ramBLe: A Parallel Framework for Constraint-Based Bayesian Network Learning via Markov Blanket Discovery

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Motivation

- Machine Learning (ML) models are being used for decision-making in a diverse set of fields – spam detection, recommender systems, etc.
    - “Black box” models are typically used for the purpose

Image Source: *XKCD – Machine Learning*
https://xkcd.com/1838/

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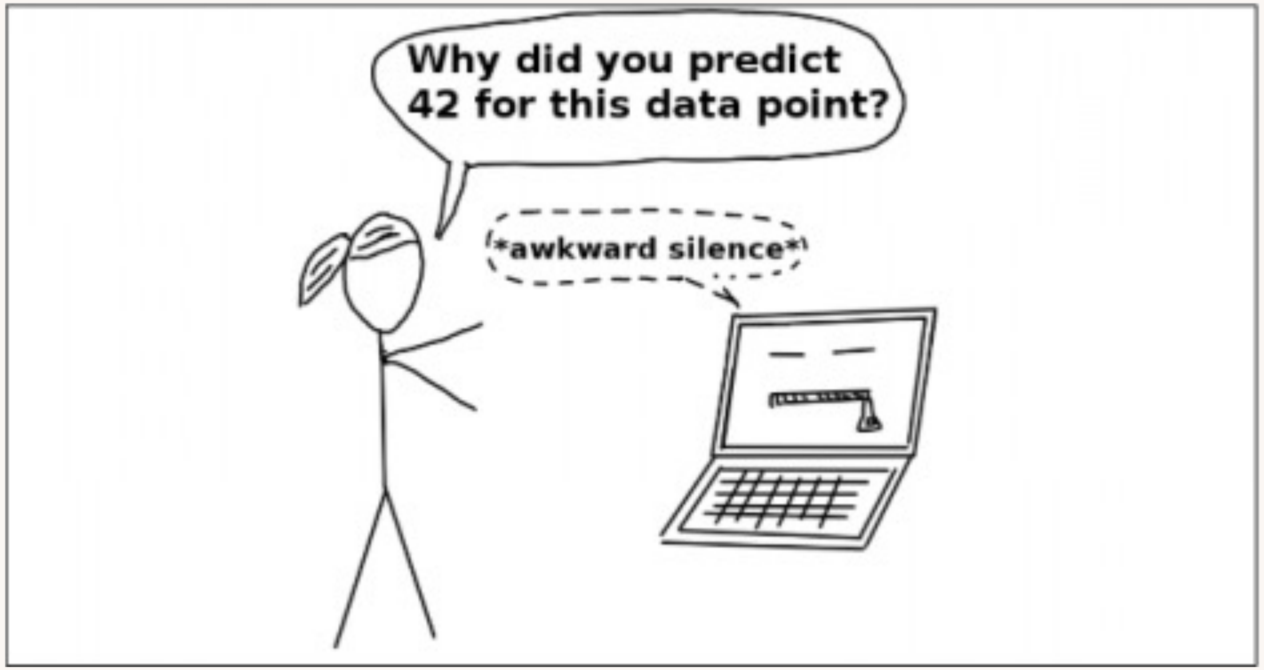

Image Source: *Interpretable Machine Learning — Fairness, Accountability, and Transparency in ML systems*
https://medium.com/@ODSC/interpretable-machine-learning-fairness-accountability-and-transparency-in-ml-systems-3ab45d961fbc

Motivation

- Machine Learning (ML) models are being used for decision-making in a diverse set of fields – spam detection, recommender systems, etc.
  - “Black box” models are typically used for the purpose – NOT interpretable
- Increasingly, ML is being used in high human-impact areas, e.g., criminal justice, healthcare, law enforcement, etc.
  - Apprehensions regarding use of black box models in these areas is growing


The New York Times

Opinion

OP-ED CONTRIBUTOR

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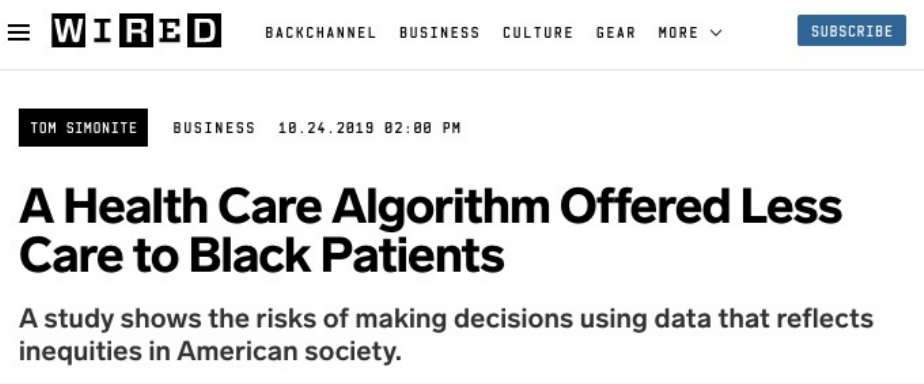
By Rebecca Wexler

June 13, 2017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- Machine Learning (ML) models are being used for decision-making in a diverse set of fields – spam detection, recommender systems, etc.
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- Increasingly, ML is being used in high human-impact areas, e.g., criminal justice, healthcare, law enforcement, etc.
  - Interpretable ML models are the need of the hour

