DFNets: Spectral CNNs for Graphs with Feedback-Looped Filters

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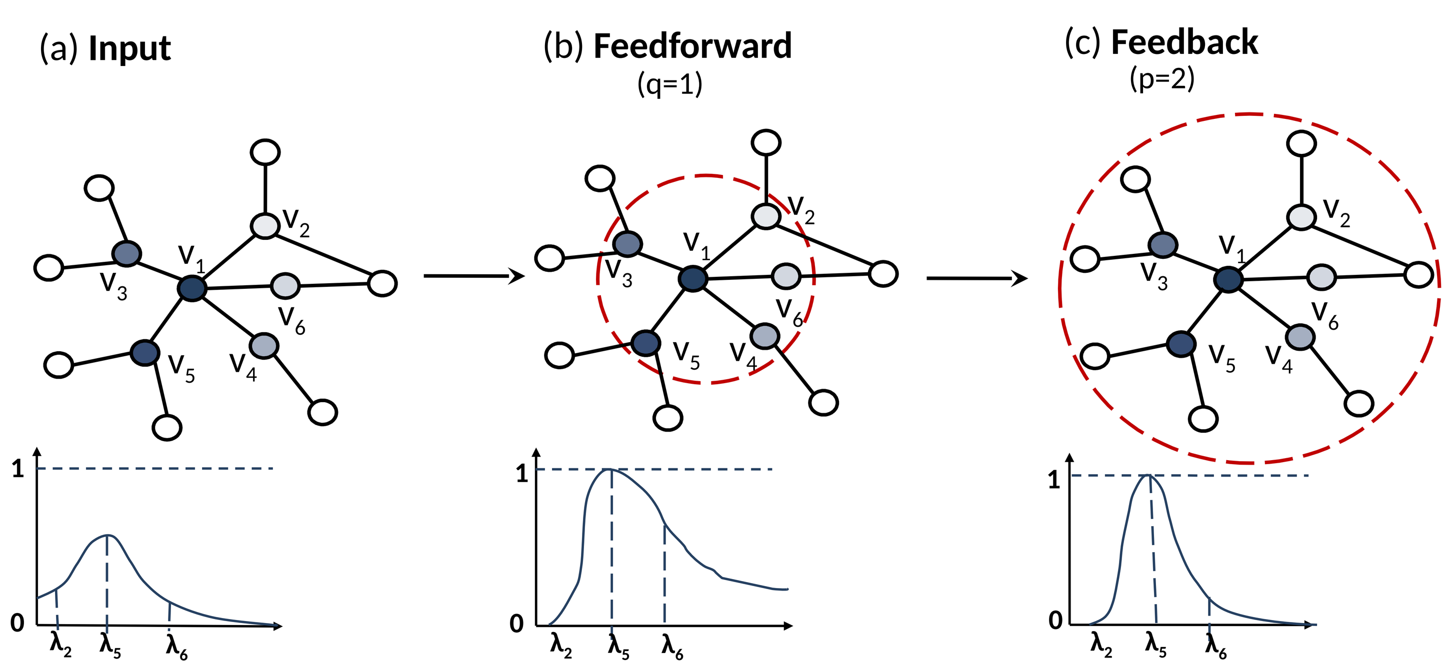
Introduction

- We propose *Distributed Feedback-Looped Network* (DFNet) which is a novel spectral CNN architecture with feedback-looped graph filters.



Feedback-Looped Filters

- Feedback-looped filters belong to a class of Auto Regressive Moving Average (ARMA) filters.

$$h_{\psi,\phi}(L)x = \Big(I + \sum_{j=1}^{p} \psi_j L^j\Big)^{-1} \Big(\sum_{j=0}^{q} \phi_j L^j\Big)x, \tag{1}$$

where p and q refer to the *feedback* and *feedforward* degrees, respectively. $\psi \in \mathbb{C}^p$ and $\phi \in \mathbb{C}^q$ are two vectors of complex coefficients.

