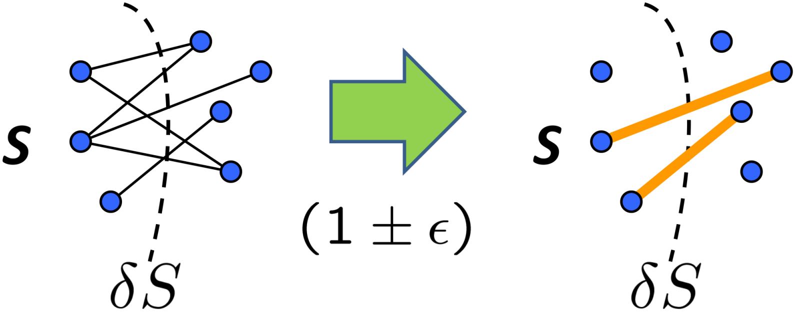

H approximates G well iff $\forall S \subset V$, sum of edges on δS remains

δS = edges leaving S

https://math.berkeley.edu/~nikhil/

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Define G and H are $(1 \pm \varepsilon)$-**cut similar** when $\forall S$

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Is this always possible? Benczúr and Karger (1996): Yes!

$\forall \varepsilon \; \exists \; (1+\varepsilon)$-cut similar $\widetilde{G}$ with $\mathcal{O}(n \log n/\varepsilon^2)$ edges s.t. $E_H \subseteq E$ and computable in $\mathcal{O}(m \log^3 n + m \log n/\varepsilon^2)$ time n nodes, m edges

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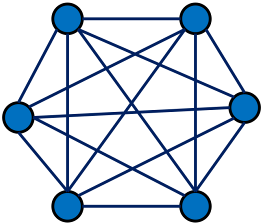
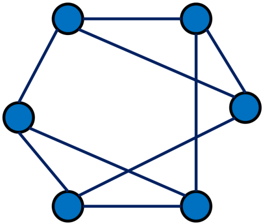
$G = K_n$



$H = d$-**regular** (random)



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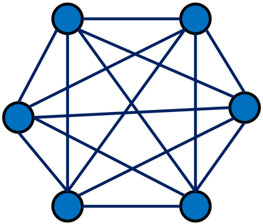

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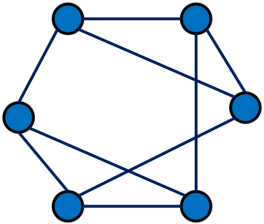

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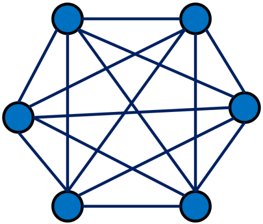

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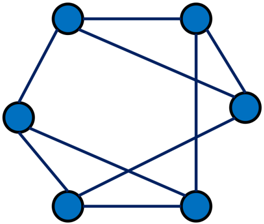

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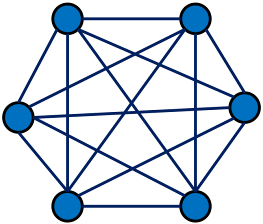

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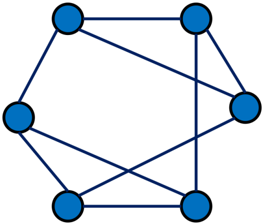

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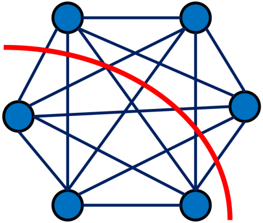

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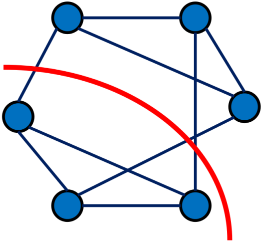

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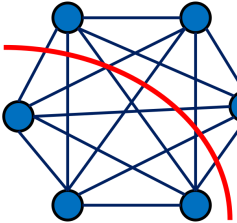

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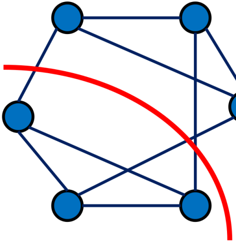

