Sparse
Pathfinder
V. Batagelj,
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Semirings

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## Pathfinder

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The Pathfinder algorithm was proposed in eighties (Schvaneveldt 1981, Schvaneveldt etal. 1989; Schvaneveldt, 1990) [14, 13, 15] for simplification of weighted networks - it removes from the network all lines that do not satisfy the triangle inequality - if for a line a shorter path exists connecting its endpoints then the line is removed. The basic idea of the Pathfinder algorithm is simple. It produces a network $\operatorname{PFnet}(\mathbf{W}, r, q)=\left(\mathcal{V}, \mathcal{L}_{P F}\right)$

```
compute \(\mathbf{W}^{(q)}\);
\(\mathcal{L}_{\text {PF }}:=\emptyset\);
for \(e(u, v) \in \mathcal{L}\) do begin
    if \(\mathbf{W}^{(q)}[u, v]=\mathbf{W}[u, v]\) then \(\mathcal{L}_{P F}:=\mathcal{L}_{P F} \cup\{e\}\)
end;
```

where $\mathbf{W}$ is a network dissimilarity matrix and $\mathbf{W}^{(q)}$ the matrix of values of all walks of length at most $q$ computed over the semiring $\left(\mathbb{R}_{0}^{+}, \oplus, \square, \infty, 0\right)$ with $a \boxtimes b=\sqrt[r]{a^{r}+b^{r}}$ and $a \oplus b=\min (a, b)$.

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## Pathfinder - theoretical results 1

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Theoretical results [7]: For a given dissimilarity matrix $\mathbf{W}$ the PFnet( $\mathbf{W}, r, q$ )

- Is unique
- Preserves geodetic distances
- Links nearest neighbors
- Contains the same information as the minimum method of hierarchical clustering
- PFnet $(\mathbf{W}, r=\infty, q=n-1)$ is the union of all MINTREES


## Pathfinder - theoretical results 2

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- Graph $\operatorname{PFnet}\left(\mathbf{W}, r_{2}, q\right)$ is a spanning subgraph of graph $\operatorname{PFnet}\left(\mathbf{W}, r_{1}, q\right)$ iff $r_{1}<r_{2}$
- Graph $\operatorname{PFnet}\left(\mathbf{W}, r, q_{2}\right)$ is a spanning subgraph of graph $\operatorname{PFnet}\left(\mathbf{W}, r, q_{1}\right)$ iff $q_{1}<q_{2}$
- Similarity transformations preserve structure: the graph $\operatorname{PFnet}(\mathbf{W}, r, q)$ is equal to the graph $\operatorname{PFnet}(\alpha \mathbf{W}, r, q)$ for $\alpha>0$.
- Monotonic transformations preserve structure for all $r=\infty$ : the graph $\operatorname{PFnet}(\mathbf{W}, r=\infty, q)$ is equal to the graph PFnet $(f(\mathbf{W}), r=\infty, q)$ where $f: \mathbb{R} \rightarrow \mathbb{R}$ is strictly increasing mapping and $f\left(\mathbf{W}=\left[f\left(w_{i j}\right)\right]\right.$.


## Pathfinder - the original algorithm

In the original algorithm the matrix $\mathbf{W}^{(q)}$ is computed on the basis of its definition

$$
\mathbf{W}^{(q)}=\sum_{i=0}^{q} \mathbf{W}^{i}
$$

by computing all its powers $\mathbf{W}^{i}, i=1, \ldots, q$. The complexity of the algorithm is $O\left(q n^{3}\right)$, therefore $O\left(n^{4}\right)$, for $q \geq n-1$. Therefore it can be applied only to relatively small (up to some hundreds vertices) networks.
Interest for Pathfinder transformation was renewed around the year 2000 by Chen [5].

## Semirings - Computing the closure over a semiring

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Because in our case the set of vertices $\mathcal{V}$ is finite, so is the set of all paths $\mathcal{E}_{u v}$. Therefore we can compute the value of all walks $w\left(\mathcal{S}_{u v}^{\star}\right)=w\left(\mathcal{E}_{u v}\right)$. One possibility is to use for large enough $k$ the equality:

$$
\mathbf{W}^{\star}=\mathbf{W}^{(k)}=(\mathbf{1}+\mathbf{W})^{k}
$$

To speed-up the computation we can consider the sequence $(\mathbf{1}+\mathbf{W})^{2^{i}}, i=1, . ., s$.
It turned out that this is not the fastest way to compute the W*.

