Agenda

- Spectral Graph for node embeddings
  - **Approximation theory** and spectral graph theory
  - **Chebyshev approximation and experiments**
    - Chevyshev fundamentals(link)
    - Chevyshev implementation (GCN v.s. GCN_cheby)
    - Parameters study by experiments
    - Other option: Lancsoz methods

Chebyshev methods

- The discussion here will mainly focus on two recent papers:
  - Defferrard et al. (**NIPS 2016**), Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering
    - **Contribution: First introduced Spectral Graph theory and Chebyshev approximation by CNN, GCN_cheby**
    - **10k nodes will burst the memory**
  - Kipf & Welling (**ICLR 2017**), Semi-Supervised Classification with Graph Convolutional Networks
    - **Contribution: Effectiveness and Efficiency Improvement GCN**
- Experimental results recap:
  - random walk + word2vec v.s. spectral graph (always better)
  - GCN(always better) v.s. GCN_cheby (**slow, and often crashes**)

What is Chebyshev Poly.

Definition 1.1 *The Chebyshev polynomial $T_n(x)$ of the first kind is a polynomial in x of degree n, defined by the relation*

$$T_n(x) = \cos n\theta \quad \text{when } x = \cos\theta.$$

Definition 1.2 *The Chebyshev polynomial $U_n(x)$ of the second kind is a polynomial of degree n in x defined by*

$$U_n(x) = \sin(n+1)\theta / \sin\theta \quad \text{when } x = \cos\theta. \tag{1.4}$$

Definition 1.3 *The Chebyshev polynomials $V_n(x)$ and $W_n(x)$ of the third and fourth kinds are polynomials of degree n in x defined respectively by*

$$V_n(x) = \cos(n+\tfrac{1}{2})\theta / \cos\tfrac{1}{2}\theta \tag{1.8}$$

and

$$W_n(x) = \sin(n+\tfrac{1}{2})\theta / \sin\tfrac{1}{2}\theta, \tag{1.9}$$

when $x = \cos\theta$.

★ $$\cos 0\theta = 1, \quad \cos 1\theta = \cos\theta, \quad \cos 2\theta = 2\cos^2\theta - 1,$$
$$\cos 3\theta = 4\cos^3\theta - 3\cos\theta, \quad \cos 4\theta = 8\cos^4\theta - 8\cos^2\theta + 1, \quad \ldots.$$

★ $$T_0(x) = 1, \quad T_1(x) = x, \quad T_2(x) = 2x^2 - 1,$$
$$T_3(x) = 4x^3 - 3x, \quad T_4(x) = 8x^4 - 8x^2 + 1, \quad \ldots.$$

★ $$T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x), \quad n = 2, 3, \ldots, \qquad \langle T_i\,, T_j \rangle = 0 \quad (i \neq j).$$

Application: minimax approximation of functions by polynomials.

Good $\|f - f^*\| \leq \epsilon$

Best $\|f - f_B^*\| \leq \|f - f^*\|$

Near-Best $\|f - f_N^*\| \leq (1+\rho)\,\|f - f_B^*\|$

Theorem 3.2 (Weierstrass's theorem) *For any given f in $C[a,b]$ and for any given $\epsilon > 0$, there exists a polynomial p_n for some sufficiently large n such that $\|f - p_n\|_\infty < \epsilon$.*

Theorem 3.3 *For any given p $(1 \leq p \leq \infty)$, there exists a unique best polynomial approximation p_n to any function $f \in \mathcal{L}_p[a,b]$ in the $\mathcal{L}_p$ norm, where $w(x)$ is taken to be unity in the case $p \to \infty$.*

How to use Chebyshev Poly.

Orthogonality(think about Fourier series)

Definition 4.1 *Two functions $f(x)$ and $g(x)$ in $\mathcal{L}_2[a,b]$ are said to be* orthogonal *on the interval $[a,b]$ with respect to a given continuous and non-negative weight function $w(x)$ if*

$$\int_a^b w(x)f(x)g(x)\,\mathrm{d}x = 0. \tag{4.1}$$

$$\langle f\,,\,g\rangle = \int_a^b w(x)f(x)g(x)\,\mathrm{d}x,$$

For the 1st kind of Chebyshev Ploy.

$$w(x) = \frac{1}{\sqrt{1-x^2}}$$

$$\begin{aligned}\langle T_i\,,\,T_j\rangle &= \int_{-1}^{1}\frac{T_i(x)T_j(x)}{\sqrt{1-x^2}}\,\mathrm{d}x\\ &= \int_0^\pi \cos i\theta\,\cos j\theta\,\mathrm{d}\theta\end{aligned}$$