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BY JEREMY KAHN

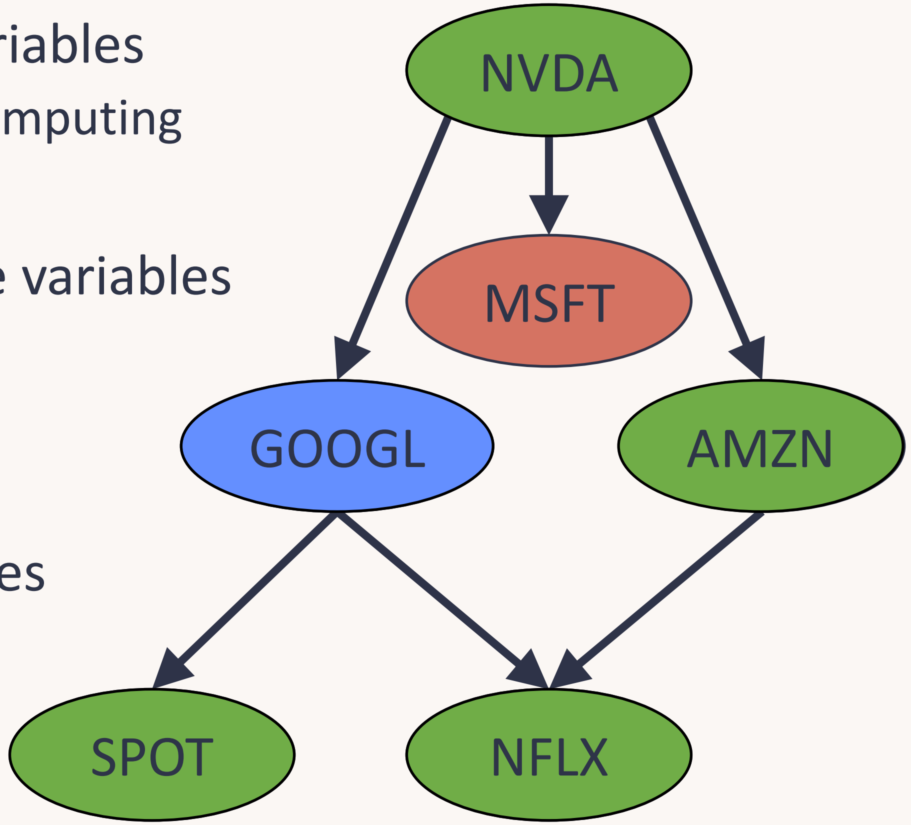
April 21, 2021 7:48 AM EDT

Motivation

- **Bayesian networks** (**BNs**) enable probabilistic reasoning about links between the variables of interest – interpretable decisions
    - Used for medical diagnosis, legal reasoning, epidemiology, etc.
- Learning structure of BNs is compute-intensive – needs parallelism
- Existing libraries for learning BNs support limited or no parallelism
    - e.g., *bnlearn*, *pcalg*, *Tetrad*
- Parallelization strategies have been proposed for various BN learning algorithms – difficult to integrate disparate strategies
    - Parallel library with support for multiple algorithms is desirable

Background – Bayesian Networks

- BN structure represents dependence graph of a set of variables
  - Case study – Stock prices of companies related to cloud computing
- **Parents and Children (PC)** set of a variable consists of the variables that are dependent on it, given any conditioning set
  - e.g., $PC(\text{GOOGL}) = \{\text{NVDA, SPOT, NFLX}\}$
- **Markov blanket (MB)** of a variable consists of the variables that render the variable independent of other variables
  - Assuming *faithfulness*
    $MB(X) = PC(X) \cup (Parents(Y)\ \forall Y \in Children(X))$
    $\Rightarrow MB(\text{GOOGL}) = \{\text{NVDA, SPOT, NFLX, AMZN}\}$



Blanket Learning Algorithms

- ***Constraint-based*** algorithms learn BN by conducting repeated CI tests using given data set of m observations for the n variables
  - Statistical tests, e.g., G^2 test for discrete data

- ***Blanket learning*** algorithms are *constraint-based* algorithms that first learn MB sets of all the variables separately to get the BN structure
  - *Grow-Shrink* (***GS***) (Margaritis and Thrun, 2000)
  - *Incremental Association MB* (***IAMB***) (Tsamardinos et al., 2003)
  - *Interleaved IAMB* (***Inter-IAMB***) (Tsamardinos et al., 2003)

Blanket Learning Algorithms

- Use variations of the *Grow-Shrink* scheme for learning MB sets
  - *Grow* phase: Add variables to candidate MB sets
  - *Shrink* phase: Remove false positive variables from candidate MB sets
- Differ in the specifics of how the scheme is iterated
  - Choosing variables to be added in *Grow* phase
    - *IAMB* and *Inter-IAMB* pick the “most dependent” variable given the current candidate MB set
    - *GS* picks the first dependent variable
  - Order of *Grow* and *Shrink* phases
    - *GS* and *IAMB* execute multiple iterations of *Grow* phase followed by one *Shrink* phase
    - *Inter-IAMB* interleaves the execution of *Grow* and *Shrink* phases in every iteration
- Perform *symmetry correction* for MB sets ($X \in MB(T) \Leftrightarrow T \in MB(X)$)
- Learn *PC from MB* sets (PC ⊆ MB)

