Sidebar: Functional PageRank (PR)

Computing PageRank (PR)

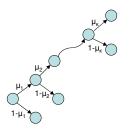
- PageRank as a random surfer process: Start surfing from a random node and keep following links with probability μ restarting with probability 1 μ; the node for restarting will be selected based on a personalization vector v. The ranking value x_i of a node i is the probability of visiting this node during surfing.
- PR can also be cast in power series representation as $x = (1 \mu) \sum_{j=0}^{k} \mu^{j} S^{j} v$; S encodes column-stochastic adjacencies.

Functional rankings

- A general method to assign ranking values to graph nodes as $x = \sum_{j=0}^{k} \zeta_j S^j v$. PR is a functional ranking, $\zeta_j = (1 \mu)\mu^j$.
- Terms attenuated by outdegrees in S and damping coefficients ζ_j .

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Functional Rankings Through Multidamping [Kollias, Gallopoulos, AG, TKDE'13]



Computing μ_j in multidamping

Simulate a functional ranking by random surfers following emanating links with probability μ_j at step j given by : $\mu_j = 1 - \frac{1}{1 + \frac{\rho_{k-j+1}}{1 - \mu_{j-1}}}, j = 1, ..., k,$ where $\mu_0 = 0$ and $\rho_{k-j+1} = \frac{\zeta_{k-j+1}}{\zeta_{k-j}}$

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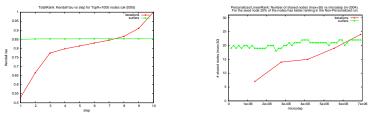
Examples

LinearRank (LR) $x^{\text{LR}} = \sum_{j=0}^{k} \frac{2(k+1-j)}{(k+1)(k+2)} S^{j} v : \mu_{j} = \frac{j}{j+2}, j = 1, ..., k.$ TotalRank (TR) $x^{\text{TR}} = \sum_{j=0}^{\infty} \frac{1}{(j+1)(j+2)} S^{j} v : \mu_{j} = \frac{k-j+1}{k-j+2}, j = 1, ..., k.$

Advantages of multidamping

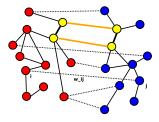
- Interpretability and Design!
- Reduced computational cost in *approximating* functional rankings using the Monte Carlo approach. A random surfer terminates with probability $1 \mu_j$ at step j.
- Inherently parallel and synchronization free computation.

Multidamping Performance



Approximate ranking: Run *n* surfers to completion for graph size *n*. How well does the computed ranking capture the "reference" ordering for top-*k* nodes, compared to standard iterations of equivalent computational cost/number of operations? *[Left]* **Approximate personalized ranking:** Run < *n* surfers to completion (each called a microstep, x-axis), but only from a selected node (personalized). How well can we capture the "reference" top-*k* nodes, i.e., how many of them are shared (y-axis), compared to the iterative approach of equivalent computational cost? *[Right]*

Sidebar: Graph Alignment



- Node similarity: Two nodes are similar if they are linked by other similar node pairs. By pairing similar nodes, the two graphs become *aligned*.
- Let \tilde{A} and \tilde{B} be the normalized adjacency matrices of the graphs (normalized by columns), H_{ij} be the independently known similarity scores (preferences matrix) of nodes $i \in V_B$ and $j \in V_A$, and μ be the fractional contribution of topological similarity.
- To compute X, IsoRank iterates:

$$X \leftarrow \mu \tilde{B} X \tilde{A}^T + (1 - \mu) H$$

Network Similarity Decomposition (NSD) [Kollias, Mohammadi, AG, TKDE'12]

Network Similarity Decomposition (NSD)

- In *n* steps of we reach $X^{(n)} = (1 - \mu) \sum_{k=0}^{n-1} \mu^k \tilde{B}^k H(\tilde{A}^T)^k + \mu^n \tilde{B}^n H(\tilde{A}^T)^n$
- Assume that $H = uv^T$ (1 component). Two phases for X:
 - u^(k) = B̃^ku and v^(k) = Ã^kv (preprocess/compute iterates)
 X⁽ⁿ⁾ = (1 μ) Σⁿ⁻¹_{k=0} μ^ku^(k)v^{(k)^T} + μⁿu⁽ⁿ⁾v^{(n)^T} (construct X)

This idea extends to *s* components, $H \sim \sum_{i=1}^{s} w_i z_i^T$.

• NSD computes matrix-vector iterates and builds X as a sum of outer products; these are much cheaper than triple matrix products.

We can then apply Primal-Dual or Greedy Matching (1/2 approximation) to extract the actual node pairs.

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NSD: Performance [Kollias, Madan, Mohammadi, AG, BMC RN'12]

| Species | Nodes | Edges |
|-------------------|-------|-------|
| celeg (worm) | 2805 | 4572 |
| dmela (fly) | 7518 | 25830 |
| ecoli (bacterium) | 1821 | 6849 |
| hpylo (bacterium) | 706 | 1414 |
| hsapi (human) | 9633 | 36386 |
| mmusc (mouse) | 290 | 254 |
| scere (yeast) | 5499 | 31898 |
| | | |

| Species pair | NSD | PDM | GM | IsoRank |
|--------------|--------|--------|--------|---------|
| | (secs) | (secs) | (secs) | (secs) |
| celeg-dmela | 3.15 | 152.12 | 7.29 | 783.48 |
| celeg-hsapi | 3.28 | 163.05 | 9.54 | 1209.28 |
| celeg-scere | 1.97 | 127.70 | 4.16 | 949.58 |
| dmela-ecoli | 1.86 | 86.80 | 4.78 | 807.93 |
| dmela-hsapi | 8.61 | 590.16 | 28.10 | 7840.00 |
| dmela-scere | 4.79 | 182.91 | 12.97 | 4905.00 |
| ecoli-hsapi | 2.41 | 79.23 | 4.76 | 2029.56 |
| ecoli-scere | 1.49 | 69.88 | 2.60 | 1264.24 |
| hsapi-scere | 6.09 | 181.17 | 15.56 | 6714.00 |

- We compute similarity matrices X for various pairs of species using Protein-Protein Interaction (PPI) networks. $\mu = 0.80$, uniform initial conditions (outer product of suitably normalized 1's for each pair), 20 iterations, one component.
- We then extract node matches using PDM and GM.
- *Three orders of magnitude speedup* from NSD-based approaches compared to IsoRank.

NSD: Parallelization [KKG JPDC'13, Submitted, KMSAG ParCo'13 Submitted]

Parallelization: NSD has been ported to parallel and distributed platforms.

- We have aligned up to million-node graph instances using over 3K cores.
- We process graph pairs of over a billion nodes and twenty billion edges each (!), on MapReduce-based distributed platforms.