

Graph Search and Learning

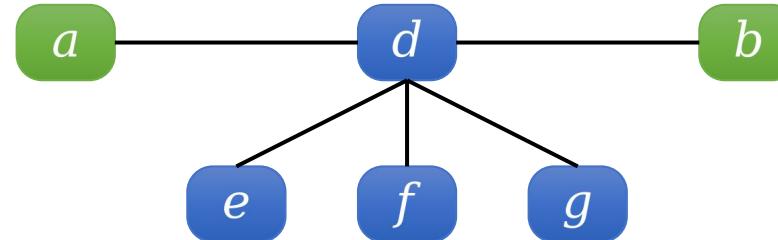
CS6101

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Map

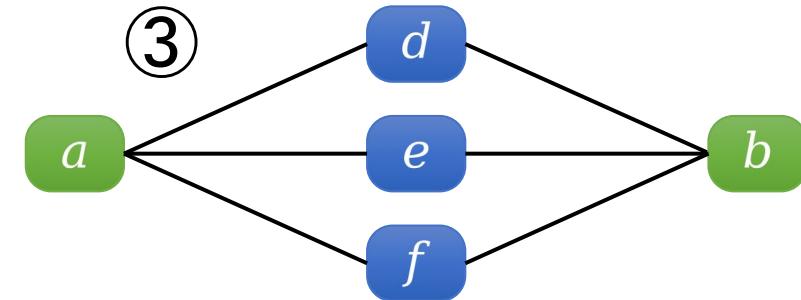
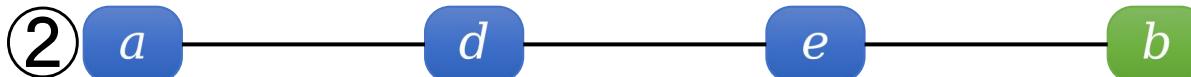
- Graphs add vital signal to local (text) features
- Useful in (at least) two task categories
 - Node property prediction
 - Page topic, spamminess, prestige, centrality, relevance
 - Edge or node-pair (property) prediction
 - Node pair relatedness
 - Edge existence, recommendation, polarity
- Starting point: How related are two given nodes?
 - Subjective, but can lay out a few axioms

Relatedness: why not shortest path?



- Shortest $a—b$ path has two hops in both cases
- In the second case, d is like someone who delivers pizza to both a and b , but many others too
- Relatedness between a and b should be larger without distraction from other nodes

Relatedness: why not max flow?



- All edges have unit edge capacity
- Max flow from a to b is 1 in ① and 3 in ③
- Most would agree a and b are more strongly related in graph ③ than graph ①
- But max flow fails to detect that relatedness is more for ① than ② (shorter path)

Relatedness: The three principles

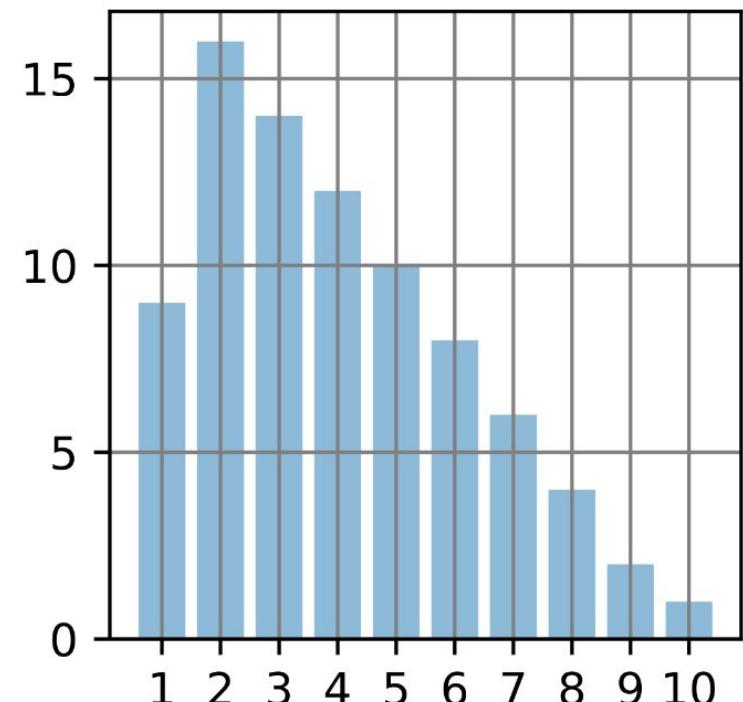
- Two nodes are more strongly related if
 - There is a short path from one to the other
 - There are many paths from one to the other
 - Paths do not have nodes on them with large degree (“low distraction paths”)
- How to combine these three considerations into a principled relatedness measure?
- That can work with rich node and text features (e.g., text) as well?
- Random walk in graphs \leftrightarrow resistive electrical networks equivalence will be useful
 - Will set up through series of warmup examples

Warmup: linear equations related to graphs

- Undirected chain graph with nodes $1, 2, \dots, n$
- Walk begins at node 1 and ends when node n is visited for the first time
- At each step, walker goes from a node to a neighbor uniformly at random
- Define $v(i)$ as the expected number of visits to node i
 - By definition, $v(n) = 1$
- Half the time surfer is at $n - 1$, they then visit n
 - $\frac{1}{2}v(n - 1) = v(n) = 1 \Rightarrow v(n - 1) = 2$
- Half the time surfer is at 2, they move to 1 next
 - $v(1) = 1 + \frac{1}{2}v(2)$ (1 for initial visit, not transition from 2)