Related Works

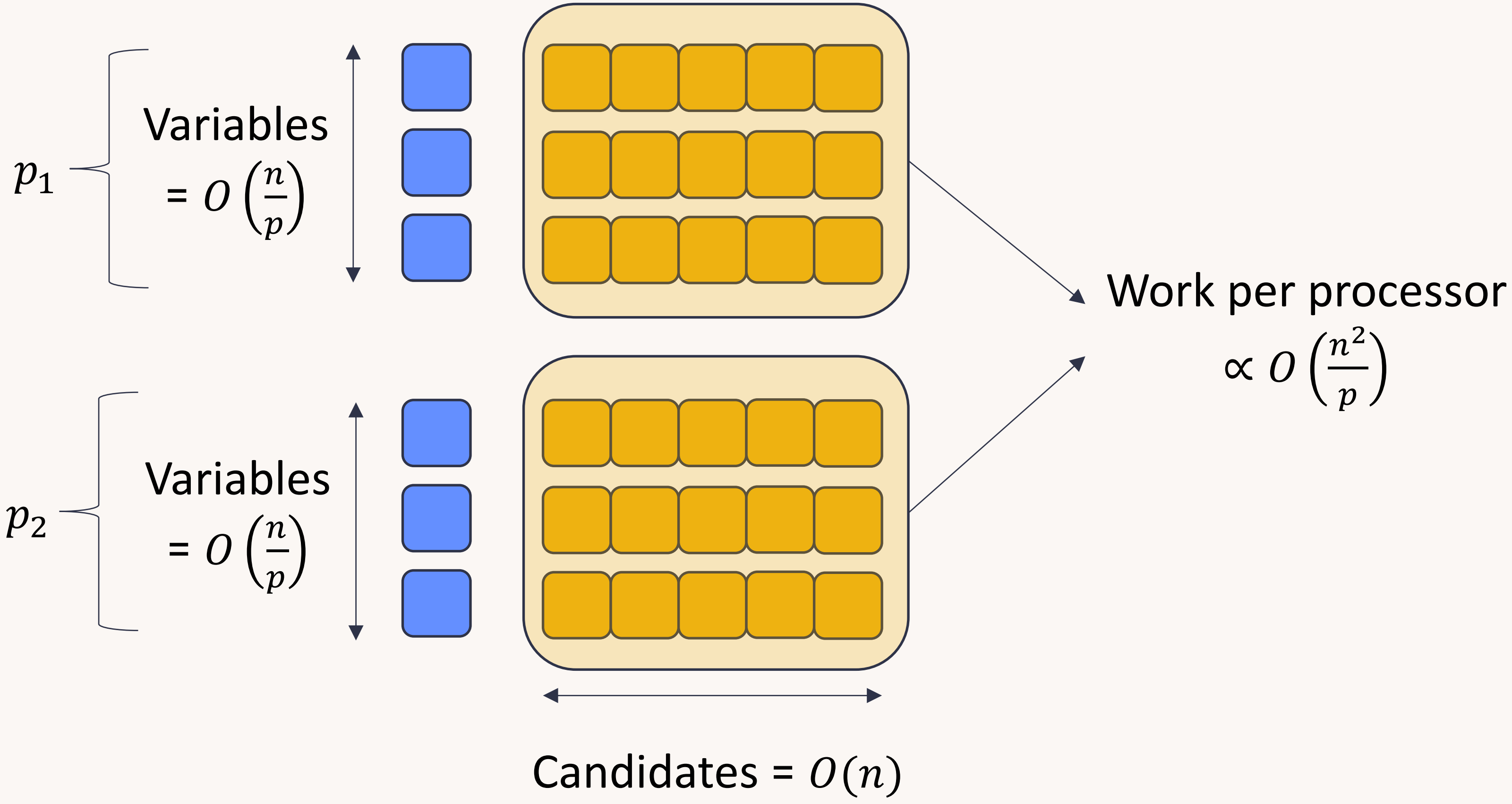
- Nikolova et al. (2011) parallelized two similar *constraint-based* algorithms: *MMPC* (Tsamardinos et al., 2006) and *GetPC* (Peña et al., 2007)
  - Scales well up to 512 cores for learning neighborhoods of 1,000 variables
  - Scaling tapers off as the number of cores or variables are increased

- *bnlearn* contains implementations of the three algorithms
  - Scutari et al. (2017) added support for parallelizing the implementations using a master-worker paradigm for small-scale parallelism

- Both these approaches distribute learning of variable neighborhoods

Parallel Framework – Key Design Ideas

- Distribute learning across processors – how?
  - Previous approaches have distributed learning neighborhoods of variables

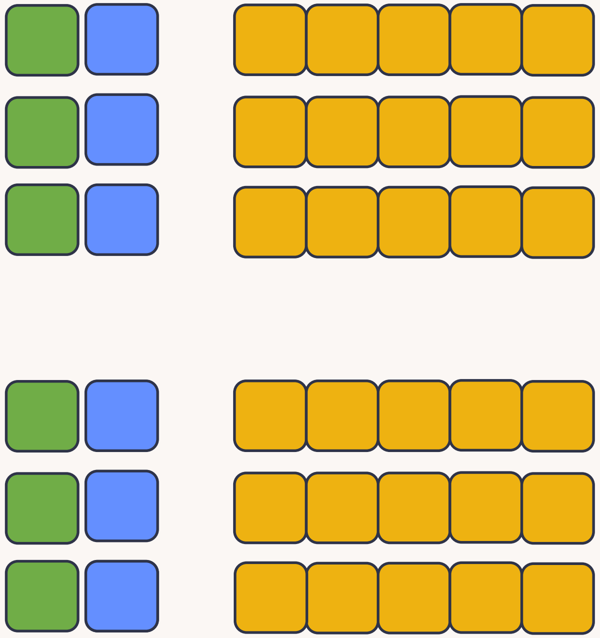


Parallel Framework – Key Design Ideas

- Distribute learning across processors – how?
  - Previous approaches have distributed learning neighborhoods of variables