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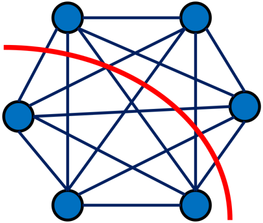

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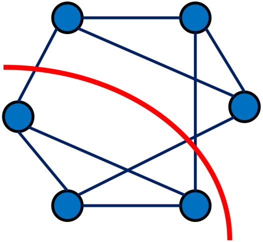

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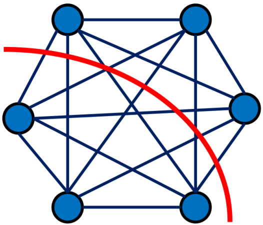

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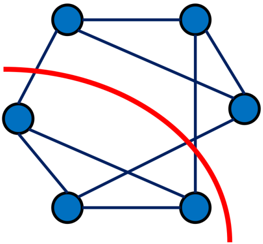

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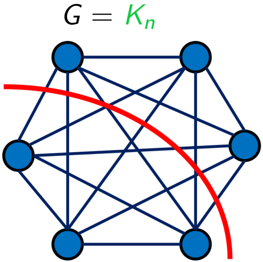

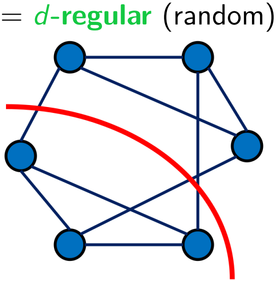

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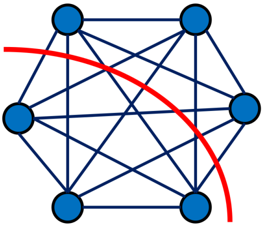

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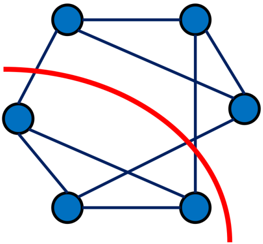

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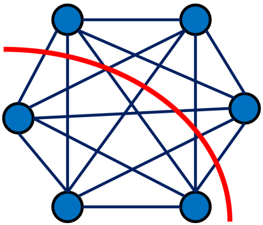

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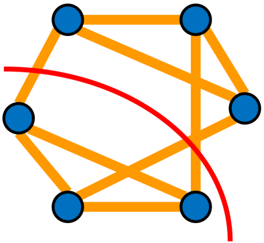

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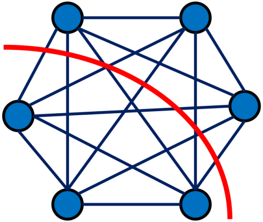

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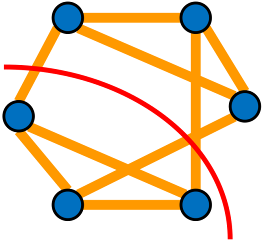

What are the cut weights for any S?

Graph Sparsification: What is good sparse?

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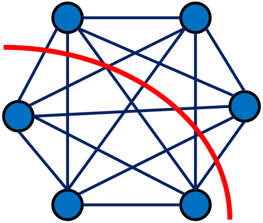

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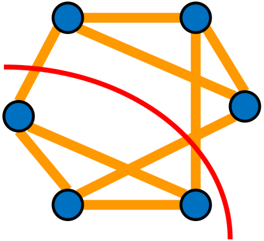

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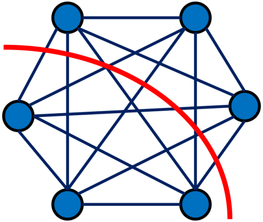

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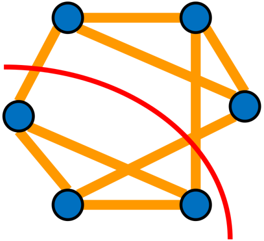

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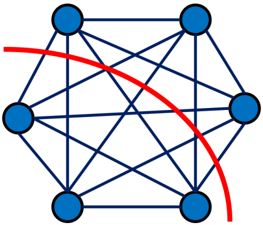

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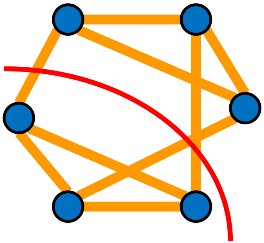

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Benczúr & Karger: Can find such H quickly for any G!