Chain graph, continued

- If surfer is at 2 now, must have been at 1 or 3 in previous time step $\Rightarrow v(2) = v(1) + \frac{1}{2}v(3)$
- For nodes $3 \leq i \leq n - 3$, $v(i) = \frac{v(i-1) + v(i+1)}{2}$
- General solution is
$$v(i) = \begin{cases} n-1 & i=1 \\ 2(n-i) & 2 \leq i \leq n-1 \\ 1 & i=n \end{cases}$$
- Before reaching n for the first time, will visit 1 expected $n-1$ times!
- Expected length of walk is $\Theta(n^2)$



Markov walks in undirected graphs

- From chain to general graph
- Nodes are states, edges are transitions
- Every time step, from a node, step to one neighbor with uniform probability (unweighted edges)
- Symmetric node-node adjacency matrix A
 - Assume single connected component
 - Positive sum for every row and column
- Convention: row = to node i , column = from node j
 - Compute column sums of A : these are node degrees $d[j]$
 - Have to go *some* node i from node j
 - Define $C[i, j] = A[i, j]/d[j] \Rightarrow$ columns of C sum to 1 ("column-stochastic")

State (multinomial) probability vector

- C is the single-step transition probability matrix (not symmetric in general)
 - $C[i, j] = C[j \rightarrow i]$ probability of walking from j to i
- $p^{(t)}[i]$ is the probability of being in node i at time step t
 - Have to be at some node: $\sum_i p^{(t)}[i] = 1$
- To be in node i at time t , must have been at some neighbor j in previous step $t - 1$
 - $p^{(t)}[i] = \sum_j p^{(t-1)}[j] C[i, j]$
- Collect into matrix-vector product $p^{(t)} = Cp^{(t-1)}$
- If a steady-state exists, $p^{(\infty)} = Cp^{(\infty)}$ is an eigenvector
 - Sometimes written as $\pi = C\pi$

Steady state and return time

- For connected undirected graph, $p^{(\infty)}$ exists
- Let M be the number of edges
- Check that $\pi[i] = d[i]/2M$ is a steady state
- I.e., visit rate is proportional to degree
 - Not generally true for directed graphs
- Return time $R(i) = \text{expected number of steps between two consecutive visits to } i$
- Claim: $R(i) = 1/\pi[i]$
 - Intuition: walk becomes a multinomial sampler π
 - Gap between getting two consecutive draws of one ‘face’ (node) — geometrically distributed
- Undirected chain graph
 - $\pi[0] = \pi[n] = 1/2n; \pi[1] = \dots = \pi[n-1] = 2/2n = 1/n$
 - $R(0) = R(n) = 2n; R(1) = \dots = R(n-1) = n$

Hitting time from node i to node k on chain

- Starting at node i , the expected number of steps to reach node j for the first time is the hitting time $H(i, j)$
- In the undirected chain graph, what is $H(k - 1, k)$?
- Walk ends when we reach k for the first time
- Therefore, nodes to the right of k effectively do not exist
- $R(k) = 2k$
- To return from k to k , we need to step to $k - 1$ and then hit k from $k - 1 \Rightarrow R(k) = 1 + H(k - 1, k)$
- Solves to $H(k - 1, k) = 2k - 1$
 - Although, w.p. $\frac{1}{2}$, we walk straight from $k - 1$ to k

Hitting time in chain graph

- How about $H(i, k)$ with $i < k \leq n - 1$?
 - To hit k , must reach $k - 1$ earlier
 - Leads to
$$\begin{aligned} H(i, k) &= H(i, k - 1) + H(k - 1, k) \\ &= H(i, k - 1) + 2k - 1 \end{aligned}$$
 - Unrolling recurrence, $H(i, k) = k^2 - i^2$
 - Confirm special case: $H(0, k) = k^2$
- Infinite random walk on integer number line
 - Start at 0, toss coin, head → +1, tail → -1
 - Coordinate is current head minus tail imbalance
 - To achieve imbalance k , have to toss k^2 times
- Commute time between i, j is $H(i, j) + H(j, i)$

Cover time

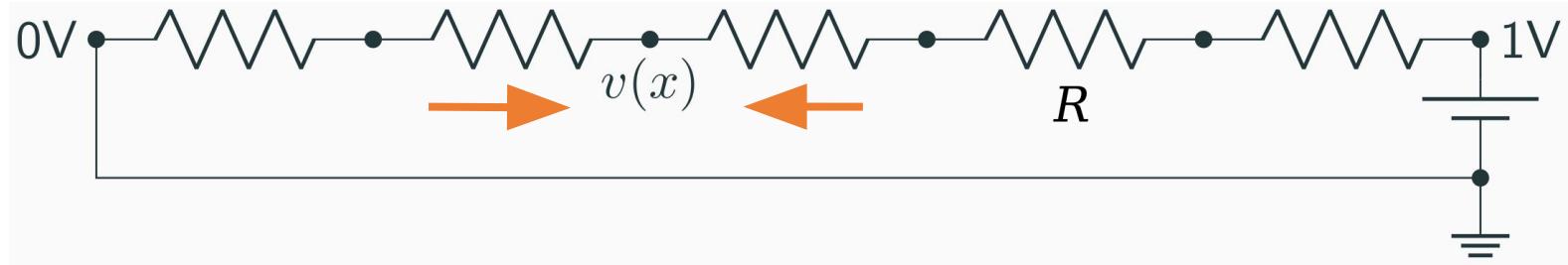
- Cover time $c(i)$ starting at node i is the expected number of steps until all nodes are visited at least once
 - In chain graph with nodes $\{0, \dots, k\}$, $c(0) = k^2$
- What is the cover time of any node in a clique?
 - The more we cover, the less likely the next step covers a new node
- Kite graph
- Dumb-bell graph