Best approx. property

Corollary 4.1B *The best $\mathcal{L}_2$ polynomial approximation p_n^B of degree n to f may be expressed in terms of the orthogonal polynomial family $\{\phi_i\}$ in the form*

$$p_n^B = \sum_{i=0}^{n} c_i\phi_i,$$

where

$$c_i = \frac{\langle f\,,\,\phi_i\rangle}{\langle \phi_i\,,\,\phi_i\rangle}.$$

Example

EXAMPLE 4.1: To illustrate Corollary 4.1B, suppose that we wish to determine the best $\mathcal{L}_2$ linear approximation p_1^B to $f(x) = 1-x^2$ on $[-1,1]$, with respect to the weight $w(x) = (1-x^2)^{-\frac12}$. In this case $\{T_i(x)\}$ is the appropriate orthogonal system and hence

$$p_1^B = c_0T_0(x) + c_1T_1(x)$$

where, by (4.17),

$$\begin{aligned} c_0 &= \frac{\langle f\,,\,T_0\rangle}{\langle T_0\,,\,T_0\rangle} = \frac{\int_{-1}^{1}(1-x^2)^{-\frac12}(1-x^2)\,\mathrm{d}x}{\pi},\\ c_1 &= \frac{\langle f\,,\,T_0\rangle}{\cancel{\langle T_0\,,\,T_0\rangle}} = \frac{\int_{-1}^{1}(1-x^2)^{-\frac12}(1-x^2)x\,\mathrm{d}x}{\frac12\pi}.\end{aligned}$$

<T1,T1>

Substituting $x = \cos\theta$,

$$\begin{aligned} c_0 &= \frac{1}{\pi}\int_0^\pi \sin^2\theta\,\mathrm{d}\theta = \frac{1}{2\pi}\int_0^\pi (1-\cos 2\theta)\,\mathrm{d}\theta = \tfrac12,\\ c_1 &= \frac{2}{\pi}\int_0^\pi \sin^2\theta\,\cos\theta\,\mathrm{d}\theta = \frac{2}{\pi}\left[\tfrac13\sin^3\theta\right]_0^\pi = 0\end{aligned}$$

and therefore

$$p_1^B = \tfrac12 T_0(x) + 0\,T_1(x) = \tfrac12,$$

so that the linear approximation reduces to a constant in this case.

How to use Chebyshev Poly.

Best approx. of Chebyshev Poly.

$$f(x) \sim \sum_{i=0}^{\infty} c_i \phi_i(x)$$

$$c_i = \langle f\,,\,\phi_i \rangle / \langle \phi_i\,,\,\phi_i \rangle$$

$$\phi_i(x) = T_i(x),\ U_i(x),\ V_i(x) \text{ or } W_i(x)$$

$$f(x) \sim {\sum_{i=0}^{\infty}}' c_i T_i(x) = \tfrac{1}{2} c_0 T_0(x) + c_1 T_1(x) + c_2 T_2(x) + \cdots$$

where

$$c_i = \frac{2}{\pi} \int_{-1}^{1} (1-x^2)^{-\frac{1}{2}} f(x) T_i(x)\,\mathrm{d}x,$$

Theorem 3.1. Chebyshev series. *If f is Lipschitz continuous on $[-1,1]$, it has a unique representation as a Chebyshev series,*

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x), \tag{3.11}$$

which is absolutely and uniformly convergent, and the coefficients are given for $k \geq 1$ by the formula

$$a_k = \frac{2}{\pi} \int_{-1}^{1} \frac{f(x) T_k(x)}{\sqrt{1-x^2}} dx, \tag{3.12}$$

and for $k = 0$ by the same formula with the factor $2/\pi$ changed to $1/\pi$.

Error bound

Theorem 5.14 *If the function $f(x)$ has $m+1$ continuous derivatives on $[-1,1]$, then $\left|f(x) - S_n^T f(x)\right| = O(n^{-m})$ for all x in $[-1,1]$.*

Example

Example 5.1: Expansion of $f(x) = \sqrt{1-x^2}$.

Here

$$\begin{aligned}
\frac{\pi}{2} c_i &= \int_{-1}^{1} T_i(x)\,\mathrm{d}x = \int_0^{\pi} \cos i\theta \sin\theta\,\mathrm{d}\theta \\
&= \tfrac{1}{2} \int_0^{\pi} [\sin(i+1)\theta - \sin(i-1)\theta]\,\mathrm{d}\theta \\
&= \tfrac{1}{2} \left[\frac{\cos(i-1)\theta}{i-1} - \frac{\cos(i+1)\theta}{i+1} \right]_0^{\pi} \quad (i \geq 1) \\
&= \tfrac{1}{2} \left(\frac{(-1)^{i-1} - 1}{i-1} - \frac{(-1)^{i+1} - 1}{i+1} \right)
\end{aligned}$$

and thus

$$c_{2k} = -\frac{4}{\pi(4k^2-1)}, \quad c_{2k-1} = 0 \quad (k = 1, 2, \ldots).$$

Also

$$c_0 = 4/\pi.$$

Hence,

$$\begin{aligned}
\sqrt{1-x^2} &\sim -\frac{4}{\pi} {\sum_{k=0}^{\infty}}' \frac{T_{2k}(x)}{4k^2-1} \\
&= \frac{4}{\pi} \left(\tfrac{1}{2} T_0(x) - \tfrac{1}{3} T_2(x) - \tfrac{1}{15} T_4(x) - \tfrac{1}{35} T_6(x) - \cdots \right)
\end{aligned}$$