- The frequency response of feedback-looped filters is defined as:

$$h(\lambda_i) = \frac{\sum_{j=0}^{q} \phi_j \lambda_i^j}{1 + \sum_{j=1}^{p} \psi_j \lambda_i^j}. \tag{2}$$

- To circumvent the issue of matrix inversion for large graphs, *feedback-looped filters* use the following approximation:

$$\bar{x}^{(0)} = x \text{ and } \bar{x}^{(t)} = -\sum_{j=1}^{p} \psi_j \tilde{L}^j \bar{x}^{(t-1)} + \sum_{j=0}^{q} \phi_j \tilde{L}^j x, \tag{3}$$

where $\tilde{L} = \hat{L} - (\frac{\hat{\lambda}_{max}}{2})I$, $\hat{L} = I - \hat{D}^{-1/2}\hat{A}\hat{D}^{-1/2}$, $\hat{A} = A + I$, $\hat{D}_{ii} = \sum_j \hat{A}_{ij}$ and $\hat{\lambda}_{max}$ is the largest eigenvalue of $\hat{L}$.

- To alleviate the issues of gradient vanishing/ exploding and numerical instabilities, we use two techniques:
  - **Scaled-normalization technique:** centralizes the eigenvalues of the Laplacian $\hat{L}$ and reduces its spectral radius bound.
  - **Cut-off frequency technique:** allows the generation of ideal high-pass filters so as to sharpen a signal by amplifying its graph Fourier coefficients.

Coefficient Optimization

- We aim to find the optimal coefficients ψ and ϕ that make the frequency response as close as possible to the desired frequency response,

$$\acute{e}(\tilde{\lambda}_i) = \hat{h}(\tilde{\lambda}_i) - \frac{\sum_{j=0}^{q} \phi_j \tilde{\lambda}_i^j}{1 + \sum_{j=1}^{p} \psi_j \tilde{\lambda}_i^j} \tag{4}$$

- Linear approximation of the error (w.r.t. ψ and ϕ) is defined as:

$$e(\tilde{\lambda}_i) = \hat{h}(\tilde{\lambda}_i) + \hat{h}(\tilde{\lambda}_i)\sum_{j=1}^{p} \psi_j \tilde{\lambda}_i^j - \sum_{j=0}^{q} \phi_j \tilde{\lambda}_i^j. \tag{5}$$

- Let $\alpha \in \mathbb{R}^{n \times p}$ with $\alpha_{ij} = \tilde{\lambda}_i^j$ and $\beta \in \mathbb{R}^{n \times (q+1)}$ with $\beta_{ij} = \tilde{\lambda}_i^{j-1}$ be two Vandermonde-like matrices. The coefficients ψ and ϕ can be learned by minimizing e as a convex constrained least-squares optimization problem:

$$\begin{aligned} &\textbf{minimize}_{\psi,\phi} \ ||\hat{h} + diag(\hat{h})\alpha\psi - \beta\phi||_2 \\ &\textbf{subject to} \ ||\alpha\psi||_\infty \leq \gamma \text{ and } \gamma < 1 \end{aligned} \tag{6}$$

Spectral Convolutional Layer

- Let $\mathbf{P} = -\sum_{j=1}^{p} \psi_j \tilde{L}^j$ and $\mathbf{Q} = \sum_{j=0}^{q} \phi_j \tilde{L}^j$. The propagation rule of a spectral convolutional layer is defined as:

$$\bar{X}^{(t+1)} = \sigma(\mathbf{P}\bar{X}^{(t)}\theta_1^{(t)} + \mathbf{Q}X\theta_2^{(t)} + \mu(\theta_1^{(t)};\theta_2^{(t)}) + b), \tag{7}$$

where σ refers to a non-linear activation function and $\bar{X}^{(0)} = X \in \mathbb{R}^{n \times f}$. $\bar{X}^{(t)}$ is a matrix of activations in the t^{th} layer.