Terminating (absorbing) walk



- Starter example: chain walk
 - If we reach bar or home, stay there for ever
 - Otherwise, step left w.p. 1/2 and right w.p. 1/2
- Start from node n : $0 < n < N$
- $p(n)$ is the probability of reaching home first
 - $p(0) = 0, p(N) = 1$
 - For $0 < n < N, p(n) = \frac{1}{2}p(n-1) + \frac{1}{2}p(n+1)$

Resistive network



- 1V battery connected to R -Ohm resistors in series
- Node 0 is at 0V, node N is at 1V
- $v(x)$ is the voltage at node x
- By Kirchoff's current law, for $0 < x < N$,

$$\frac{v(x-1) - v(x)}{R} + \frac{v(x+1) - v(x)}{R} = 0$$

- (No charge accumulates at node x)
- Solves to $v(x) = \frac{1}{2}v(x-1) + \frac{1}{2}v(x+1)$, exactly the same form as $p(n)$

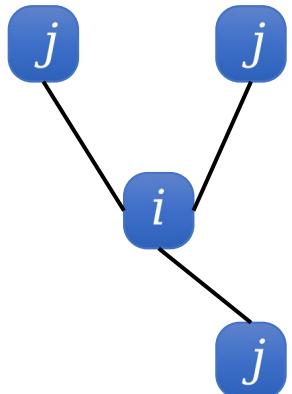
Escape probability

- Designated sink node s , target node t , start node j
- $E(s, t; j)$ the probability of reaching t before ever visiting s
- Base cases $E(s, t; s) = 0$, $E(s, t; t) = 1$
- For $j \neq s, t$ we move to a neighbor i of j and recurse from i
 - With unweighted edges, we get
$$E(s, t; j) = \frac{1}{d(j)} \sum_{i: (i,j) \in E} E(s, t; i)$$
 - With edge transition probabilities $C[* , j]$, we get $E(s, t; j) = \sum_{i: (i,j) \in E} C[i, j] E(s, t; i)$
- Recall $C[i, j] = \frac{A[i, j]}{\sum_l A[l, j]}$, this lets us write
$$E(s, t; j) = \frac{\sum_{i: (i,j) \in E} A[i, j] E(s, t; i)}{\sum_{i: (i,j) \in E} A[i, j]}$$
- E.P. at node j is edge-weighted average of E.P. of neighbors i of j

Harmonic functions on graphs

- In general, for node j with neighbors $\{i\}$, Kirchoff's current law says (for non-battery, non-ground nodes)

$$\sum_{i:(i,j) \in E} \frac{v(i) - v(j)}{R_{ij}} = 0$$



- For easier notation, use conductance $g_{ij} = 1/R_{ij}$ and rewrite as

$$\sum_{j:(i,j) \in E} g_{ij}(v(i) - v(j)) = 0$$

- Collecting terms, we get

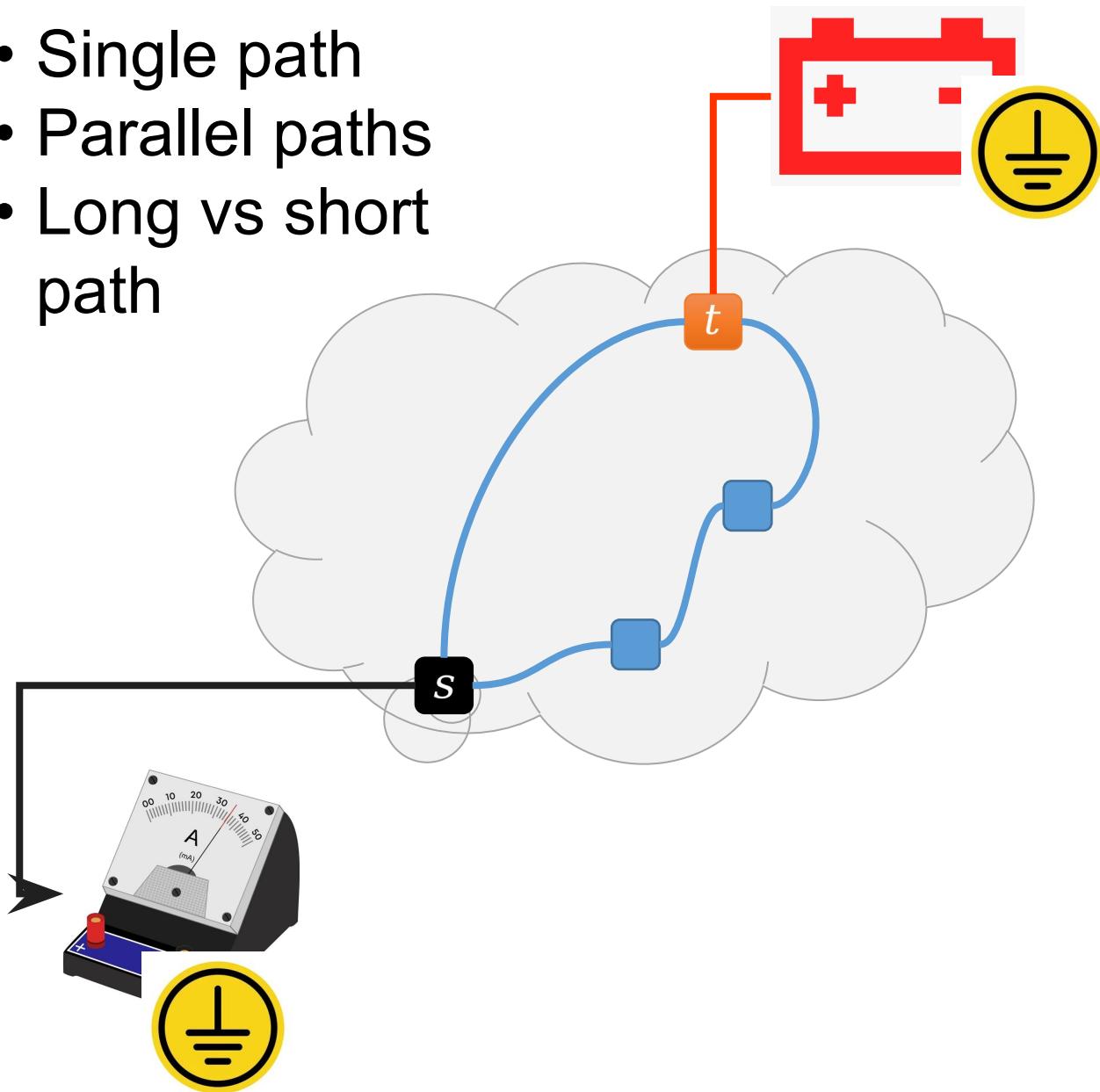
$$v(j) = \frac{\sum_{i:(i,j) \in E} g_{ij} v(i)}{\sum_{i:(i,j) \in E} g_{ij}}$$

