Networks for machine learning

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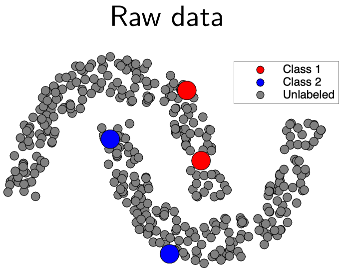
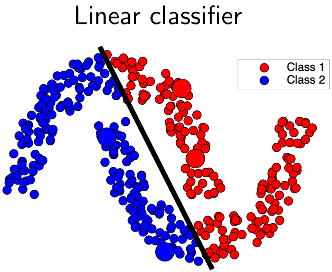
The big data era

- Modern systems generate massive amounts of data
  - Sensor systems
  - Internet of things
  - Digital documents
- Technological progress permits to store and effortlessly access it
- Valuable source of information to better solve real world problems
- To get insights from all these data, we need to first organize it
  - Separate emails that are spam from those that are not
  - Organize documents by topic
  - Identify bank transactions that are fraud
- Numerous classification techniques have been proposed over the years
- Classifiers need to learn from annotated data.
- Issue: annotated data do not follow the big data trend

The scarcity of labelled data





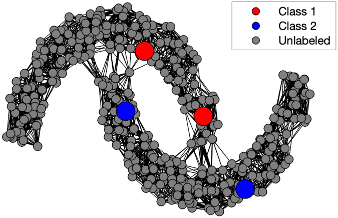
Labelled examples are insufficient to learn
something about the data

Q: How to learn from limited amounts of labelled data?

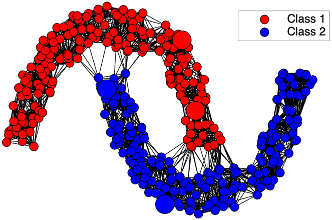
A: Use a similarity graph to learn from both labelled and unlabelled data

Graph node classification

Graph from data



Label propagation



Graphs are powerful objects to represent data

Q: How to propagate the labelled data in the graph?

A: Google's PageRank!

PageRank for data classification

The PageRank assigns a score function to graph vertices according to

$$\arg\min_{f} \{ \underbrace{\sum_{u,v \in \mathcal{G}} W_{uv} \left(\frac{f_u}{D_{uu}} - \frac{f_v}{D_{vv}} \right)^2}_{\text{Smoothness}} + \mu \underbrace{\sum_{u \in \mathcal{G}} \frac{1}{D_{uu}} (f_u - y_u)^2}_{\text{Fitting}} \}$$

- y: indicator function of annotated nodes (1 if annotated, 0 otherwise)
- μ: regularization parameter
- f: PageRank vector
- Smoothness: similar vertices should have similar values in f
- Fitting: f should be consistent with labelled data

The solution of this problem coincides with the equilibrium state of a random walk process

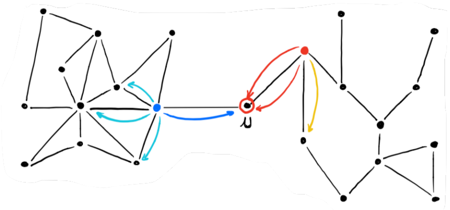
PageRank as a diffusion process

The solution of the PageRank problem is a random walk process:

$$f^T = \sum_{k=0}^{\infty}(1-\alpha)\alpha^k y^T P^k,$$

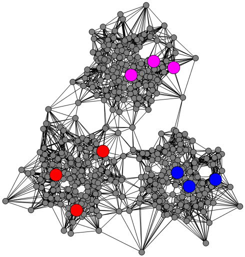
where $\alpha = 1/(1+\mu)$

- $k = 0$: walker at a label with probability one
- $k+1$: walkers decides to jump to a neighbor with probability α, or to restart to the labels with probability $(1-\alpha)$
- $f_u \propto$ probability of finding a walker, at equilibrium, at node u

