Faster Local Solvers for Graph Diffusion Equations

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Background: Graph Diffusion Equations

Definition Given a propagation matrix $\boldsymbol{M}$ associated with an undirected graph $\mathcal{G}(\mathcal{V}, \mathcal{E})$, a general graph diffusion equation is defined as

$$\boldsymbol{f} \triangleq \sum_{k=0}^{\infty} c_k \boldsymbol{M}^k \boldsymbol{s},$$

where $\boldsymbol{f}$ is the diffusion vector of a source vector $\boldsymbol{s}$, and $c_k \geq 0$.

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Many graph learning tools can be represented as diffusion vectors. What's more, to compute $\boldsymbol{f}_{\text{PPR}}$ and $\boldsymbol{f}_{\text{KATZ}}$, it is equivalent to solving the linear system $\boldsymbol{Qx} = \boldsymbol{s}$.

Equ.	$\boldsymbol{M}$	c_k	$\boldsymbol{s}$
PPR	$\boldsymbol{AD}^{-1}$	$\alpha(1-\alpha)^k$	$\boldsymbol{e}_s$
Katz	$\boldsymbol{A}$	α^k	$\boldsymbol{e}_s$
HK	$\boldsymbol{AD}^{-1}$	$e^{-\tau}\tau^k/k!$	$\boldsymbol{e}_s$
IPR	$\boldsymbol{AD}^{-1}$	$\frac{\theta^k}{(\theta^k+\theta^{10})^2}$	$\boldsymbol{e}_s$
APPNP	$\boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{AD}^{-\frac{1}{2}}$	$\alpha(1-\alpha)^k$	$\boldsymbol{x}$

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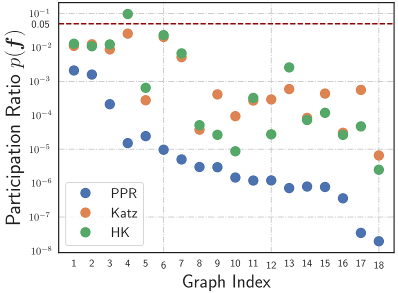
where $\boldsymbol{f}$ is the diffusion vector of a source vector $\boldsymbol{s}$, and $c_k \geq 0$.

A key property of $\boldsymbol{f}$ is the high localization of its entry magnitudes. We measure the localization by participation ratio $p(\boldsymbol{f}) = (\sum_{i=1}^{n} |f_i|^2)^2 / (n \sum_{i=1}^{n} |f_i|^4)$.



Faster Solvers via Local Diffusion Process

We propose a novel graph diffusion framework via a *local diffusion process* for efficiently approximating GDEs.

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The *local diffusion process* is defined as a process of updates $\{(\boldsymbol{x}^{(t)}, \boldsymbol{r}^{(t)}, \mathcal{S}_t)\}_{0 \le t \le T}$.

$$\left(\boldsymbol{x}^{(t+1)}, \boldsymbol{r}^{(t+1)}, \mathcal{S}_{t+1}\right) = \phi\left(\boldsymbol{x}^{(t)}, \boldsymbol{r}^{(t)}, \mathcal{S}_t; \boldsymbol{s}, \epsilon, \mathcal{G}, \mathcal{A}_\theta\right), \quad 0 \le t \le T.$$

We say this process *converges* when $\mathcal{S}_T = \emptyset$ if there exists such T; the generated sequence of active nodes are $\mathcal{S}_t$. The total number of operations of local solver $\mathcal{A}_\theta$ is

$$\mathcal{T}_{\mathcal{A}_\theta} = \sum_{t=0}^{T-1} \operatorname{vol}(\mathcal{S}_t) = T \cdot \overline{\operatorname{vol}}(\mathcal{S}_T).$$