Voltage at a node is the conductance-weighted average of voltages at neighboring nodes

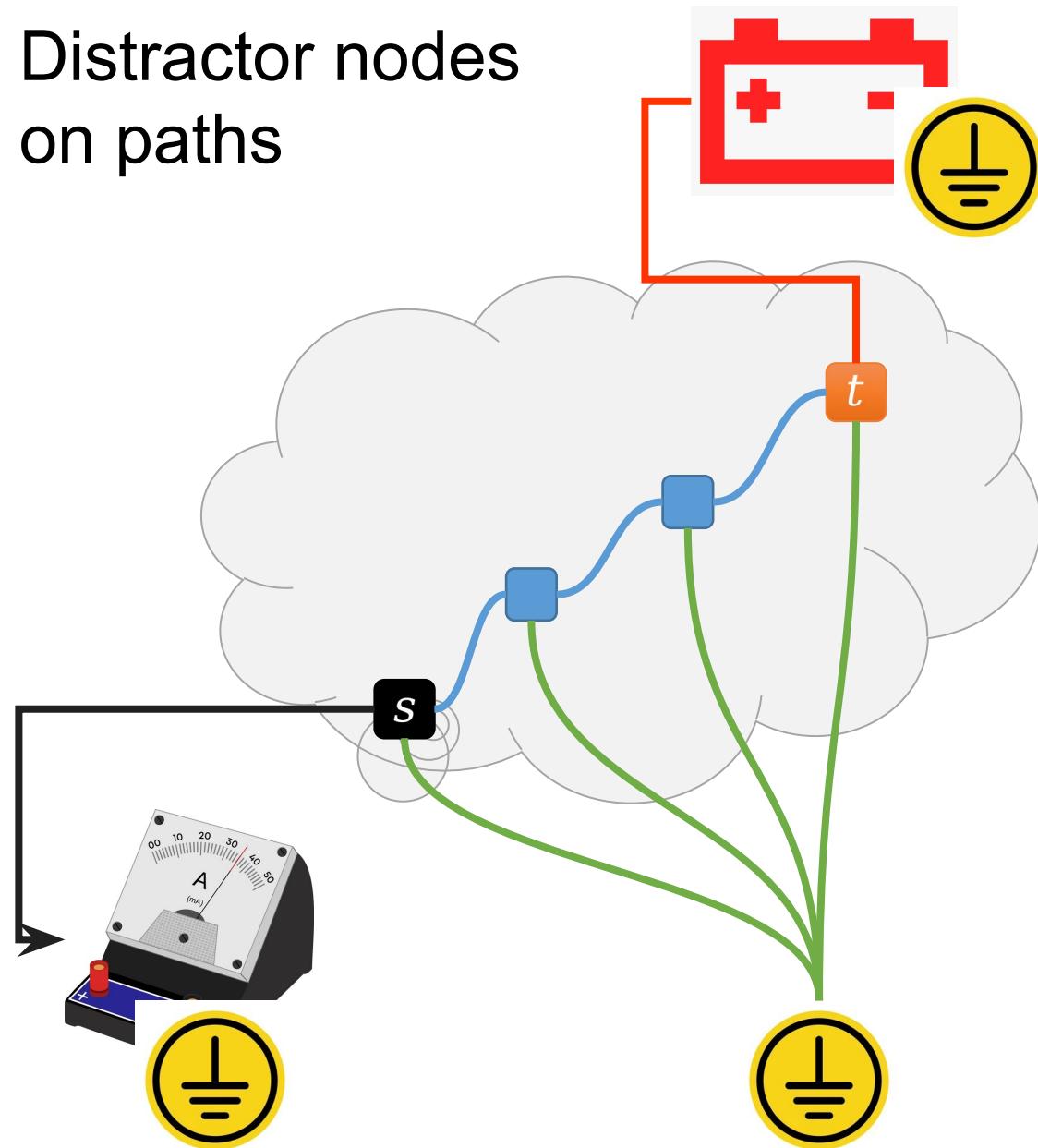
- Except for boundary conditions $v(s) = 0$, $v(t) = 1$