Theoretical Analysis

- DFNets has several nice properties:
  - Improved localization
  - Efficient computation
  - Guaranteed stability
  - Linear convergence
  - Universal design
  - Dense architecture

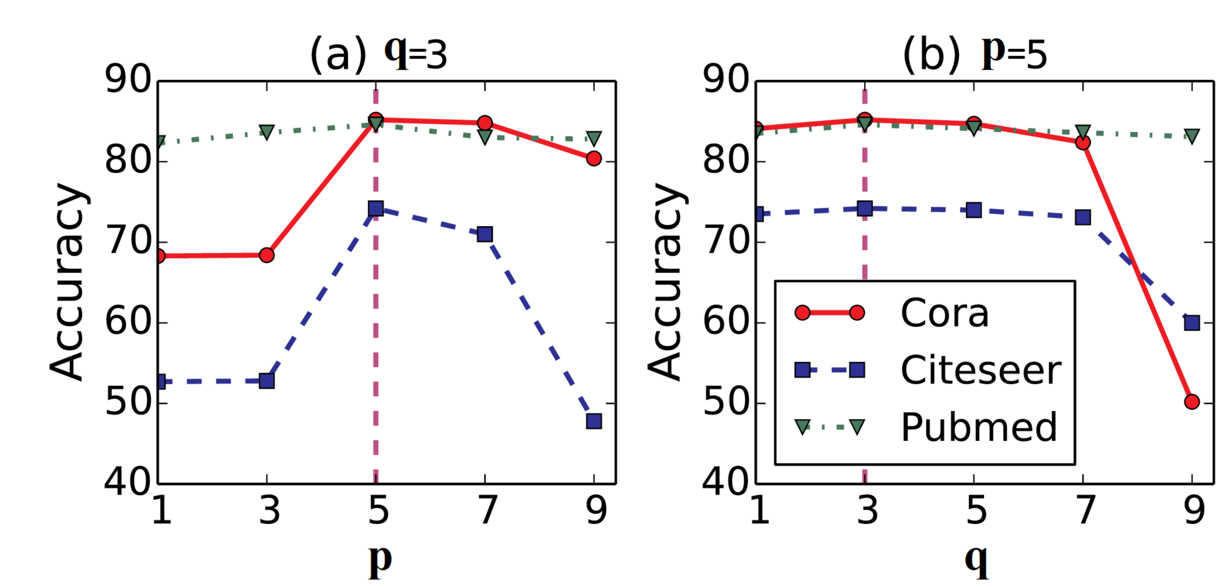
Spectral Graph Filter	Type	Learning Complexity	Time Complexity	Memory Complexity
Chebyshev filters	Polynomial	$O(k)$	$O(km)$	$O(m)$
Lanczos filters		$O(k)$	$O(km^2)$	$O(m^2)$
Cayley filters	Rational polynomial	$O((r+1)k)$	$O((r+1)km)$	$O(m)$
ARMA_1 filters		$O(t)$	$O(tm)$	$O(m)$
d parallel ARMA_1 filters		$O(t)$	$O(tm)$	$O(dm)$
Feedback-looped filters (ours)		$O(tp+q)$	$O((tp+q)m)$	$O(m)$

Numerical Experiments

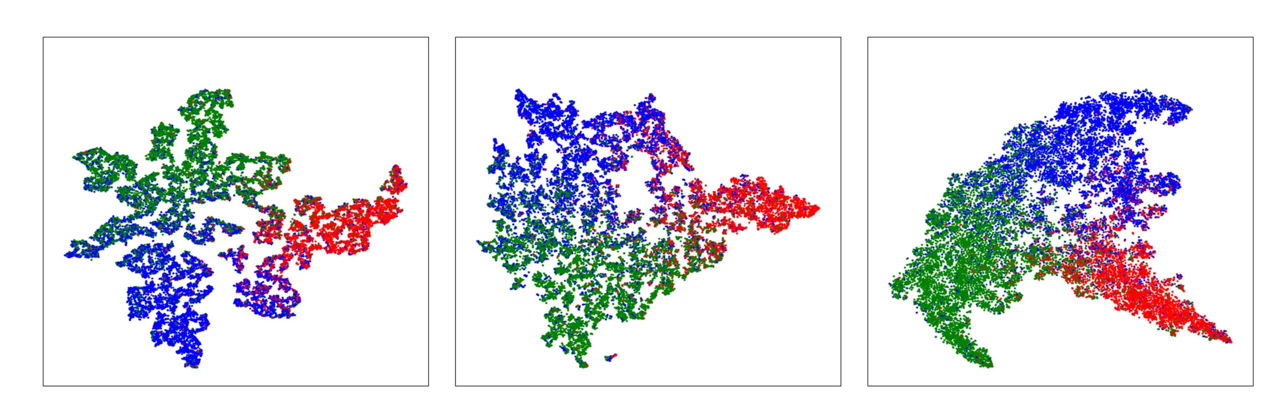
- Comparison with the state-of-the-art methods.