Chebyshev methods

- Defferrard et al. (**NIPS 2016**), Convolutional Neural Networks on Graphs with Fast Localized Spectral Filtering, GCN_cheby
- INPUT:
  - s: raw nodes features
  - L: graph Laplacian
- OUTPUT:
  - s': new embeddings of s

Chebyshev methods

2.2 Graph filters

In the classic setting, applying a filter to a signal is performed by convolution, which corresponds to point-wise multiplication in the spectral domain. Similarly, filtering a graph-signal is peformed by multiplication with a filter in the graph Fourier domain. A graph filter is defined by a continuous function $g : \mathbb{R}_+ \to \mathbb{R}$. To obtain its discrete coefficients, this function is evaluated at each eigenvalue: $g(\lambda_\ell)$ for $\ell = 0, \ldots, N-1$. The filtering operation then corresponds to $\hat{s}'(\ell) = g(\lambda_\ell) \cdot \hat{s}(\ell)$, where s' is the filtered signal. Equivalently, using matrix notation, we have

$s \in \mathbb{R}^n$ assigning a value to each vertex

$U = [u_0, \ldots, u_{n-1}] \in \mathbb{R}^{n \times n}$

graph Fourier transform $\hat{s} = U^* s \in \mathbb{R}^n$

$$s' = U g(\Lambda) U^* s, \qquad (1)$$

inverse $s = U\hat{s}$.

where $g(\Lambda)$ is the diagonal matrix containing the coefficients $g(\lambda_\ell)$ on the diagonal. In terms of matrix functions [11], the relation (1) can be compactly expressed as $s' = g(\mathcal{L})s$ with $g(\mathcal{L}) := U g(\Lambda) U^*$.

$g_\theta(\Lambda) = \mathrm{diag}(\theta) \quad \theta \in \mathbb{R}^n$

$g_\theta(\Lambda)\, \hat{s} = \theta \odot \hat{s}$

Chebyshev methods

$$g_{\theta'} \star s = s' = U g(\Lambda) U^* s$$

$\mathcal{O}(N^3)$

$$g_{\theta'}(\Lambda) \approx \sum_{k=0}^{K} \theta'_k T_k(\tilde{\Lambda})$$

$$(U \Lambda U^\top)^k = U \Lambda^k U^\top$$

$$g_{\theta'} \star s \approx \sum_{k=0}^{K} \theta'_k T_k(\tilde{L})$$

$$s' = U g(\Lambda) U^* s = \left(a_0 I + a_1 \mathcal{L} + \cdots + a_M \mathcal{L}^M\right) s$$

Chebyshev methods

- **GCN_cheby**
  - **calculate normalized graph Laplacian** $L = I_N - D^{-\frac{1}{2}} A D^{-\frac{1}{2}} = U \Lambda U^\top$
  - **calculate eigenvalues of normalized graph Laplacian (time consuming)**
  - **shift the normalized Laplacian to [-1,1]** $\tilde{L} = \frac{2}{\lambda_{\max}} L - I_N$
  - **apply Chebyshev polynomial** $g_{\theta'} \star x \approx \sum_{k=0}^{K} \theta'_k T_k(\tilde{L}) x$
- **GCN**
  - **calculate normalized graph Laplacian** $L = I_N - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$
  - **assume lambda_max=2, shift the L** $\tilde{L} = \quad L - I_N$
  - **apply Chebyshev polynomial** $g_{\theta'} \star x \approx \theta'_0 x + \theta'_1 \left(L - I_N\right) x = \theta'_0 x - \theta'_1 D^{-\frac{1}{2}} A D^{-\frac{1}{2}} x$
  - $\theta = \theta'_0 = -\theta'_1$ $\quad g_\theta \star x \approx \theta \left(I_N + D^{-\frac{1}{2}} A D^{-\frac{1}{2}} \right) x$

renormalization trick: $I_N + D^{-\frac{1}{2}} A D^{-\frac{1}{2}} \rightarrow \tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}}$

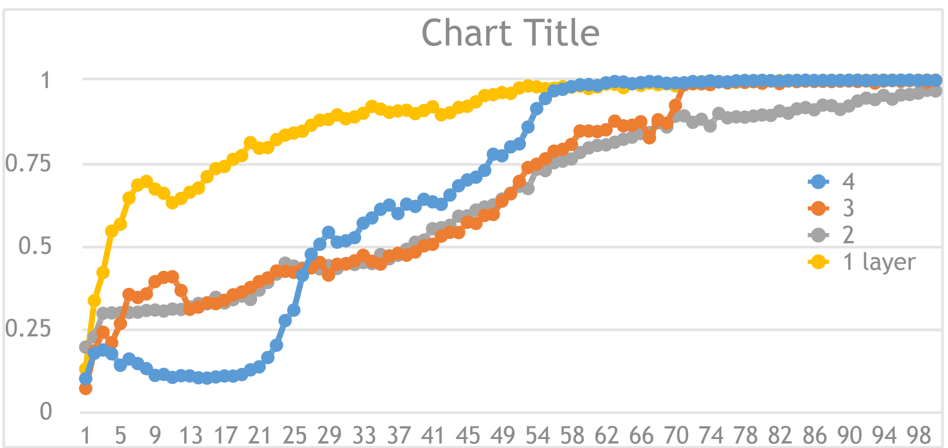
$\tilde{A} = A + I_N$ and $\tilde{D}_{ii} = \sum_j \tilde{A}_{ij}$