Effective conductance

- Single path
- Parallel paths
- Long vs short path



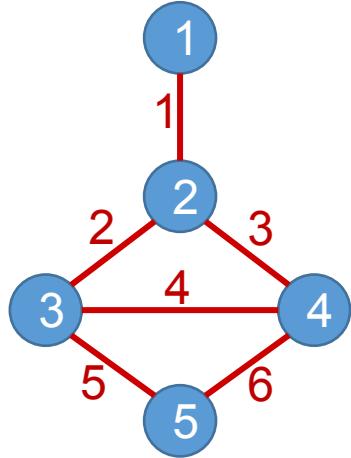
- Distractor nodes on paths



Pseudo-relevance feedback

- Node i = doc, relevance $r(i)$ wrt a query
 - May be produced by a neural scoring network
- Edge = doc-doc similarity $a(i, j) \geq 0$
 - May be output by another network
- For now, assume $r(i)$ and $a(i, j)$ are fixed
- Final score for ranking purpose is $f(i)$ (“decision variables”) with two-part objective
 - $f(i)$ should approximate $r(i)$: $\sum_i (f(i) - r(i))^2$
 - $f(i)$ should be smooth across edges:
$$\sum_{i,j} a(i, j)(f(i) - f(j))^2$$

Node-edge adjacency matrix B



$$A = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \left[\begin{matrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{matrix} \right] \end{matrix}$$

$$B = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \left[\begin{matrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{matrix} \right] \end{matrix}$$

Orient each edge arbitrarily, one -1 and one $+1$ in each column

$$B B^T = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \left[\begin{matrix} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{matrix} \right] \end{matrix} \quad \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix} & \left[\begin{matrix} & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \end{matrix} \right] \end{matrix}$$

$$= \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \left[\begin{matrix} 5 & -1 & -1 & -1 & -1 \\ -1 & 5 & -1 & -1 & -1 \\ -1 & -1 & 5 & -1 & -1 \\ -1 & -1 & -1 & 5 & -1 \\ -1 & -1 & -1 & -1 & 5 \end{matrix} \right] \end{matrix}$$

Off-diagonals are $-A$

Diagonals hold node degrees

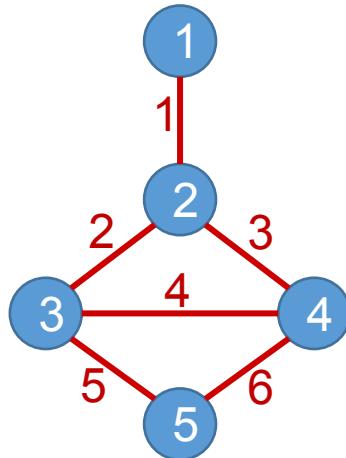
Why is BB^\top interesting?

- Smoothness loss is $(f_1 - f_2)^2 + (f_2 - f_3)^2 + (f_2 - f_4)^2 + \dots$
- One term for each edge
- Let $f^\top = [f_1 \ f_2 \ f_3 \ f_4 \ f_5]$
- What is $f^\top B$?

1	2	3	4	5

1	2	3	4	5	6
1					
2					
3					
4					
5					

$$= \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix}$$



- Smoothness loss is therefore $f^\top B = f^\top B B^\top f$
- $B B^\top$ is positive semidefinite
- Therefore this is a convex quadratic term

PageRank

- Query-independent score of ‘authority’ of a page (node) in the Web graph of hyperlinks (directed edges)
- Seeley, 1949: “... we are involved in an “infinite regress”: [an actor’s status] is a function of the status of those who choose him; and their [status] is a function of those who choose them, and so ad infinitum.
- Edge direction is critical: $i \rightarrow j$ increases authority of j but not i
- What if node-node adjacency matrix A is allowed to be asymmetric?
 - Normalize columns as before to get C , and find fixpoint $p^{(\infty)} = Cp^{(\infty)}$ as before
 - What can go wrong?

Directed walks (e.g., on Web graph)

- Complications: dead ends and cycles
- Markov walk on such graphs may lead to problematic (non-unique, degenerate, or non-convergent) $p^{(\infty)}$
- Two sufficient conditions avoid these problems
 - Single strongly connected component (directed path from any node to another) $\rightarrow p^{(\infty)}$ is well-defined and unique
 - Aperiodic (cycles of almost all lengths exist) $\rightarrow p^{(\infty)}$ converges starting from any $p^{(0)}$

Teleport

- Hyperparameter (walk probability) $\alpha \in (0,1)$
- Random walker currently at node j
 - If j has out-neighbors, total probability of walking to neighbors is α
 - If j is a dead end, probability of walking out is 0
- With the remaining probability ($1 - \alpha$ or 1), teleport (jump) to any node in the graph
 - Choose target uniformly at random, or
 - Sample a multinomial ‘personalization’ teleport distribution r
- “Random walk with restart” (RWR)
- Effectively superpose a complete directed graph on top of the input graph, satisfying both requirements