Faster Solvers via Local Diffusion Process

The standard Gauss-Seidel iterative method with Successive Overrelaxation can be localized via *local diffusion process* as

$$\text{LocalSOR} : \boldsymbol{x}^{(t+t_{i+1})} = \boldsymbol{x}^{(t+t_i)} + \omega \cdot \tilde{\boldsymbol{e}}_{u_i}^{(t+t_i)}, \quad \boldsymbol{r}^{(t+t_{i+1})} = \boldsymbol{r}^{(t+t_i)} - \omega \cdot \boldsymbol{Q} \cdot \tilde{\boldsymbol{e}}_{u_i}^{(t+t_i)},$$

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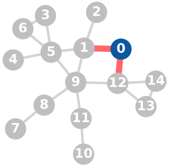
If we reformulate $\boldsymbol{Q}\boldsymbol{x} = \boldsymbol{s}$ as $\boldsymbol{x}_t^* = \arg\min_{\boldsymbol{x}\in\mathbb{R}^n} f(\boldsymbol{x}) \triangleq \frac{1}{2}\boldsymbol{x}^\top \boldsymbol{Q}\boldsymbol{x} - \boldsymbol{s}^\top \boldsymbol{x}$. The standard gradient descent and Chebyshev methods can be localized as the following

$$\text{LocalGD}: \qquad \boldsymbol{x}^{(t+1)} = \boldsymbol{x}^{(t)} + \boldsymbol{r}_{\mathcal{S}_t}^{(t)}, \qquad \boldsymbol{r}^{(t+1)} = \boldsymbol{r}^{(t)} - \boldsymbol{Q}\boldsymbol{r}_{\mathcal{S}_t}^{(t)},$$

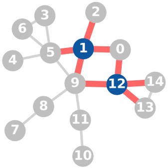
$$\text{LocalCH}: \boldsymbol{\pi}^{(t+1)} = \boldsymbol{\pi}^{(t)} + \frac{2\delta_{t+1}}{1-\alpha}\boldsymbol{D}^{1/2}\boldsymbol{r}_{\mathcal{S}_t}^{(t)} + \delta_{t:t+1}(\boldsymbol{\pi}^{(t)} - \boldsymbol{\pi}^{(t-1)})_{\mathcal{S}_t}, \delta_{t+1} = \left(\frac{2}{1-\alpha} - \delta_t\right)^{-1}$$

$$\boldsymbol{D}^{1/2}\boldsymbol{r}^{(t+1)} = \boldsymbol{D}^{1/2}\boldsymbol{r}^{(t)} - (\boldsymbol{\pi}^{(t+1)} - \boldsymbol{\pi}^{(t)}) + (1-\alpha)\boldsymbol{A}\boldsymbol{D}^{-1}(\boldsymbol{\pi}^{(t+1)} - \boldsymbol{\pi}^{(t)}).$$

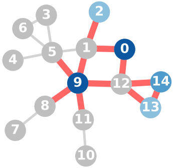
Local Diffusion Process



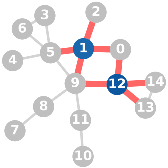
$\mathcal{S}_0 = \{0\}$



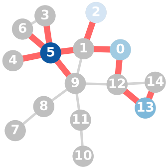
$\mathcal{S}_1 = \{1, 12\}$



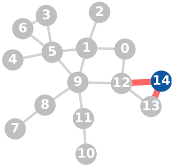
$\mathcal{S}_2 = \{0, 2, 9, 13, 14\}$



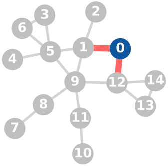
$\mathcal{S}_3 = \{1, 12\}$



$\mathcal{S}_4 = \{0, 2, 5, 13\}$



$\mathcal{S}_5 = \{14\}$



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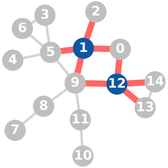
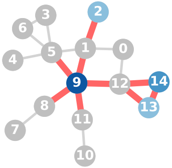