$g_\theta \star x \approx \theta \left(\tilde{D}^{-\frac{1}{2}} \tilde{A} \tilde{D}^{-\frac{1}{2}} \right) x$

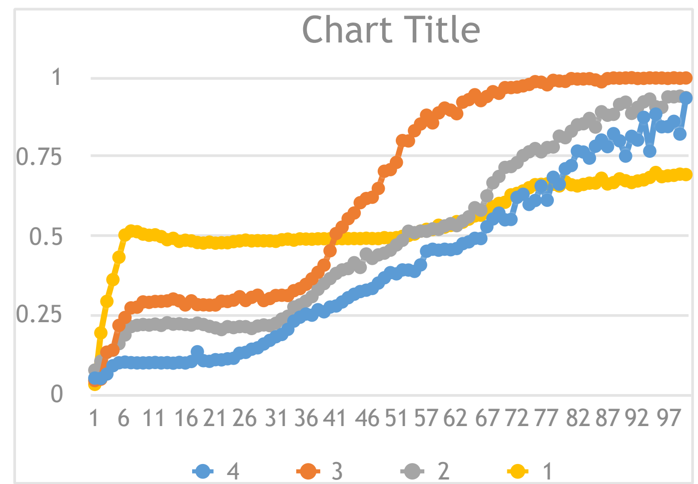
Chebyshev experiments

Performance under difference numbers of layers(GCN)

10k dp	1k feat	10class



20class



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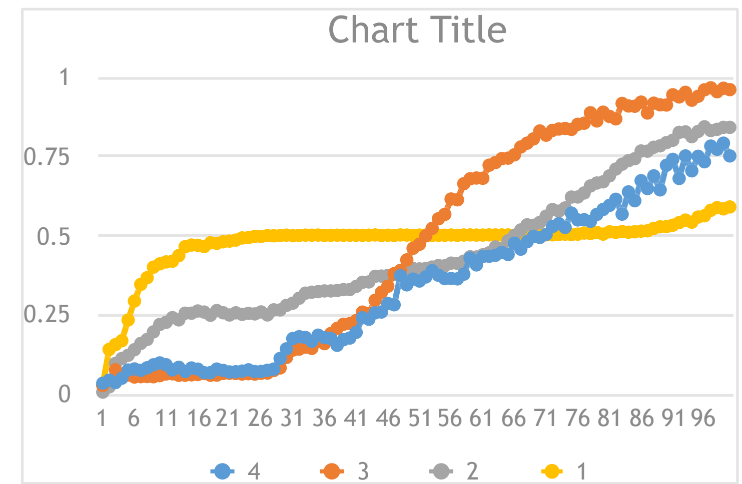
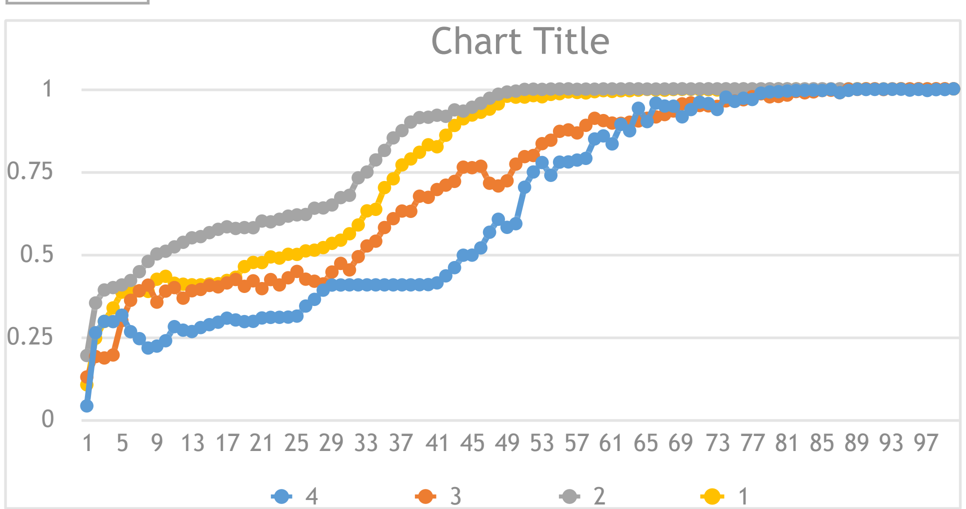
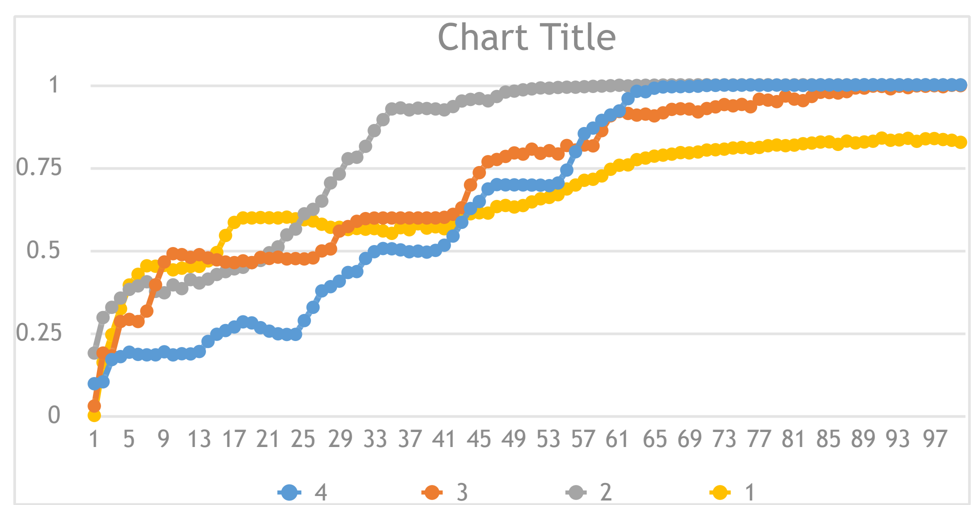