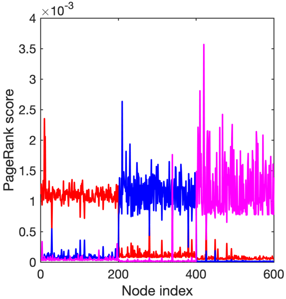


Illustration

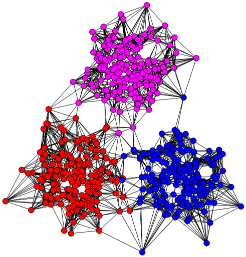
Data



PageRank vectors



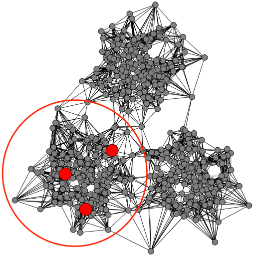
$u \in S_k : argmax_k F_{uk}$



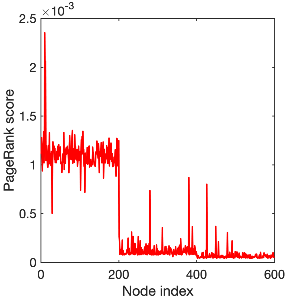
Reducing the number of labelled points

In practice, unfeasible to collect labelled data for hundreds or thousands of classes. Can we indentify classes individually?

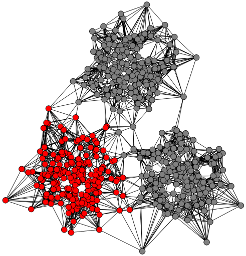
Data



PageRank vector



Final decision?

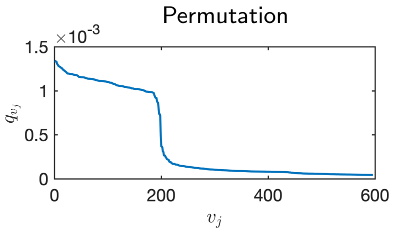


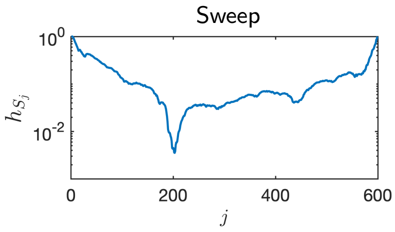
The sweep-cut algorithm

Sweep-cut

A sweep-cut is a procedure to identify individual classes from a PageRank vector.

- Let $v_1, \dots, v_N$ be a rearrangement of the vertices in descending order, so that the permutation vector q satisfies $q_{v_i} = f_{v_i}/d_{v_i} \geq q_{v_{i+1}} = f_{v_{i+1}}/d_{v_{i+1}}$
- Let $S_j = \{v_1, \dots, v_j\}$ be the set of vertices indexed by the first j elements of q.
- Let $\tau(f) = \min_j h_{S_j}$, where h_{S_j} is the ratio of external and internal links of S_j.
- Retrieve $\hat{S}_{gt} = S_j$ for the set S_j achieving $\tau(f)$

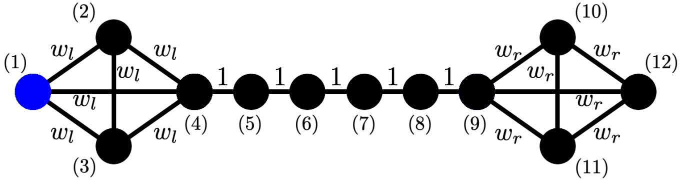




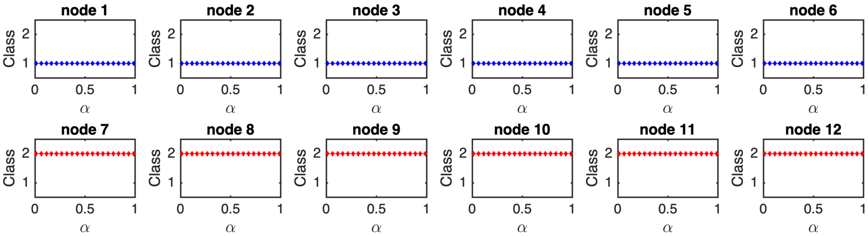
Drawbacks?

- Unbalanced data settings lead to classification biases
- RW properties (e.g. Mixing rate, mean passage times, etc) highly sensitive to non-trivial network structure
- Reliable classifications with few labelled data only under simple data settings
- Curse of dimensionality issue causes flat functions
- Avoid sweep-cuts to retrieve sub-classes conforming one bigger class

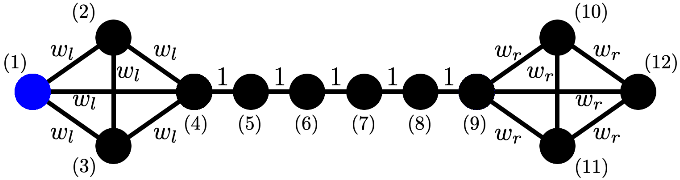
Sensitivity to non-trivial network structures