p_1

p_2



Selected Candidate Variables

Iteration 1

Parallel Framework – Key Design Ideas

- Distribute learning across processors – how?
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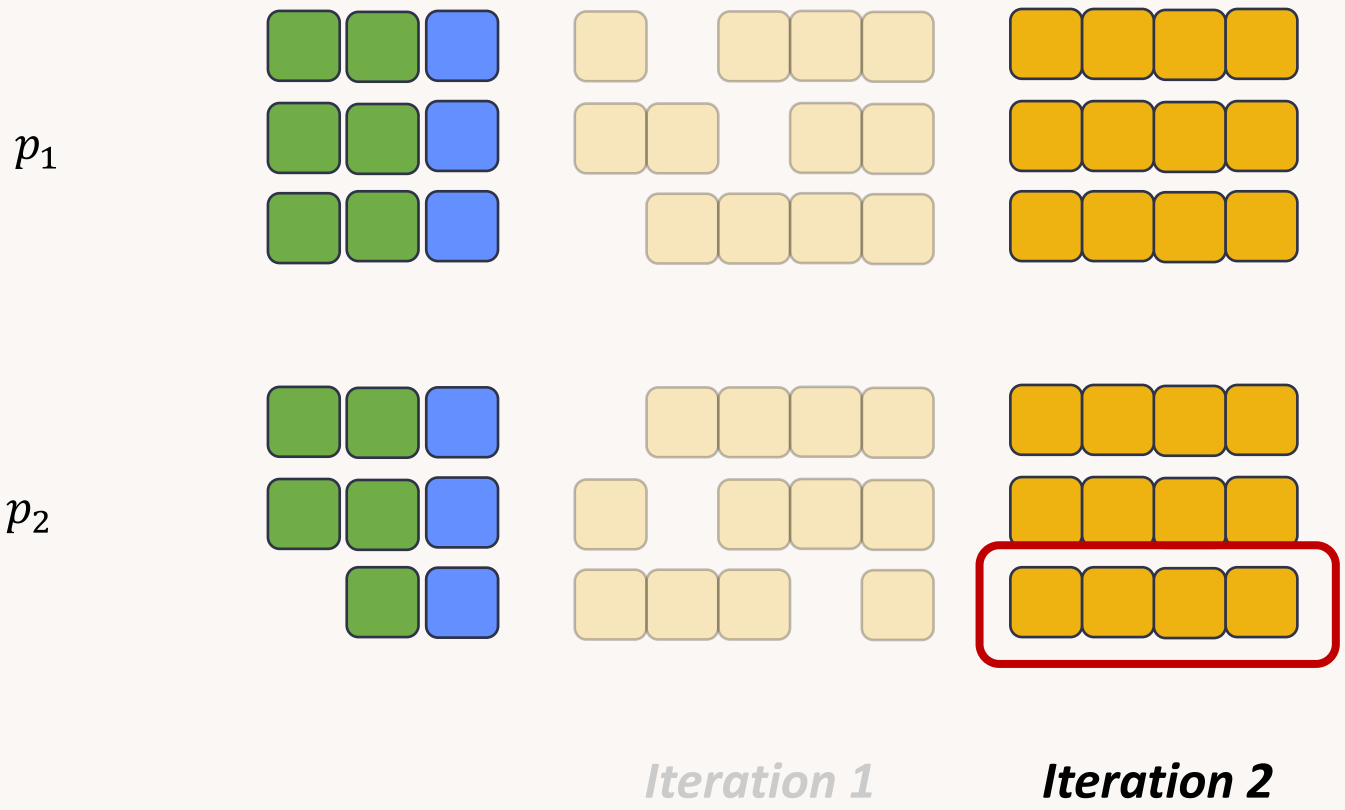

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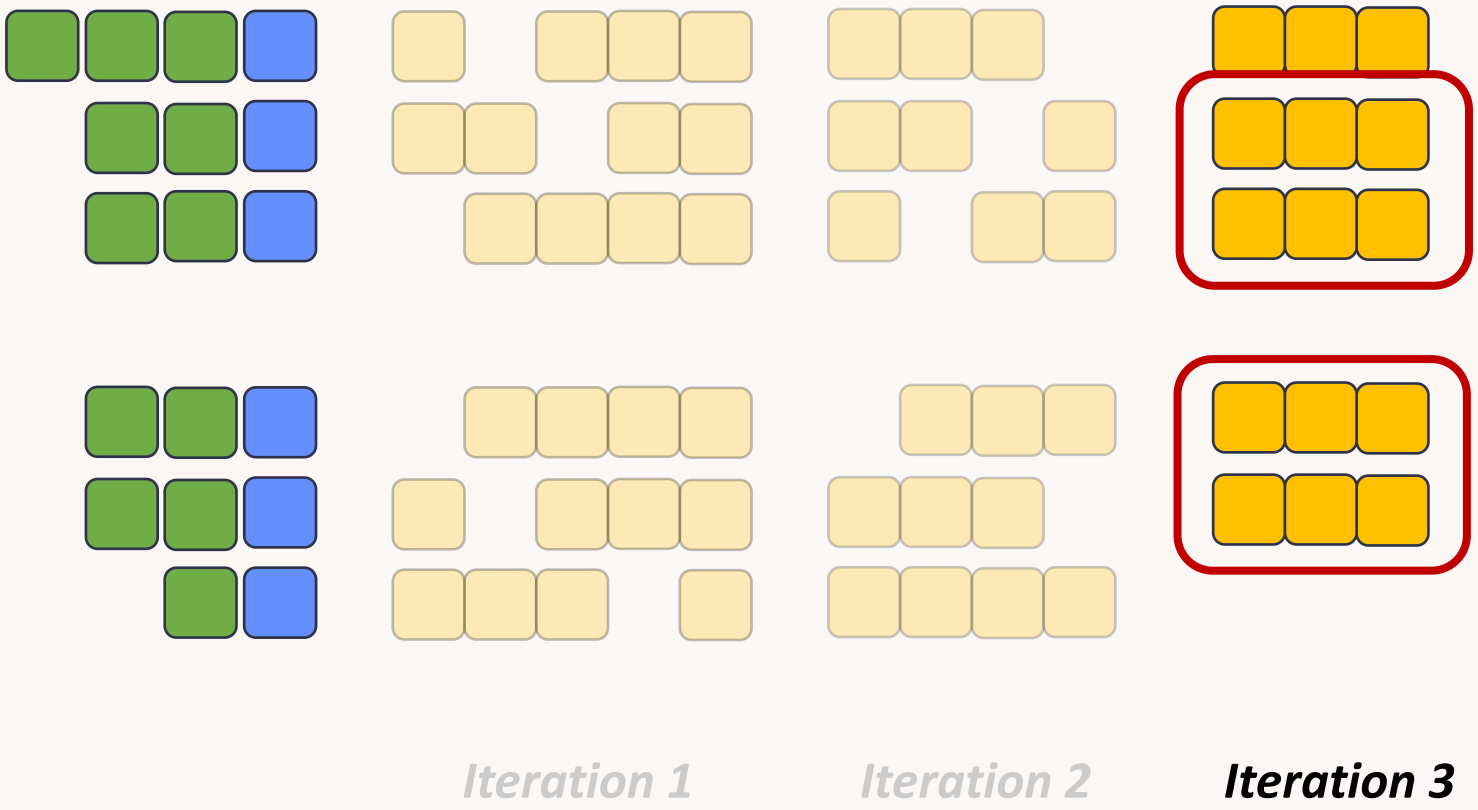