$\mathcal{S}_1 = \{0, 1, 12\}$



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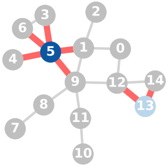

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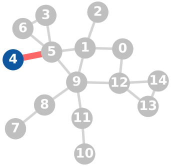

$\mathcal{S}_4 = \{4, 12\}$

Properties of LocalSOR

Let $\boldsymbol{Q} \triangleq \boldsymbol{I} - \beta \boldsymbol{P}$ where $P_{uv} \neq 0$ if $(u, v) \in \mathcal{E}$; 0 otherwise, and $\boldsymbol{P} \geq \boldsymbol{0}_{n \times n}$. Define maximal value $P_{\max} = \max_{u \in \mathcal{V}} \|\boldsymbol{P}\boldsymbol{e}_u\|_1$. Assume that $\boldsymbol{r}^{(0)} \geq \boldsymbol{0}$ is nonnegative and $P_{\max}$, β are such that $\beta P_{\max} < 1$, then the local diffusion process via LocalSOR with $\omega \in (0, 1)$ has the following properties

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If the local diffusion process converges (i.e., $\mathcal{S}_T = \emptyset$), then T is bounded by

$$T \leq \frac{1}{\omega \overline{\gamma}_T (1 - \beta P_{\max})} \ln \frac{\|\boldsymbol{r}^{(0)}\|_1}{\|\boldsymbol{r}^{(T)}\|_1}, \text{ where } \overline{\gamma}_T \triangleq \frac{1}{T} \sum_{t=0}^{T-1} \left\{ \gamma_t \triangleq \frac{\sum_{i=1}^{|\mathcal{S}_t|} r_{u_i}^{(t+t_i)}}{\|\boldsymbol{r}^{(t)}\|_1} \right\}.$$

Properties of LocalSOR

- For $\alpha \in (0,1), \omega = 1$, the run time of LocalSOR for solving PPR with the stop condition $\|\boldsymbol{D}^{-1}\boldsymbol{r}^{(T)}\|_\infty \leq \alpha\epsilon$ and initials $\boldsymbol{x}^{(0)} = \boldsymbol{0}$, $\boldsymbol{r}^{(0)} = \alpha\boldsymbol{e}_s$ is bounded as

$$\mathcal{T}_{\text{LocalSOR, PPR}} \leq \min\left\{\frac{1}{\epsilon\alpha}, \frac{\overline{\text{vol}}(\mathcal{S}_T)}{\alpha\bar{\gamma}_T} \ln\frac{C_{\text{PPR}}}{\epsilon}\right\}, \qquad \text{where } \frac{\overline{\text{vol}}(\mathcal{S}_T)}{\bar{\gamma}_T} \leq \frac{1}{\epsilon}.$$

  The estimate $\boldsymbol{x}^{(T)}$ satisfies $\|\boldsymbol{D}^{-1}(\boldsymbol{x}^{(T)} - \boldsymbol{f}_{\text{PPR}})\|_\infty \leq \epsilon$.

- For $\alpha \in (0, 1/d_{\max}), \omega = 1$, the run time of LocalSOR for solving Katz with the stop condition $\|\boldsymbol{D}^{-1}\boldsymbol{r}^{(T)}\|_\infty \leq \epsilon$ and $\boldsymbol{x}^{(0)} = \boldsymbol{0}$ and $\boldsymbol{r}^{(0)} = \boldsymbol{e}_s$ is bounded as

$$\mathcal{T}_{\text{LocalSOR, Katz}} \leq \min\left\{\frac{1}{\epsilon(1-\alpha d_{\max})}, \frac{\overline{\text{vol}}(\mathcal{S}_T)}{(1-\alpha d_{\max})\bar{\gamma}_T} \ln\frac{C_{\text{Katz}}}{\epsilon}\right\}, \text{ where } \frac{\overline{\text{vol}}(\mathcal{S}_T)}{\bar{\gamma}_T} \leq \frac{1}{\epsilon}.$$

  The estimate $\hat{\boldsymbol{f}}_{\text{Katz}} = \boldsymbol{x}^{(T)} - \boldsymbol{e}_s$ satisfies $\|\hat{\boldsymbol{f}}_{\text{Katz}} - \boldsymbol{f}_{\text{Katz}}\|_2 \leq \|(\boldsymbol{I} - \alpha\boldsymbol{A})^{-1}\boldsymbol{D}\|_1 \cdot \epsilon$.