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As a consequence, $\arg\min_{\mathbf{x}} \|\mathbf{L}_H\mathbf{x} - \mathbf{b}\| \approx \arg\min_{\mathbf{x}} \|\mathbf{L}_G\mathbf{x} - \mathbf{b}\|$

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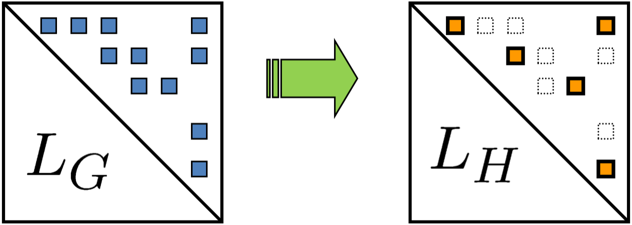

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Then $\sum_{e\in E} s_e\mathbf{v}_e\mathbf{v}_e^\mathsf{T} \approx \mathbf{I} \iff \sum_{e\in E} s_e\mathbf{a}_e\mathbf{a}_e^\mathsf{T} \approx \mathbf{A}$

multiplying by $\mathbf{A}^{1/2}$ on both sides

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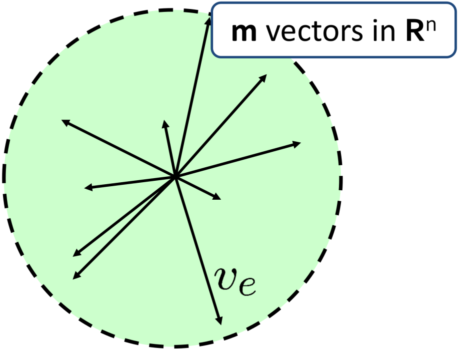

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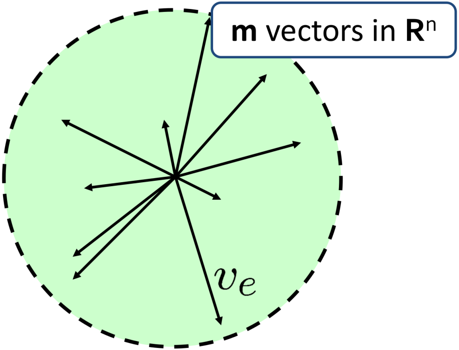

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moment ellipse is a sphere

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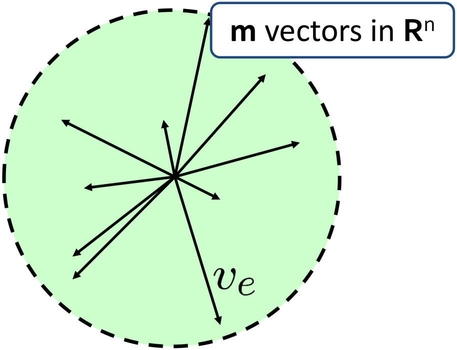
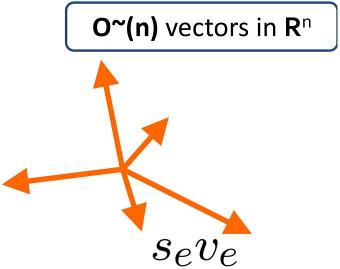
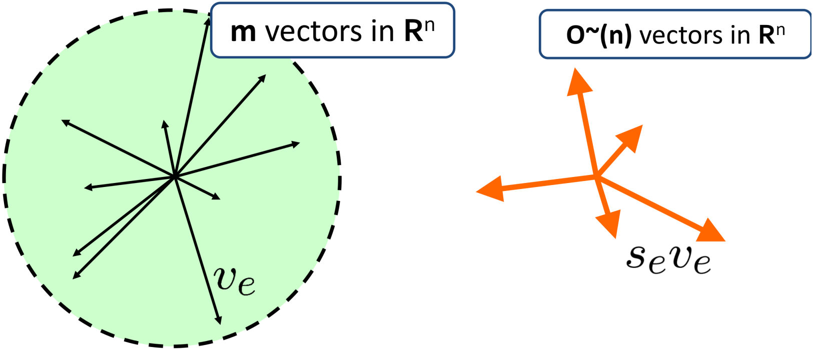




Spectral Graph Sparsification: Intuition

What are we doing by choosing H?