Load Imbalance

Unclear how to fix

Parallel Framework – Key Design Ideas

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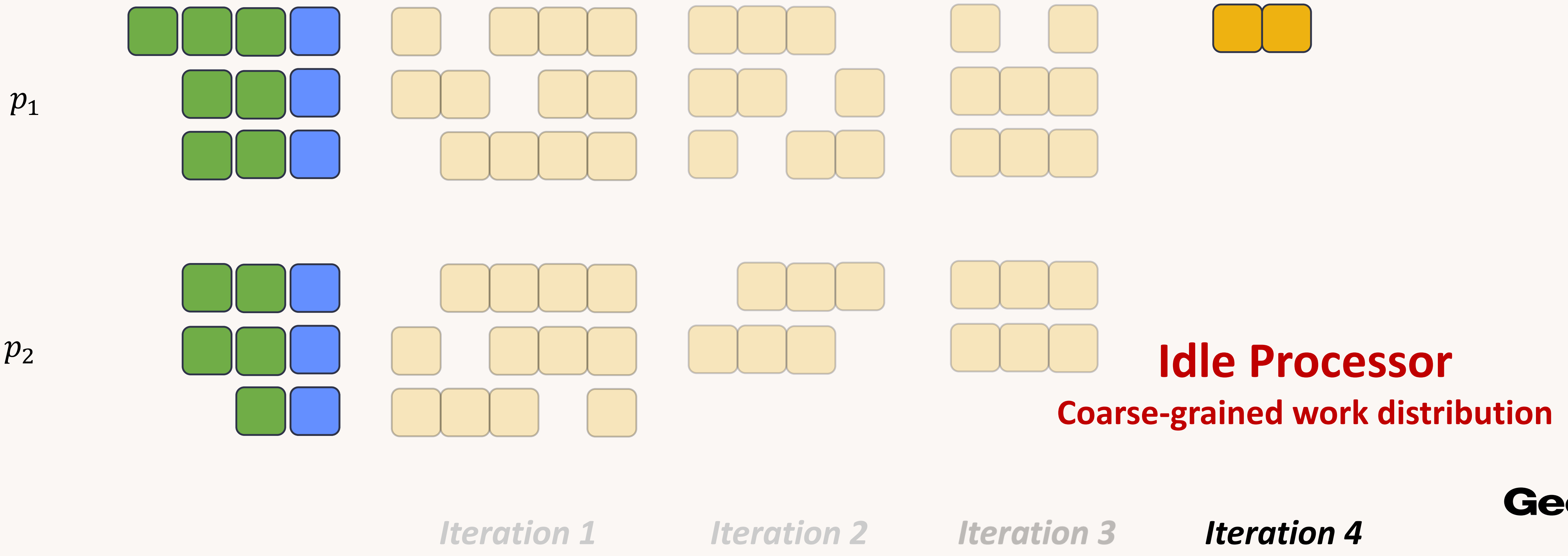