## Semirings - Computing the closure over a complete semiring

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Kleene, Warshall, Floyd and Roy contributed to the development of the procedure which final form was given by Fletcher [6].

```
\(\mathbf{C}_{0}:=\mathbf{W}\);
for \(k:=1\) to \(n\) do begin
    for \(i:=1\) to \(n\) do for \(j:=1\) to \(n\) do
        \(c_{k}[i, j]:=c_{k-1}[i, j]+c_{k-1}[i, k] \cdot\left(c_{k-1}[k, k]\right)^{\star} \cdot c_{k-1}[k, j] ;\)
        \(c_{k}[k, k]:=1+c_{k}[k, k] ;\)
end;
\(\mathbf{W}^{\star}:=\mathbf{C}_{n}\);
```

If we delete the statement $c_{k}[k, k]:=1+c_{k}[k, k]$ we obtain the algorithm for computing the strict closure $\overline{\mathbf{W}}=\mathbf{W} \mathbf{W}^{\star}$.

## Semirings - Dissimilarities

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Joly and Le Calvé theorem [8]:
For any even dissimilarity measure $d$ there is a unique number $p \geq 0$, called its metric index, such that: $d^{r}$ is metric for all $r \leq p$, and $d^{r}$ is not metric for all $r>p$.

In the opposite direction we can say: Let $d$ be a dissimilarity and for $x, y$ and $z$ we have $d(x, z)+d(z, y) \geq d(x, y)$ and $d(x, y)>\max (d(x, z), d(z, y))$ then there exists a unique number $p \geq 0$ such that for all $r>p$

$$
d^{r}(x, z)+d^{r}(z, y)<d^{r}(x, y)
$$

or equivalently

$$
d(x, z) \boxtimes d(z, y)<d(x, y)
$$

## Semirings - Minkowski operation

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Minkowski operation $a \boxtimes b=\sqrt[r]{a^{r}+b^{r}}$ :
$r=1 \Rightarrow a \square b=a+b$,
$r=2 \Rightarrow a \square b=\sqrt{a^{2}+b^{2}}$,
$r=\infty \Rightarrow a \boxminus b=\max (a, b)$.
And let $a \oplus b=\min (a, b)$.
The structure $\left(\mathbb{R}_{0}^{+}, \oplus, \square, \infty, 0\right)$ is a complete semiring with $a^{\star}=0$. It is called also Pathfinder semiring.

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Since the Pathfinder semiring is idempotent it holds

$$
\mathbf{W}^{(q)}=(\mathbf{1} \oplus \mathbf{W})^{q}
$$

This power can be computed faster using binary algorithm (for example, to compute $a^{57}=a^{32} \cdot a^{16} \cdot a^{8} \cdot a^{1}$ we need only 8 multiplications instead of 56). This improvement was proposed by Guerrero-Bote etal. (2006) [7] and reduces complexity to $O\left(n^{3} \log q\right)$. When $q \geq n-1, \mathbf{W}^{(q)}=\mathbf{W}^{\star}$ and it can be determined by the Fletcher's algorithm over Pathfinder semiring. This improvement was proposed by Quirin etal. (2008) [9] and reduces complexity to $O\left(n^{3}\right)$. Additional improvement can be made for undirected networks in the case $q \geq n-1$ and $r=\infty$. In this case the network $P F$ is the union of all minimal spanning trees of $N$. It can be obtained using an adapted version of Kruskal's minimal spanning tree algorithm as described in Quirin etal. (2008) [10]. The complexity of this algorithm is $O(m \log n)$ where $m$ is the number of edges.