PageRank recurrence

- For notational simplicity assume no dead-end nodes
- If random walker is now at node i , then
 - Either walking in from a neighbor j , along edge (j, i) , with probability $\alpha C[i, j]$
 - Or jumped from some arbitrary node k , with probability $(1 - \alpha)r[i]$
- If steady state probability of visiting node i is $p[i]$,

$$p[i] = \sum_{j:(j,i) \in E} \alpha C[i, j] p[j] + \sum_{j \in V} (1 - \alpha) p[j] r[i]$$

- Or, in compact matrix form,

$$p = \alpha C p + (1 - \alpha) r$$

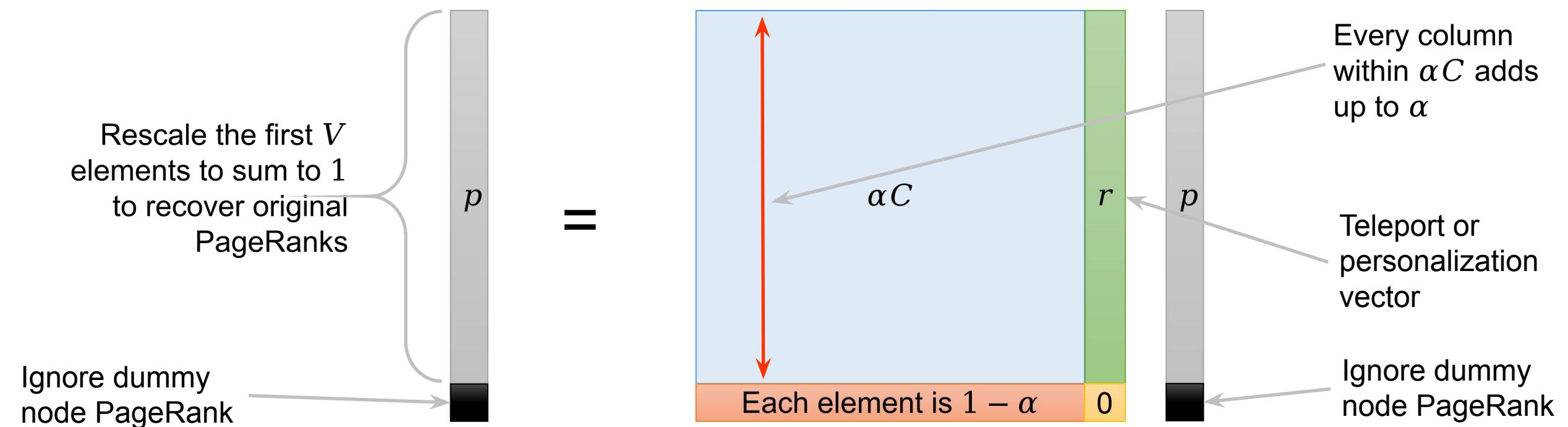
- Solve for p efficiently, with $|V| \approx 10^{10}$, $|E| \approx 10^{12}$
- Use $p[i]$ as a static (query independent) feature in learning to rank
- How to tune α ? Why are some values suitable?

Solving the recurrence

- PageRank equation $p = \alpha C p + (1 - \alpha)r$
 - $\mathbb{I}p - \alpha C p = (\mathbb{I} - \alpha C)p = (1 - \alpha)r$ or
 $p = (1 - \alpha)(\mathbb{I} - \alpha C)^{-1}r$
 - Here $(\mathbb{I} - \alpha C)^{-1} \in \mathbb{R}^{V \times V}$, $r \in \mathbb{R}^V$
 - Does matrix inverse of $(\mathbb{I} - \alpha C)$ always exist?
 - Even if it exists, it is dense and impractical to store or manipulate
- A more practical form is $p = (1 - \alpha) \sum_{n \geq 0} \alpha^n C^n r$
 - Converges because C is column-stochastic and $\alpha < 1$

A homogeneous form

- Instead of all-to-all teleport, use a dummy node
 - All-to-dummy then dummy-to-all ‘walk’ edges
- Leads to a padded $\widehat{C} \in \mathbb{R}^{(V+1) \times (V+1)}$ and corresponding padded $\widehat{p} \in \mathbb{R}^{(V+1)}$ in the homogeneous form $\widehat{p} = \widehat{C}\widehat{p}$
- Rescale non-dummy nodes in \widehat{p} to add up to 1 to recover p



Power iteration

- To solve $\hat{p} = \widehat{C}\hat{p}$ via power iteration
- Initialize $\hat{p}^{(0)}$ ‘suitably’
 - Can be initially random
 - Later, warm start from previous runs
 - (Hope is that Web graph is changing relatively slowly)
- Repeat for $t = 1, 2, \dots$
 - $\hat{p}^{(t)} \leftarrow \widehat{C}\hat{p}^{(t-1)}$
- Until $\|\hat{p}^{(t)} - \hat{p}^{(t-1)}\|$ is “small enough”
- Postprocess “ $\hat{p}^{(\infty)}$ ” to recover PageRanks

RAM-friendly, IO-friendly matrix-vector product

- Luckily, \hat{C} is sparse with $O(V + E)$ nonzeros
- Store as a list on disk, with records $\langle i, j, \hat{c}_{i,j} \rangle$
- Need to hold $\hat{p}^{(t)}, \hat{p}^{(t-1)}$ in RAM
 - Otherwise need repeated sorts, more expensive
- Repeat
 - Initialize $\hat{p}^{(t)}$ to all zeros
 - Scan edge list; for each $\langle i, j, \hat{c}_{i,j} \rangle$
 - $\hat{p}^{(t)}[i] += \hat{c}_{i,j} \hat{p}^{(t-1)}[j]$
 - Check for convergence and quit loop if done
 - Swap (pointers to) $\hat{p}^{(t)}, \hat{p}^{(t-1)}$