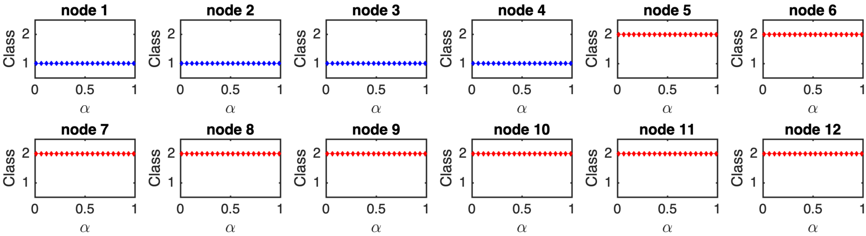
Balanced setting: $w_l = w_r = 1$



Sensitivity to non-trivial network structures



Skewed setting: $w_l = 10; w_r = 1$



How to solve this issue?

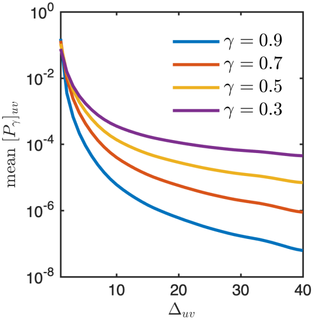
Tweaking random walk dynamics: Lévy flights?

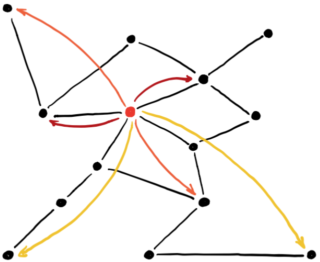
Lévy flights

Lévy flights induced by L^γ for $0 < \gamma < 1$ (Riascos, Phys. Rev. E 90, 2014)

$$L^\gamma = (D - W)^\gamma = Q\Lambda^\gamma Q^T = D_\gamma - W_\gamma$$

$$(P_\gamma)_{uv} = (D_\gamma^{-1} W_\gamma)_{uv} \propto \Delta_{uv}^{-\gamma}.$$





Extending PageRank to Lévy flights

Proposition: extending PageRank to Lévy flights

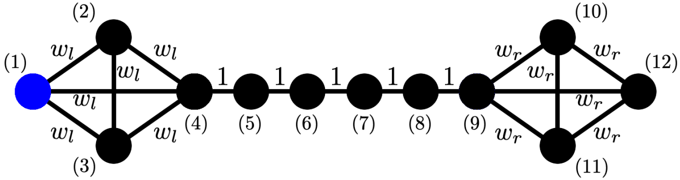
$$\arg\min_f \left\{ \sum_{u,v\in\mathcal{G}} (W_\gamma)_{uv} \left(\frac{f_u}{(D_\gamma)_{uu}} - \frac{f_v}{(D_\gamma)_{vv}} \right)^2 + \mu \sum_{u\in\mathcal{G}} \frac{1}{(D_\gamma)_{uu}} (f_u - y_u)^2 \right\}$$

Solution: equilibrium state of Lévy flight process

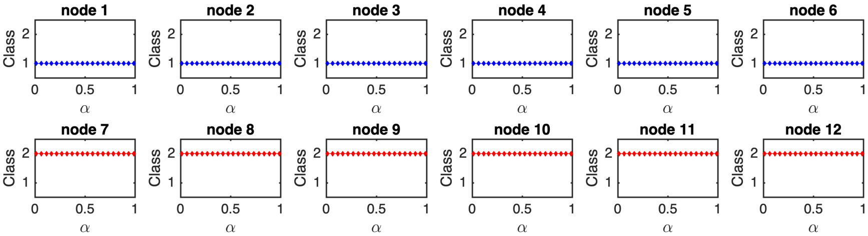
$$f^T = \sum_{k=0}^{\infty} (1-\alpha)\alpha^k y^T P_\gamma^k,$$

where $\alpha = 1/(1+\mu)$

Revisiting the skewed graph via Lévy flights



Skewed setting: $w_l = 10$; $w_r = 1$ and $\gamma = 0.01$



Recap

- Graphs are useful objects to represent data
- Graphs allow to learn from labelled and unlabelled data to improve classifiers
- Random walkers are a simple yet effective approach to propagate information in the graph (PageRank algorithm)
- Random walkers can be sensitive to trapping regions in the graph
- Anomalous diffusion processes, like Lévy flights, may carry a better alternative in certain applications