We take a subset of these $\mathbf{e}_e$s and scale them!

https://math.berkeley.edu/~nikhil/

Spectral Graph Sparsification: Intuition

What kind of scaling go we want?

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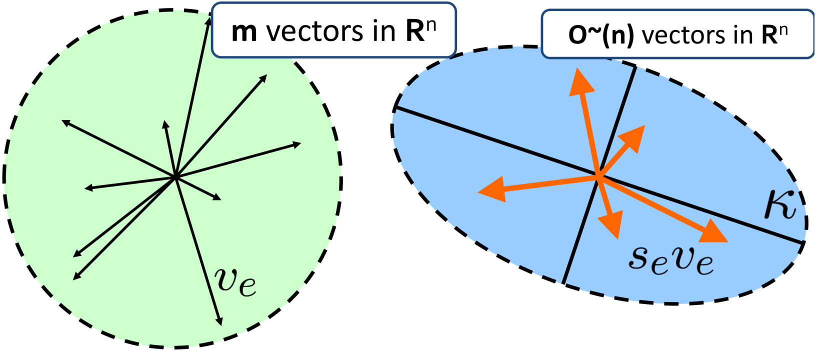

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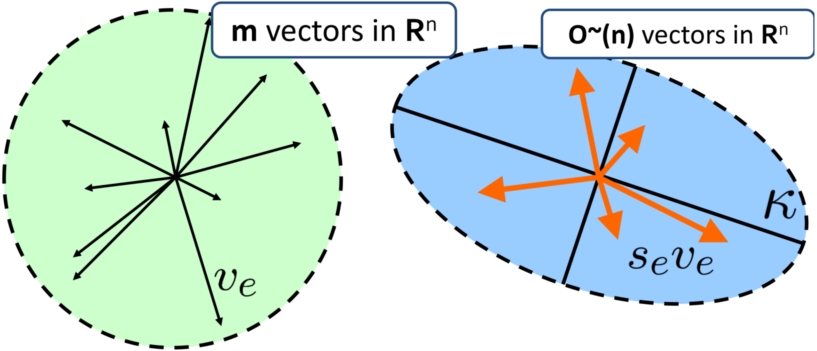

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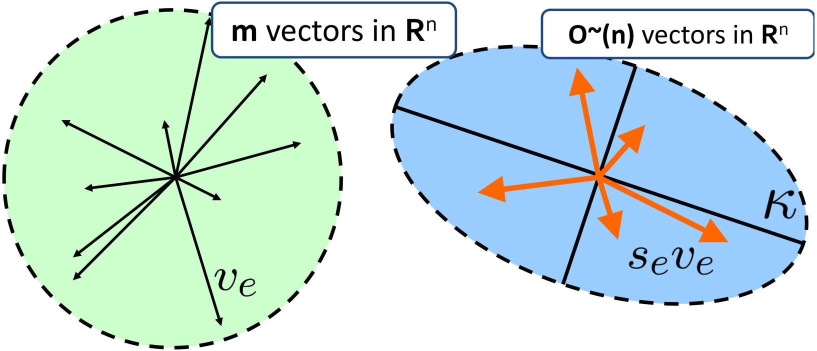

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the blue eigenvalues are between 1 and κ

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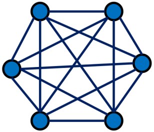
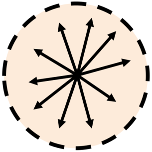
K_n graph



$\sum_{e \in E} \mathbf{b}_e \mathbf{b}_e^\mathsf{T} = \mathbf{L}_G$



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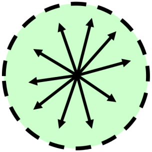