Power iterations to find dominant eigenvector

- Simple notation $p \leftarrow Cp$
- If C is column-stochastic, renormalizing p is not required in principle
- May still do it in practice, for numerical stability
- C 's eigenvalues satisfy $1 = \lambda_1 > |\lambda_2| > |\lambda_3| > \dots$
- Corresponding eigenvectors u_1, u_2, u_3, \dots form orthonormal basis
- Express $p^{(0)} = a_1 u_1 + a_2 u_2 + a_3 u_3 + \dots$ where a_1, a_2, a_3, \dots are coordinates in the new basis

$$\begin{aligned} p^{(1)} &= Cp^{(0)} = a_1 Cu_1 + a_2 Cu_2 + a_3 Cu_3 + \dots \\ &= a_1 u_1 + a_2 \lambda_2 u_2 + a_3 \lambda_3 u_3 + \dots \end{aligned}$$

- After k iterations, $p^{(1)} = a_1 u_1 + a_2 \lambda_2^k u_2 + a_3 \lambda_3^k u_3 + \dots$
- Observe that only $a_1 u_1$ does not shrink, all other terms do
- Can we shrink lower eigenvectors faster?

Acceleration

- Suppose, after some number of iterations, we got lucky and all but top two eigenvectors are gone:

$$p^{(k-2)} = u_1 + a_2 u_2$$

- In the next two iterations,

$$\begin{aligned} p^{(k-1)} &= Cp^{(k-2)} = u_1 + a_2 \lambda_2 u_2 \\ p^{(k)} &= Cp^{(k-1)} = u_1 + a_2 \lambda_2^2 u_2 \end{aligned}$$

- Using these, we can solve for u_1

- $$\begin{aligned} u_1[i] &= p^{(k-2)}[i] - a_2 u_2[i] \\ &= p^{(k-2)}[i] - \frac{(p^{(k-1)}[i] - p^{(k-2)}[i])^2}{p^{(k)}[i] - 2p^{(k-1)}[i] + p^{(k-2)}[i]} \end{aligned}$$

- Periodically, force $p^{(k)}$ to this value

TotalRank: More principled choice of α

- Here we fix teleport r for simplicity
- Instead write $p(\alpha)$ as a function of α
- Since we don't know α , marginalize
- $$\begin{aligned} \int_0^1 p(\alpha) d\alpha &= \int_0^1 \left[\sum_{k \geq 0} (1 - \alpha) \alpha^k C^k \right] r d\alpha \\ &= \sum_{k \geq 0} C^k r \int_0^1 (1 - \alpha) \alpha^k d\alpha \\ &= \left[\sum_{k \geq 0} \frac{C^k}{(k + 1)(k + 2)} \right] r \end{aligned}$$
- How to compute this infinite sum?

Recap

- Random walk in graphs \leftrightarrow electrical networks
- Node-to-node relatedness
 - Hitting, commute, cover times, escape probability
- Node popularity or prestige
 - Steady state visit rates
- PageRank
 - Need for teleport (irreducible, aperiodic)
 - Dominant eigenvector, (accelerated) power method
 - Next: (query-time) personalization

Personalized PageRank

- General recurrence $p_r = \alpha C p_r + (1 - \alpha)r$
- Subscript r in p_r because PageRank will be regarded as a function of r
- Teleport vector r can be designed from application needs
 - $r[i]$ proportional to query relevance of doc i
 - $r[i] > 0$ if user has visited page i (often)
- Recall we can write $p_r = (1 - \alpha)(\mathbb{I} - \alpha C)^{-1}r$
- The highlighted part is a matrix M
- Thus, p_r is a linear function of r : $p_r = Mr$

Impulse teleport vector

- For a fixed node i , a special value $r = \delta_i$ is defined as

$$\delta_i[j] = \begin{cases} 1 & j = i \\ 0 & j \neq i \end{cases}$$

- “Impulse teleport” to only one node i
- Corresponding p_{δ_i} is called the personalized PageRank vector $\text{PPV}(i) \in \mathbb{R}^V$
- $\text{PPV}(i)$ is a kind of soft “reachability map” from node i to all V nodes
- Imagine we have precomputed and stored $\text{PPV}(i)$ for all nodes i
- From these, can we recover p_r for any r ?

Linearity and superposition

- Thanks to linearity
 - $M(ur) = p_{ur} = up_r = u(Mr)$ with $u \in \mathbb{R}$
 - (Although ur may not be a valid multinomial teleport distribution)
 - Likewise, $p_{r+r'} = p_r + p_{r'}$ (ditto for $r + r'$)
- Given arbitrary teleport r , we can decompose it among the basis $\{\delta_i : i \in V\}$ as $r = \sum_i u_i \delta_i$
- Accordingly, $p_r = \sum_i u_i \text{PPV}(i)$
- “We have precomputed and stored $\text{PPV}(i)$ for all nodes i ” — can be prohibitively expensive

Pushdown and “backward propagation”