Applications

Our accelerated local solvers are ready for many applications such as

- Solve GDEs with discrete-time dynamic graph.
- Accelerate the message propagation in GNN networks.

Alg 1 InstantGNN(LocalGS) $(\mathcal{G}, \boldsymbol{p}, \boldsymbol{r}, \epsilon, \alpha, s, \beta)$

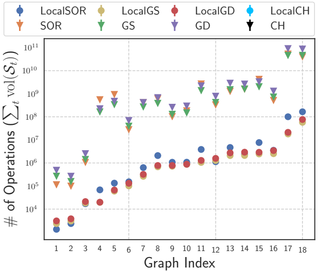
1: **while** $\max_u |r[u]| \geq \epsilon d_{\text{out}}^{1-\beta}[u]$ **do**
2: $\quad$ Push(u)
3: **return** $(\boldsymbol{p}, \boldsymbol{r})$

4: **procedure** Push(u):
5: $\quad p[u] \leftarrow p[u] + \alpha \cdot r[u]$
6: $\quad r[u] \leftarrow 0$
7: $\quad$ **for** v in $\mathcal{N}_{\text{out}}(u)$ **do**
8: $\quad\quad r_s[v] \leftarrow r[v] + \frac{(1-\alpha)\cdot r[u]}{d_{\text{out}}^{1-\beta}[u] d_{\text{out}}^{\beta}[v]}$

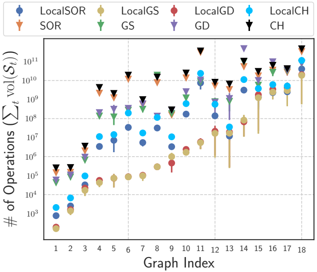
Alg 2 InstantGNN(LocalSOR)$(\mathcal{G}, \boldsymbol{p}, \boldsymbol{r}, \epsilon, \alpha, s, \beta, \omega)$

1: **while** $\max_u |r[u]| \geq \epsilon d_{\text{out}}^{1-\beta}[u]$ **do**
2: $\quad$ Push(u)
3: **return** $(\boldsymbol{p}, \boldsymbol{r})$

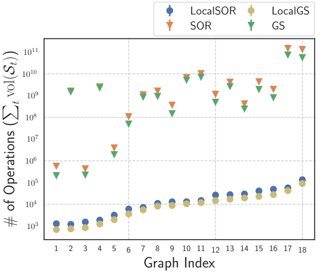
4: **procedure** Push(u):
5: $\quad p[u] \leftarrow p[u] + \alpha \cdot \omega \cdot r[u]$
6: $\quad r[u] \leftarrow r[u] - \omega \cdot r[u]$
7: $\quad$ **for** v in $\mathcal{N}_{\text{out}}(u)$ **do**
8: $\quad\quad r[v] \leftarrow r[v] + \omega \cdot \frac{(1-\alpha)\cdot r[u]}{d_{\text{out}}^{1-\beta}[u] d_{\text{out}}^{\beta}[v]}$



PPR($\alpha = 0.1, \epsilon = \frac{1}{n}$)



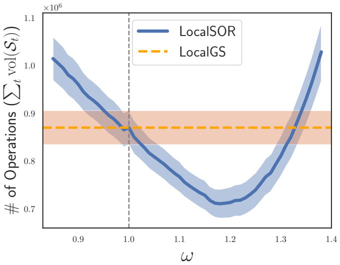
Katz($\alpha = \frac{1}{1+\|\boldsymbol{A}\|_2}, \epsilon = \frac{1}{m}$)