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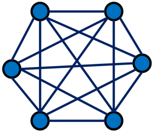

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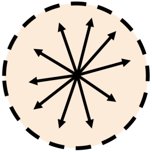

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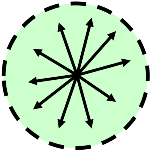

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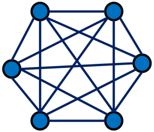

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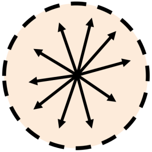

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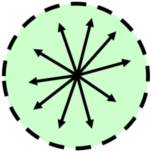

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rescaling $\mathbf{v}_e = \mathbf{L}^{-1/2}\mathbf{b}_e$ does not change the shape

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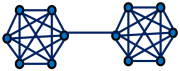

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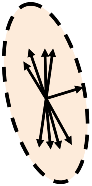

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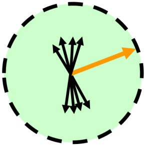

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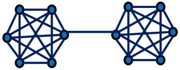

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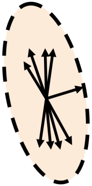

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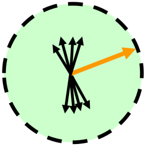

The vector corresponding to the link gets stretched!

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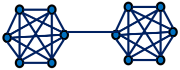

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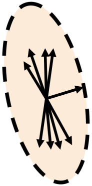

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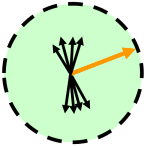

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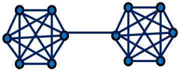

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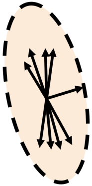

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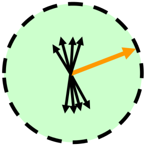

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rescaling reveals the vectors that are critical

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Edges with higher R_{eff} are more **electrically significant**!

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    still unfeasible when m is large

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Computing $\widetilde{R}_{\text{eff}}$ using the sparsifier is fast ($m = \boldsymbol{O}(n\log(n))$), and not too many iterations are necessary.

What can I use sparsifiers for?

- Graph linear systems: minimum cut, maximum flow, Laplacian regression, SSL

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- More in general, solving Strongly Diagonally Dominant (SDD) linear systems

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But what if my problems have no use for spectral guarantees?

Or if my boss does not trust approximation methods

Distributed graph processing

Large graphs do not fit in memory

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Needs to be scalable

↳ minimimize pass over data / communication costs

Needs to be consistent

↳ updates should propagate properly

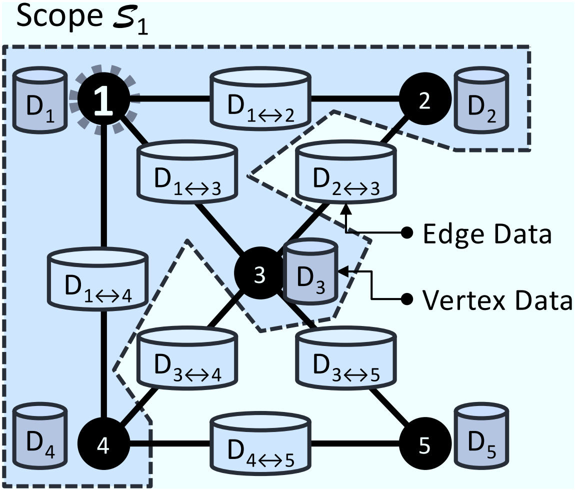
Distributed graph processing

Different choices have different impacts: for example splitting the graph according to nodes or according to edges.