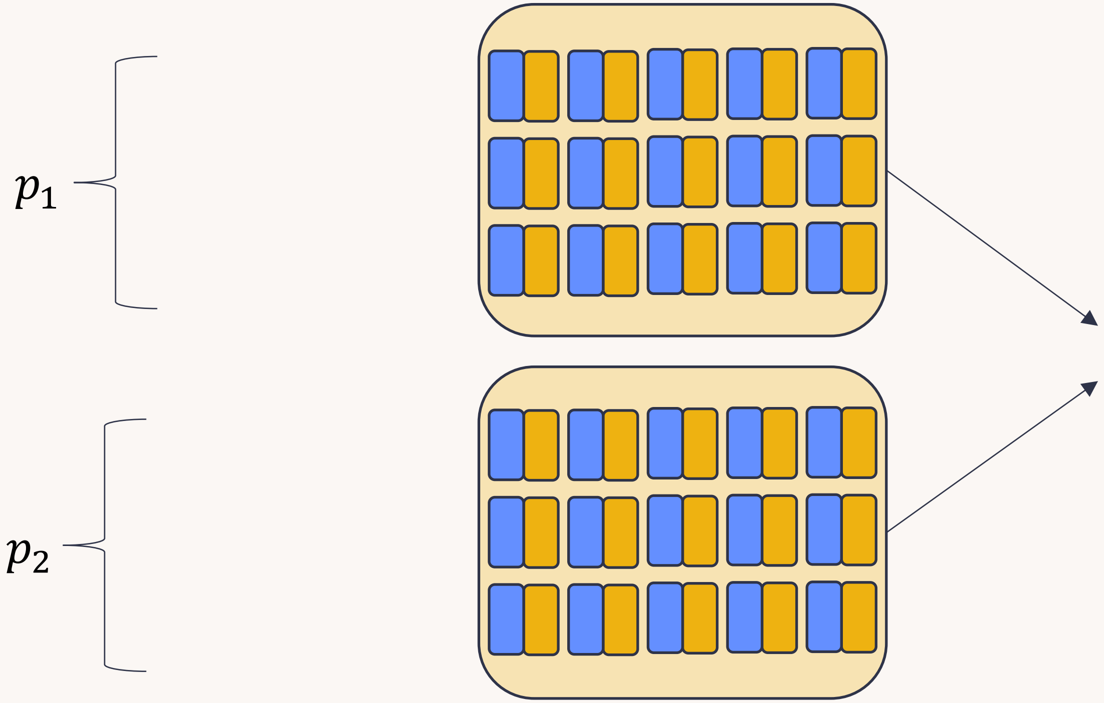
Parallel Framework – Key Design Ideas

- Distribute learning across processors – how?
  - Previous approaches have distributed learning neighborhoods of variables

- ***Observation***: **Variables have different neighborhood sizes – distributing variables to processors is suboptimal**
- ***Idea***: ***Distribute all the target and candidate variable pairs in parallel***