100feat



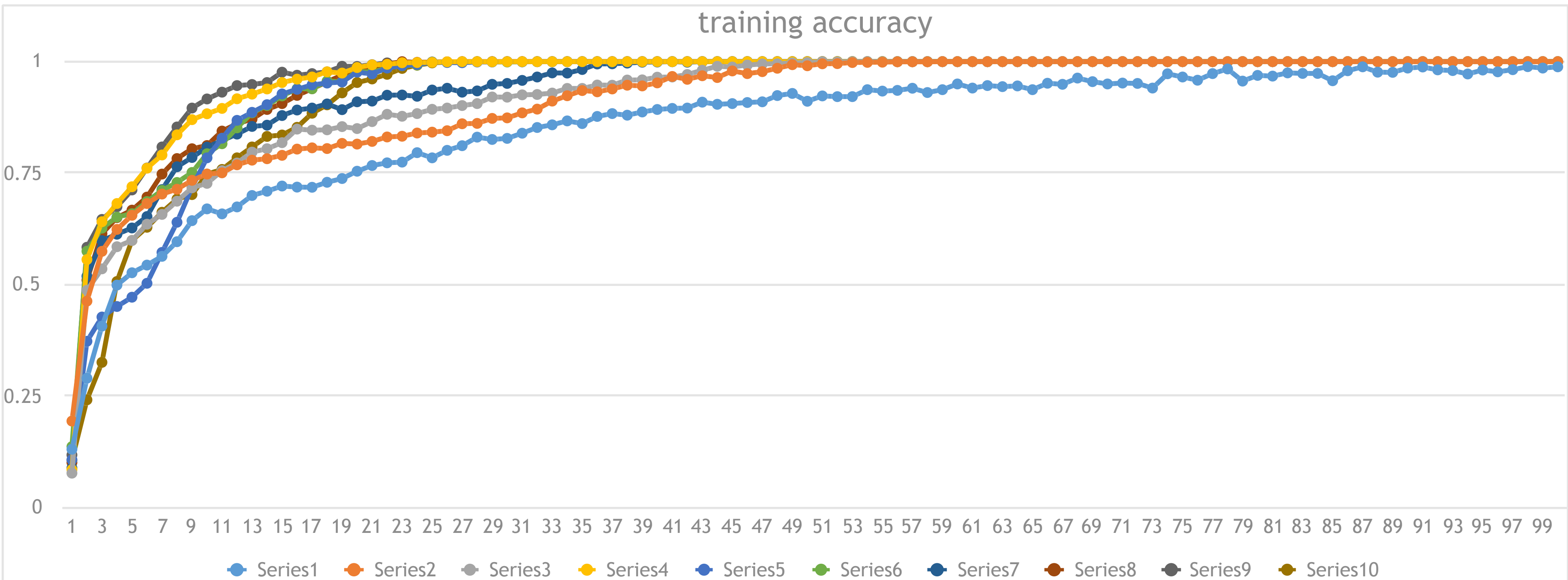
20k dp

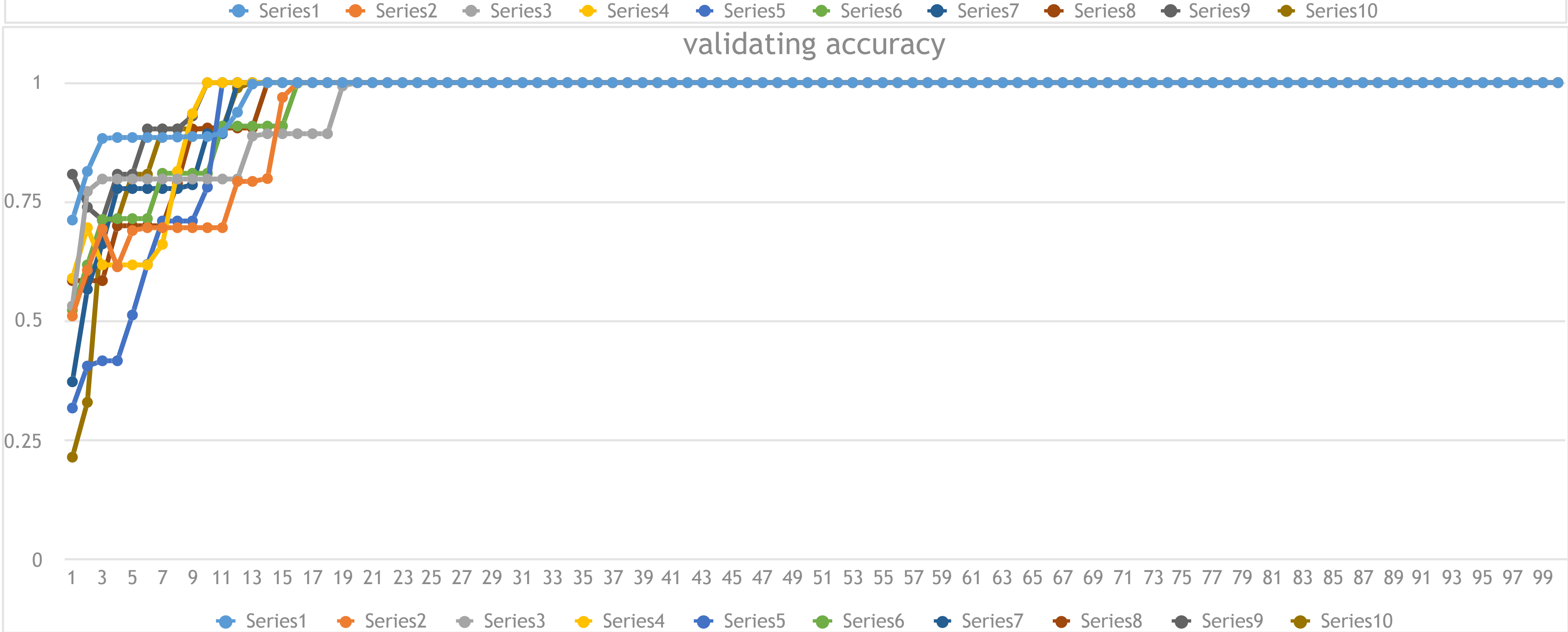


Chebyshev experiments

Performance under difference numbers of Chebyshev orders