Model	Cora	Citeseer	Pubmed	NELL
SemiEmb	59.0	59.6	71.1	26.7
LP	68.0	45.3	63.0	26.5
DeepWalk	67.2	43.2	65.3	58.1
ICA	75.1	69.1	73.9	23.1
Planetoid*	64.7	75.7	77.2	61.9
Chebyshev	81.2	69.8	74.4	-
GCN	81.5	70.3	79.0	66.0
LNet	79.5	66.2	78.3	-
AdaLNet	80.4	68.7	78.1	-
CayleyNet	81.9*	-	-	-
ARMA_1	84.7	73.8	81.4	-
GAT	83.0	72.5	79.0	-
GCN + DenseBlock	82.7 ± 0.5	71.3 ± 0.3	81.5 ± 0.5	66.4 ± 0.3
GAT + Dense Block	83.8 ± 0.3	73.1 ± 0.3	81.8 ± 0.3	-
DFNet (ours)	**85.2 ± 0.5**	**74.2 ± 0.3**	**84.3 ± 0.4**	**68.3 ± 0.4**
DFNet-ATT (ours)	**86.0 ± 0.4**	**74.7 ± 0.4**	**85.2 ± 0.3**	**68.8 ± 0.3**
DF-ATT (ours)	83.4 ± 0.5	73.1 ± 0.4	**82.3 ± 0.3**	**67.6 ± 0.3**

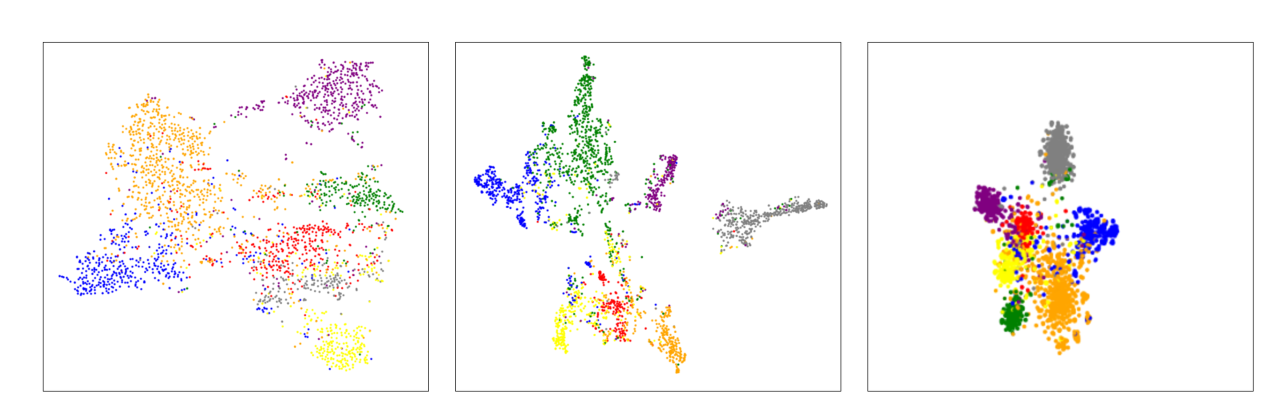
- Comparison under different polynomial orders (DFNet).



- Node embeddings (top: Pubmed ; bottom: Cora).



(a) GCN (b) GAT (c) DFNet (ours)



(a) GCN (b) GAT (c) DFNet (ours)