Parallel Framework – Key Design Ideas

- ***Idea*: Distribute all the target and candidate variable pairs in parallel**

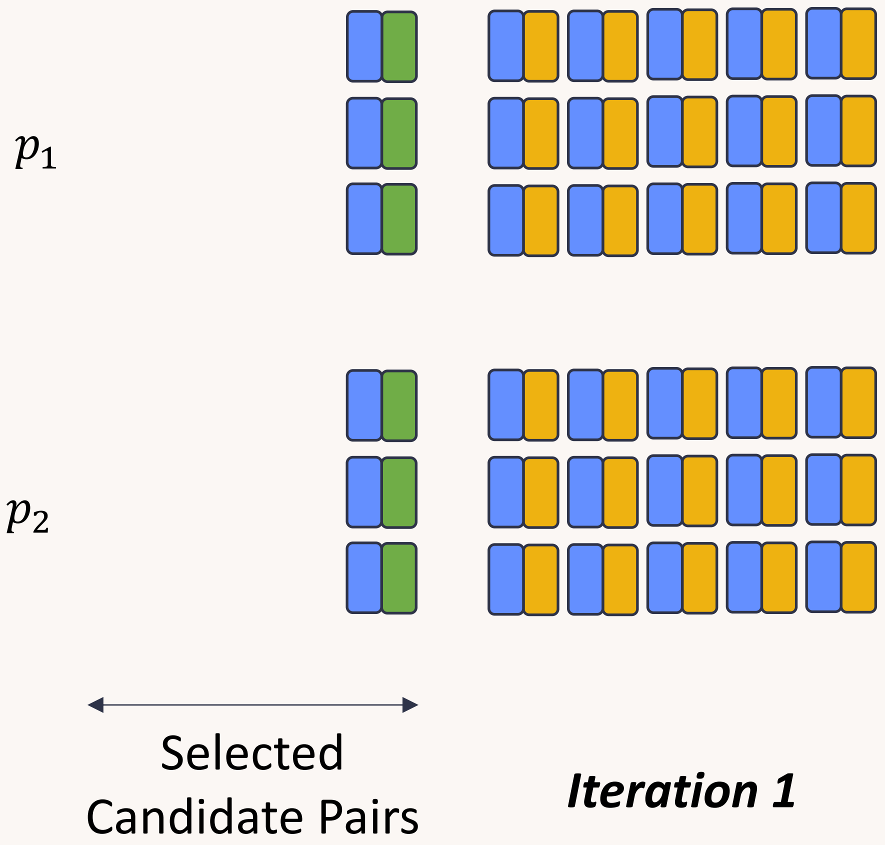


Work per processor ∝ Pairs per processor

$$= O\left(\frac{n^2}{p}\right)$$

Parallel Framework – Key Design Ideas

- ***Idea*: Distribute all the target and candidate variable pairs in parallel**



Parallel Framework – Key Design Ideas

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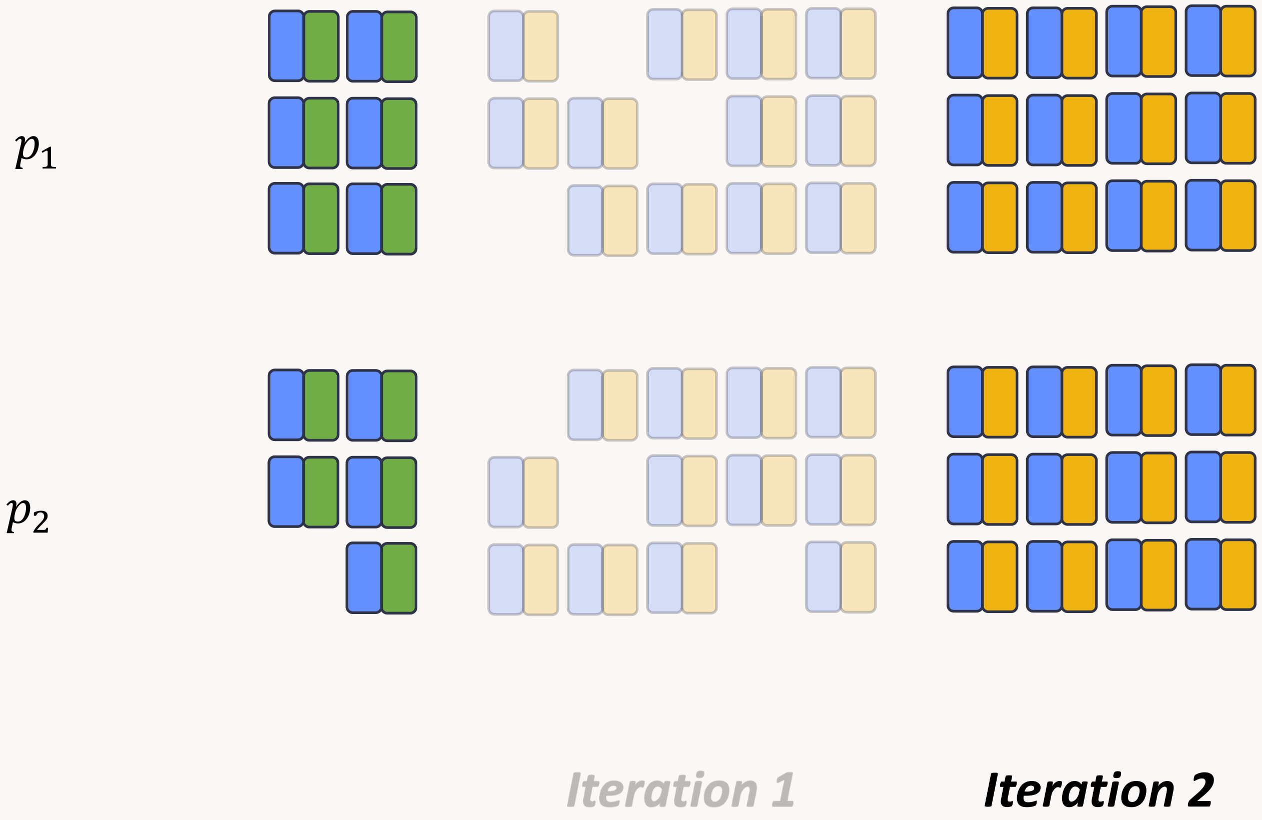

Parallel Framework – Key Design Ideas

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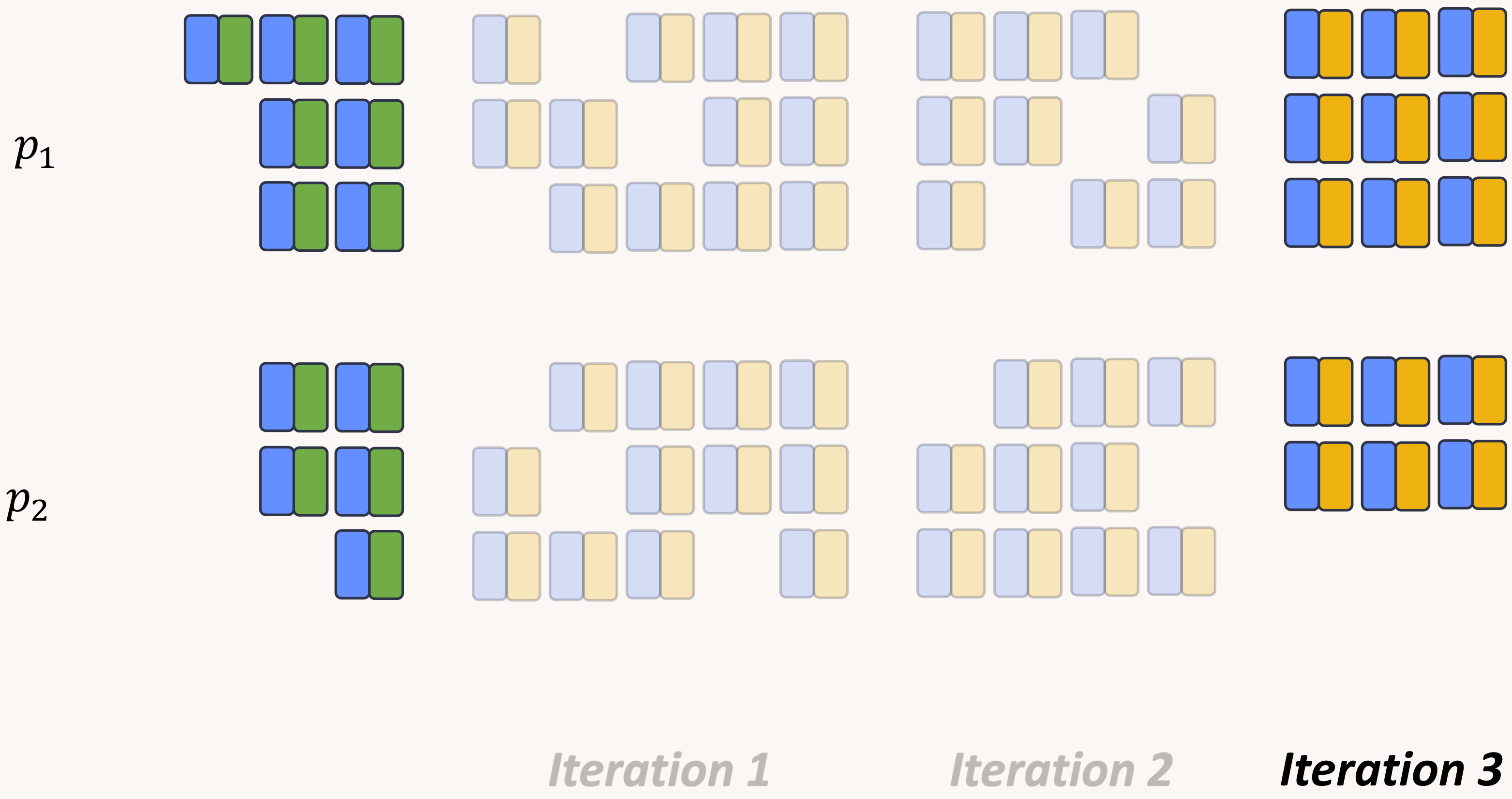
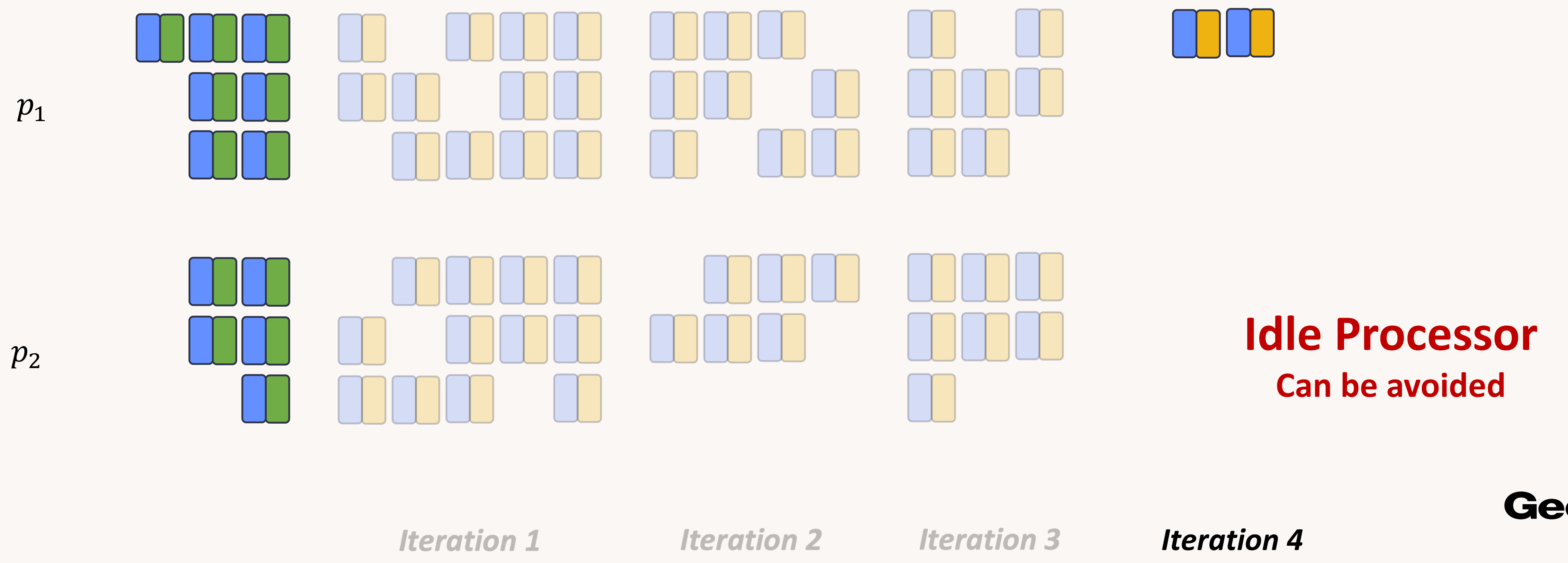