5k dp	0.5k feat	10class

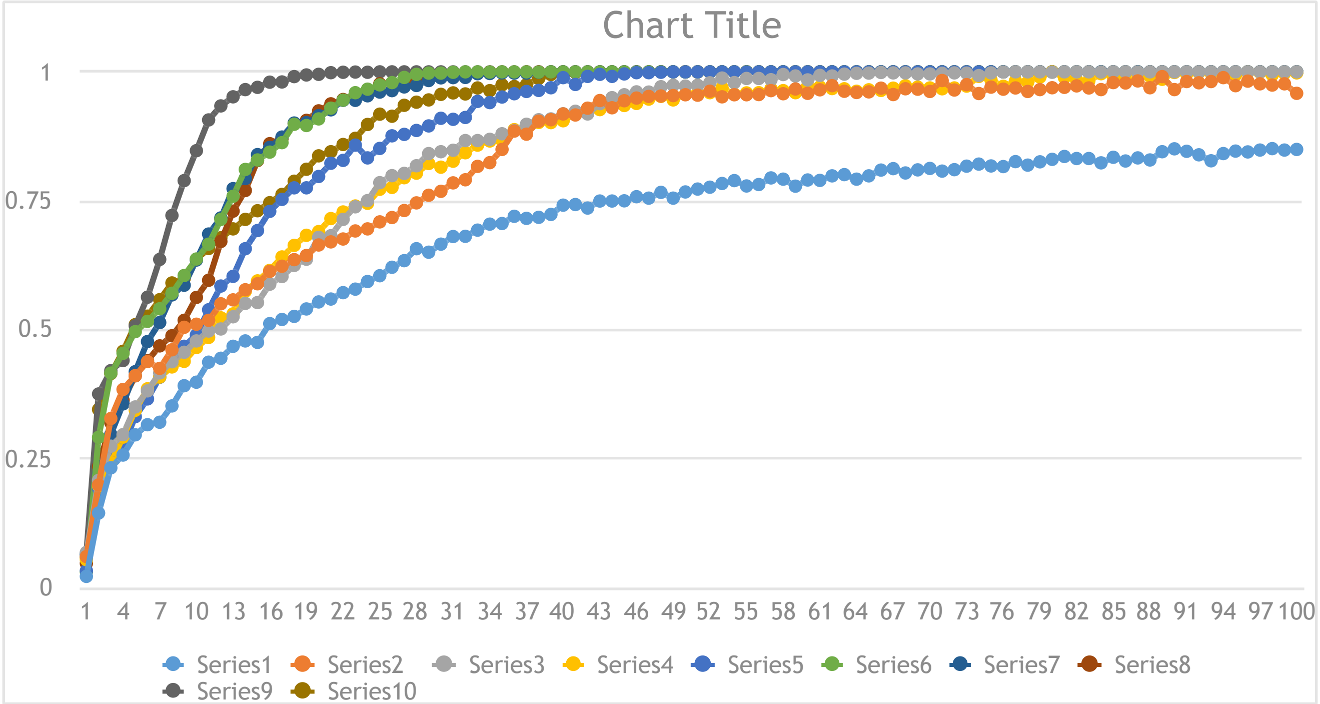




Chebyshev experiments

Performance under difference numbers of Chebyshev orders