Many computation models (academic and commercial) each with its pros and cons

- MapReduce
- MPI
- Pregel
- **Graphlab**

The GraphLab abstraction



The GraphLab abstraction

```
In [1]: import sframe

In [2]: edges = sframe.SFrame.read_csv('/media/sf_share/td3_example_edges.csv')

In [3]: vertices = sframe.SFrame.read_csv('/media/sf_share/td3_example_vertices.csv')

In [4]: G = sframe.SGraph(edges= edges, vertices=vertices, src_field='src', dst_field='dst')

In [5]: G

Out[5]: SGraph({'num_edges': 26, 'num_vertices': 9})
        Vertex Fields:['__id', 'f']
        Edge Fields:['__src_id', '__dst_id', 'weight']
```

The GraphLab abstraction

Under the hood: tabular representation

```
Columns:
    __id int
    f float

Rows: 9

Data:
+------+------+
| __id |  f   |
+------+------+
|  5   | 0.51 |
|  7   | 0.82 |
|  10  | 0.08 |
|  2   | 0.82 |
|  6   | 0.85 |
|  9   | 0.83 |
|  3   | 0.18 |
|  1   | 0.35 |
|  4   | 0.36 |
+------+------+
[9 rows x 2 columns]
```

```
Columns:
    __src_id int
    __dst_id int
    weight float

Rows: 26

Data:
+----------+----------+----------+
| __src_id | __dst_id |  weight  |
+----------+----------+----------+
|    7     |    5     | 0.13185  |
|    5     |    7     | 0.13185  |
|    7     |    7     | 0.026779 |
|    10    |    7     | 0.57121  |
|    7     |    10    | 0.57121  |
|    10    |    2     | 0.94047  |
|    7     |    6     | 0.64528  |
|    5     |    3     | 0.93374  |
|    10    |    3     | 0.31713  |
|    5     |    1     | 0.57796  |
+----------+----------+----------+
[26 rows x 3 columns]
Note: Only the head of the SFrame is printed.
```

The GraphLab abstraction

```
In [1]: import sframe

In [2]: G = sframe.SGraph()

In [3]: G

Out[3]: SGraph({'num_edges': 0, 'num_vertices': 0})
        Vertex Fields:['__id']
        Edge Fields:['__src_id', '__dst_id']
```

The GraphLab abstraction

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In [1]: import sframe

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In [4]: G.add_edges(sframe.Edge(1,2))

Out[4]: SGraph({'num_edges': 1, 'num_vertices': 2})
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        Edge Fields:['__src_id', '__dst_id']
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- Functional programming approach

The GraphLab abstraction

```
triple_apply(triple_apply_fn, mutated_fields, input_fields=None)
```

processes all edges asyncronously and in parallel

```
>>> PARALLEL FOR (source, edge, target) AS triple in G:
...     LOCK (triple.source, triple.target)
...     (source, edge, target) = triple_apply_fn(triple)
...     UNLOCK (triple.source, triple.target)
... END PARALLEL FOR
```

- No guarantees on order of execution

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- Updating (src,edge,dst) violates immutability
- triple_apply_fn receives a copy of (src,edge,dst)
  ↳ returns an updated (src',edge',dst')
  use return values to build a new graph

The GraphLab abstraction

triple_apply_fn is a pure function

Function in the mathematical sense, same input gives same output.

```
def triple_apply_fn(src, edge, dst):
    #can only access data stored in src, edge, and dst,
    #three dictionaries containing a copy of the
    #fields indicated in mutated_fields
    f = dst['f']

    #inputs are copies, this does not change original edge
    edge['weight'] = g(f)

    return ({'f': dst['f']}, edge, dst)
```

The GraphLab abstraction

An example, computing degree of nodes

```
def degree_count_fn (src, edge, dst):
    src['degree'] += 1
    dst['degree'] += 1
    return (src, edge, dst)

G_count = G.triple_apply(degree_count_fn, 'degree')
```

The GraphLab abstraction

Slightly more complicated example, suboptimal pagerank

```
#assume each node in G has a field 'degree' and 'pagerank'
#initialize 'pagerank' = 1/n for all nodes

def weight_count_fn (src, edge, dst):
    dst['degree'] += edge['weight']
    return (src, edge, dst)

def pagerank_step_fn (src, edge, dst):
    dst['pagerank'] += (edge['weight']*src['pagerank']
                                     /dst['degree'])
    return (src, edge, dst)

G_pagerank = G.triple_apply(weight_count_fn, 'degree')

while not converged(G_pagerank):
    G_pagerank = G_pagerank.triple_apply(
                        pagerank_step_fn, 'pagerank')
```

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```

How many iterations to convergence?

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