## Sparse Pathfinder

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For sparse networks in general case there is still some space for improvements. We rewrite the basic Pathfinder algorithm in the form

$$
\begin{aligned}
& \mathcal{L}_{P F}:=\emptyset ; \\
& \text { for } v \in \mathcal{V} \text { do begin } \\
& \quad \text { compute the list } S=\left(\left(u, d_{u}\right): u \in N(v)\right) \text {, where } d_{u}=\mathbf{W}^{(q)}[v, u] ; \\
& \quad \text { for }\left(u, d_{u}\right) \in S \text { do } \\
& \quad \text { if } d_{u}=\mathbf{W}[v, u] \text { then } \mathcal{L}_{P F}:=\mathcal{L}_{P F} \cup\{(v, u)\} \\
& \text { end; }
\end{aligned}
$$

$N(v)$ denotes the set of successors of vertex $v$.
For determining the values $d_{u}=\mathbf{W}^{(q)}[v, u]$ for $q=n-1$ we can use an adapted Dijkstra's algorithm that determines the list $S$ in a single run. The job is done when all values of vertices from $N(v)$ are determined. Only a (small) portion of network should be inspected for each vertex $v$. To efficiently implement this algorithm a special data structure Indexed Priority Queue is needed.

## Sparse Pathfinder - BFS algorithm

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In the case $q<n-1$ a variant of BFS (Breath First Search) algorithm is used to determine the list $S$. The FIFO queue $Q$ is composed of triples $(t, d, I): t$ is a vertex, $d$ is a dist-length and $/$ is a line-length.
To make the implementation fast all the structures: the queue $Q$ and lists Plist and Vlist are represented with arrays.

## Sparse Pathfinder - BFS algorithm compute the list $S$

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```
\(S:=\emptyset ; T:=N(v)\); emptyQ; dMax \(:=\max \left\{w_{v u}: u \in T\right\}\);
putLastQ( \(v, 0,0)\); \(\operatorname{dist}[v]:=0\); level \(:=0\);
while size \(Q()>0\) do begin
    \(\left(u, d_{u}, l\right):=\) firstFromQ(); \(l:=I+1\);
    if \(I>\) level then begin
        level \(:=1\);
        for \(v \in\) Plist do \(P[v]:=0\);
        \(n\) Plist \(:=0\);
    end
    for \(t \in N(u)\) do begin
        \(d N e w:=d_{u}\) 占 \(w(u, t)\);
        if \(d\) New \(\leq d M a x\) then begin
            if \(V[t]\) then begin
            if \(d N e w<\operatorname{dist}[t]\) then begin
                    \(\operatorname{dist}[t]:=d N e w ;\)
                        if \(l<q\) then begin
                        if \(P[t]>0\) then update \(\mathrm{Q}(t, d N e w)\)
                        else putLastQ \((t, d N e w, I)\);
                        end
            end
            end else begin
                \(\operatorname{dist}[t]:=d N e w ;\) if \(I<q\) then putLastQ \((t, d N e w, l)\);
            end
        end
    end
end;
for \(v \in\) Plist do \(P[v]:=0\); for \(v \in\) Vlist do \(V[v]:=\) false;
\(n\) Plist \(:=0 ; n\) Vlist \(:=0\);
for \(t \in T\) do \(S:=S \cup\{(t, \operatorname{dist}[t])\}\);
```


## Tests $-q=2$ and $q=3$

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$q=2$

n
$q=3$

n
eatRSd5.net: $n=23219, \overline{\operatorname{deg}}=28.048$ Edinbourgh Associtive Thesaurus, $d_{5}$ Cluster1.net: $n=37689, \overline{\mathrm{deg}}=15.875$ Citations in Clustering $d(u, v)=1-n(u, v) / \max ($ inS $(u)$, inS $(v)$, outS $(u)$, outS $(v))$
Cluster2.net: $n=37690, \overline{\mathrm{deg}}=16.016$ Citations in Clustering $d(u, v)=1 / n(u, v)$

## Tests $-q=4$ and $q=5$

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## Tests $-q=10$ and $q=\max$

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## Conclusions

- the tests with sparse random networks of Erdos-Renyi type show that the new algorithms extend the range of sparse networks for which we can determine the Pathfinder network in reasonable time to at least $n=50000$.
- it seems that on real-life networks (green marks) the algorithm works much faster than on random networks with the same average degree.


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