20class



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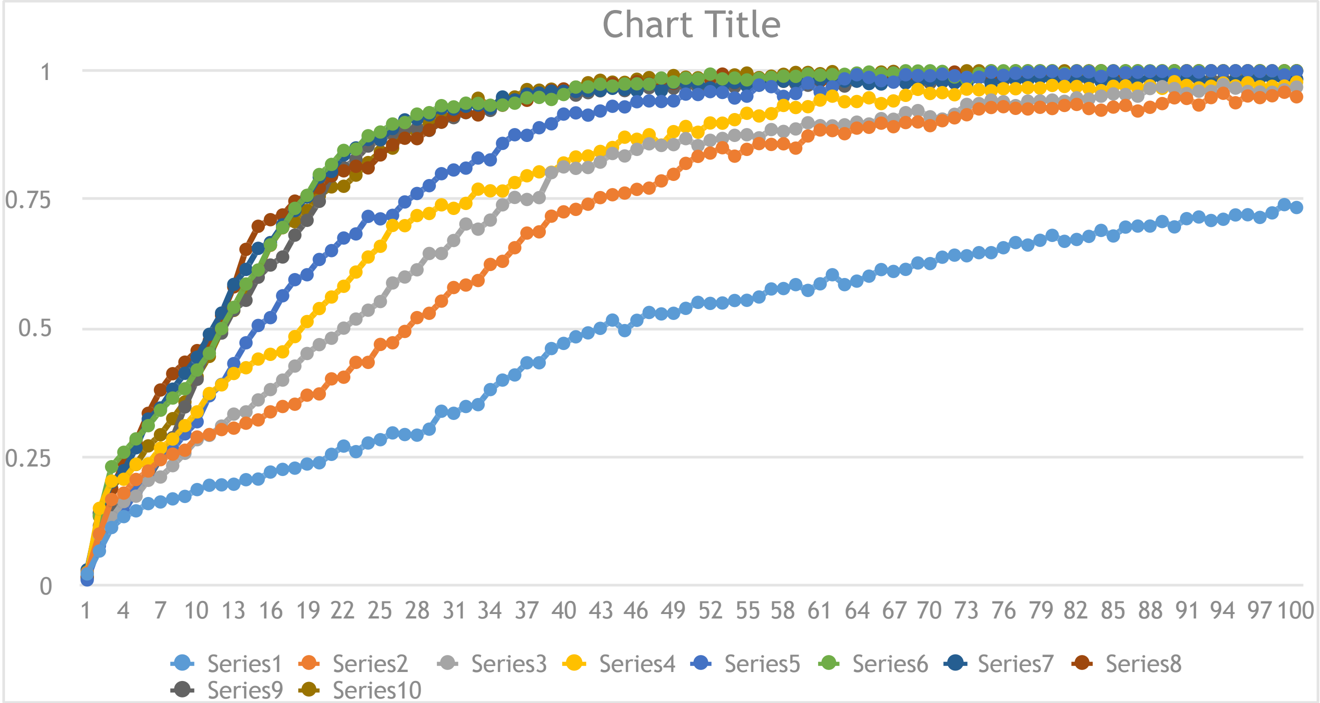
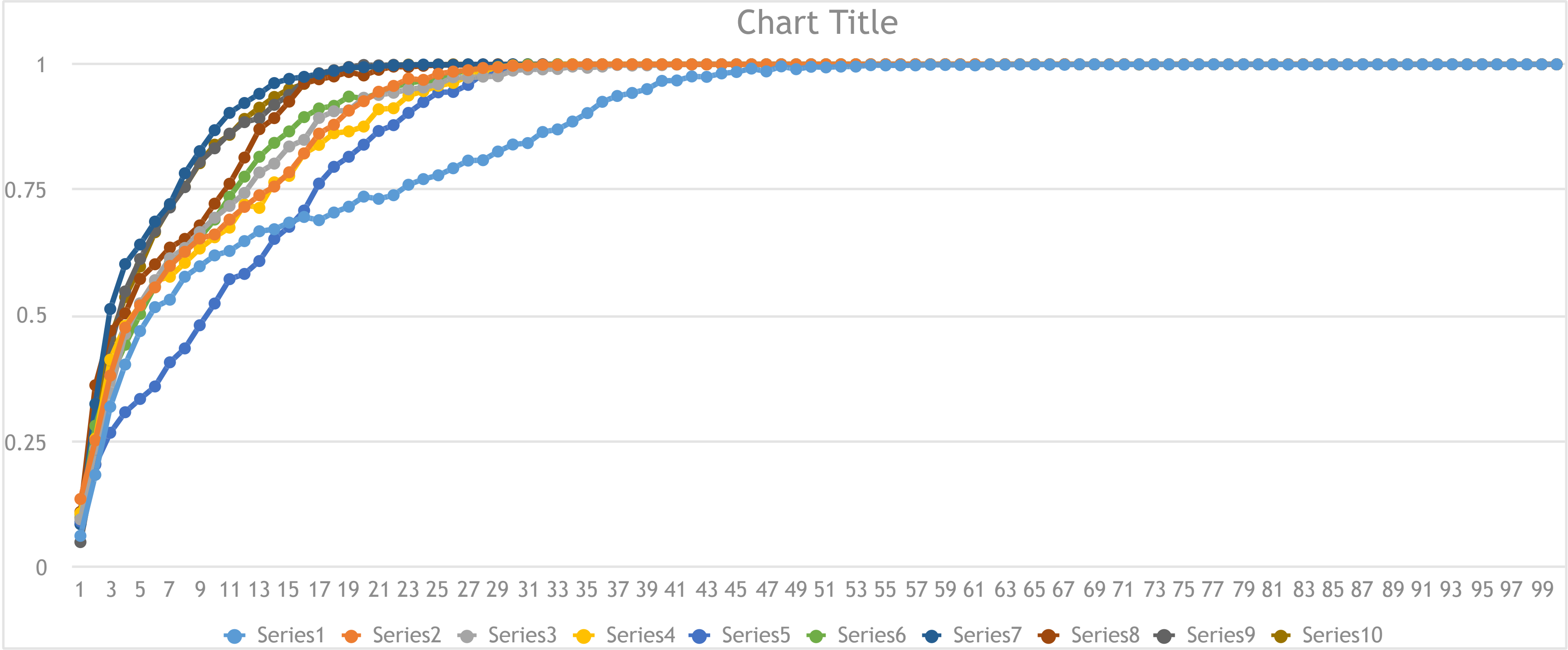