- Recall $p_r = p_{\alpha C r} + (1 - \alpha)r$
- Aside: $\sum_{v:(u,v) \in E} C[v, u] \delta_v = C \delta_u$ (verify this)
- Using the pushdown property,
$$\sum_{v:(u,v) \in E} \alpha C[v, u] p_{\delta_v} = p_{\sum_{(u,v) \in E} \alpha C[v, u] \delta_v}$$
- Therefore we can write
$$\alpha \sum_{v:(u,v) \in E} C[v, u] p_{\delta_v} = p_{\alpha C \delta_u} = \alpha C p_{\delta_u}$$
- leading to
$$p_{\delta_u} = \alpha \sum_{v:(u,v) \in E} C[v, u] p_{\delta_v} + (1 - \alpha) \delta_u$$
- Note, vector p_{δ_u} is being expressed in terms of vectors p_{δ_v} of out-neighbors v where $(u, v) \in E$

Synchronous and asynchronous PageRank

- | | |
|--|--|
| <ul style="list-style-type: none">• $q \leftarrow r, p \leftarrow 0$• while q is large do<ul style="list-style-type: none">• $p \leftarrow p + (1 - \alpha)q$• $q \leftarrow \alpha C q$ | <ul style="list-style-type: none">• $q \leftarrow r, p \leftarrow 0$• while some $q(u)$ is large<ul style="list-style-type: none">• $\hat{q} \leftarrow q(u); q(u) \leftarrow 0$• $p(u) += (1 - \alpha)\hat{q}$• for out-neighbors v<ul style="list-style-type: none">• $q(v) += \alpha C[v, u]\hat{q}$ |
|--|--|

Iter		

Similar loop
invariants can be
set up in both
forms

What is $\text{PPV}_v = p_{r=\delta_v} \in \Delta^{|V|-1}$?

- If unit heat is injected into node v , how much heat goes lands up at all nodes?
- By linearity, if h “heat units” are injected into v , node w will get $p_{\delta_v}[w]$ “heat units”
- Can short-cut if p_{δ_v} is available

Forward propagation

- For input teleport distribution vector r , PageRank is a solution to $p = \alpha C p + (1 - \alpha)r$
- p is a (linear) function of r , and we write it as p_r
- If $\{u\}$ link to v and we know all $p_r[u]$, we can compute $p_r[v]$ via “forward propagation” as

$$\begin{aligned} & \sum_{u:(u,v) \in E} \alpha C[v, u] p_r[u] + \sum_u r[u] (1 - \alpha) \\ &= \sum_{u:(u,v) \in E} \alpha C[v, u] p_r[u] + (1 - \alpha) \end{aligned}$$

- Note, scalar quantity $p_r[v]$ is expressed in terms of scalar quantities $p_r[u]$ of in-neighbors u of node v

SimRank motivation

- Recall $p_{\delta_i}[j]$ is the PageRank of node j when teleport is to only node i
 - How often a RWR restarting at i visits j
 - Incorporates all three relatedness principles
 - But not generally symmetric: $p_{\delta_i}[j] \neq p_{\delta_j}[i]$
- Some applications need a symmetric measure of node-node similarity based on their graph neighborhoods
 - Here we focus on edges from other nodes into i, j
 - Call them the in-neighbors $N(i), N(j)$
 - (Can incorporate also out-links, local features, etc.)

SimRank formulation

- A node is maximally similar to itself: $s(i, i) = 1$
- To compute $s(i, j)$ with $i \neq j$
 - Let $i' \in N(i)$, $j' \in N(j)$
 - Recursively compute $s(i', j')$
 - $s(i', j')$ ‘suitably’ contributes to $s(i, j)$

$$s(i, j) = \frac{1}{|N(i)||N(j)|} \sum_{i' \in N(i), j' \in N(j)} \alpha s(i', j')$$

- $\alpha \in (0, 1)$ is a dampener much like in PageRank
- Is $s(i, j)$ well-defined and convergent?
- Possible to compute efficiently for all i, j pairs?

Hyperlink induced topic search (HITS)

- Query dependent graph collection stage
 - Pages with high text match scores
 - Their in- and out-neighbors (one hop)
- Each node u has two kinds of prestige score
 - Authority score $a[u]$, similar to PageRank, groundbreaking papers
 - Hub score $h[u]$, “reflected glory”, good survey paper
- Mutual recurrence
 - Good hubs endorse good authorities:
$$h[u] = \sum_{v:(u,v) \in E} a(v) \text{ or } \mathbf{h} = \mathbf{E} \mathbf{a}$$
 - Good authorities endorsed by good hubs:
$$a[v] = \sum_{u:(u,v) \in E} h(u) \text{ or } \mathbf{a} = \mathbf{E}^\top \mathbf{h}$$

HITS calculations

- Equivalently, $\mathbf{h} = \mathbf{E}\mathbf{a} = \mathbf{E}\mathbf{E}^\top \mathbf{h}$
and $\mathbf{a} = \mathbf{E}^\top \mathbf{h} = \mathbf{E}^\top \mathbf{E}\mathbf{a}$
- Unlike PageRank, $\mathbf{E}\mathbf{E}^\top$ and $\mathbf{E}^\top \mathbf{E}$ are not stochastic; norm control needed
- Initialize $\mathbf{h} \leftarrow \mathbf{1}$, $\mathbf{a} \leftarrow \mathbf{1}$
- Some number of iterations:
 - $\mathbf{h}_\diamond \leftarrow \mathbf{E}\mathbf{a}$; $\mathbf{h} \leftarrow \mathbf{h}_\diamond / \|\mathbf{h}_\diamond\|_1$ // hub update
 - $\mathbf{a}_\diamond \leftarrow \mathbf{E}^\top \mathbf{h}$; $\mathbf{a} \leftarrow \mathbf{a}_\diamond / \|\mathbf{a}_\diamond\|_1$ // authority update

Stability

Learning to rank in graphs