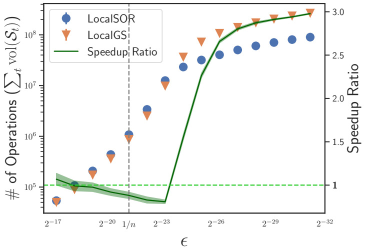


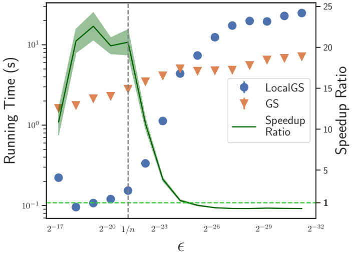
HK($\tau = 10, \epsilon = \frac{1}{\sqrt{n}}$)

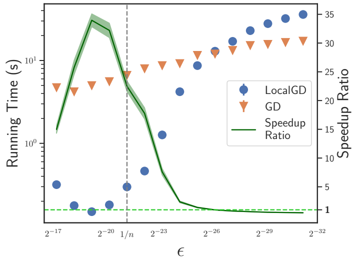
All local methods significantly speed up their global counterparts on all datasets.

Experiments









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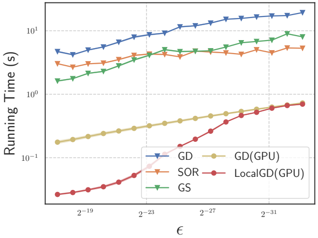

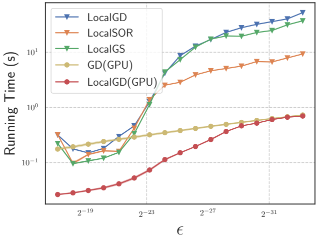

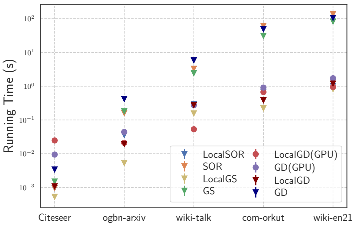

LocalGD (GPU) can be much faster than GD (GPU) and other methods based on CPUs.

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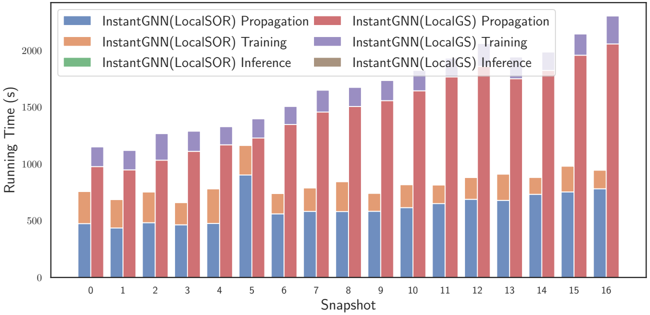

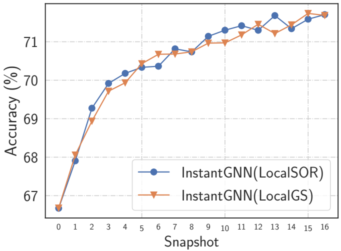

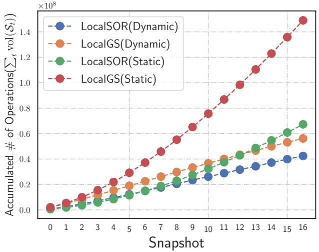

Thanks!

- Our code is publicly available at `https://github.com/JiaheBai/Faster-Local-Solver-for-GDEs`.
- If you have any questions, contact us:
  Jiahe Bai, jhbai20@fudan.edu.cn;
  Baojian Zhou, bjzhou@fudan.edu.cn.