100feat



Any option for Chebyshev?

- 2nd, 3rd and 4th Chebyshev polynomials

Definition 1.2 *The Chebyshev polynomial $U_n(x)$ of the second kind is a polynomial of degree n in x defined by*

$$U_n(x) = \sin(n+1)\theta / \sin\theta \quad \text{when } x = \cos\theta. \tag{1.4}$$

Definition 1.3 *The Chebyshev polynomials $V_n(x)$ and $W_n(x)$ of the third and fourth kinds are polynomials of degree n in x defined respectively by*

$$V_n(x) = \cos(n+\tfrac{1}{2})\theta / \cos\tfrac{1}{2}\theta \tag{1.8}$$

and

$$W_n(x) = \sin(n+\tfrac{1}{2})\theta / \sin\tfrac{1}{2}\theta, \tag{1.9}$$

when $x = \cos\theta$.

- Fourier series equal to Chebyshev series when g is even

$$g(\theta) \sim \tfrac{1}{2}a_0 + \sum_{k=1}^{\infty}(a_k \cos k\theta + b_k \sin k\theta) \tag{5.41}$$

where

$$a_k = \frac{1}{\pi}\int_{-\pi}^{\pi} g(\theta)\cos k\theta \, d\theta, \quad b_k = \frac{1}{\pi}\int_{-\pi}^{\pi} g(\theta)\sin k\theta \, d\theta, \quad (k = 0, 1, 2, \ldots). \tag{5.42}$$

$\Rightarrow$

$$g(\theta) \sim {\sum_{k=0}^{\infty}}' a_k \cos k\theta$$

where

$$a_k = \frac{2}{\pi}\int_0^{\pi} g(\theta)\cos k\theta \, d\theta.$$

$\Rightarrow$

$$f(x) \sim {\sum_{k=0}^{\infty}}' a_k T_k(x)$$

where

$$a_k = \frac{2}{\pi}\int_{-1}^{1}(1-x^2)^{-\frac{1}{2}} f(x) T_k(x) \, dx.$$

- Lanczos method (mentioned in **GCN_cheby**):
  - Complexity comparison with GCN: $\mathcal{O}(K|\mathcal{E}|)$ v.s. $\mathcal{O}(M \cdot |\mathcal{E}|)$

Given a continuous function $g : [0, \lambda_{\max}] \to \mathbb{R}$ and a vector s, the following approximation to $g(\mathcal{L})s$ was proposed by Gallopoulos and Saad in [6]:

$$g(\mathcal{L})s \approx \|s\|_2 V_M g(H_M) e_1 := g_M, \tag{4}$$

  - Lanczos approximation can be expected to perform significantly better because of its ability to adapt to the eigenvalues of L. (This phenomenon is well-understood for Krylov subspace approximations to solutions of linear system.)

Susnjara, Ana, et al. "Accelerated filtering on graphs using lanczos method." *arXiv preprint arXiv:1509.04537* (2015).