Load Imbalance

Can be alleviated

Parallel Framework – Key Design Ideas

- ***Idea*: Distribute all the target and candidate variable pairs in parallel**



Parallel Framework – Primary Data Structure

- $c\text{–}scores$ is a list of tuples $< X, Y, \theta_{XY} >$ s.t. $X \in \mathcal{X}, Y \in \mathcal{X} \setminus \{X\}$
  - θ_{XY} is the score of Y for addition to the MB set of X
  - Tuples with the same X are contiguously arranged in the list

- Work distribution in parallel by distributing the tuples
  - $c\text{–}scores$ is block-distributed across processors – $c\text{–}scores_j$ on processor j

Parallel Framework – Components

- Parallel *Grow* phase on processor j
  - Update θ_{XY} for all the tuples $\in c\text{–}scores_j$
    - Computation of θ_{XY} is dependent on the algorithm
  - Add Y to the MB of X corresponding to the best θ_{XY}
    - Can be identified using two segmented parallel prefix operations for all the variables
- Parallel *Shrink* phase on processor j
  - Candidate MBs are available for local target variables – no communication
- Parallel *Symmetry Correction* using algorithm by Nikolova et al. (2011)
- Parallel *PC from MB* for local target variables on processor j

Parallel Skeleton – Blanket Learning

function PARALLEL-SKELETON-INTERIAMB():
  Input: $\mathcal{X}$, D, APPLY-HEURISTIC, REDUCE-HEURISTIC
  Output: $\mathcal{PC}(T)$ sets for all $T \in \mathcal{X}$
  parallel j = *processor's rank* **do**
    Initialize *c-scores*$_j$, *variables*$_j$, $\mathcal{MB}(\cdot)$ as described in subsection 3.2.1
    Initialize *neighbors* as empty list of tuples
    repeat
      GROW-PHASE(D, *c-scores*, *variables*, $\mathcal{MB}$, APPLY-HEURISTIC, REDUCE-HEURISTIC)
      + SHRINK-PHASE(D, *variables*, $\mathcal{MB}$)
    until *no* $\mathcal{MB}(X)$ *changes on any of the processors*
    - SHRINK-PHASE(D, *variables*, $\mathcal{MB}$)
    SYMMETRY-CORRECTION(*variables*, $\mathcal{MB}$)
    Synchronize $\mathcal{MB}(\cdot)$ across all the processors
    CONSTRUCT-PC(D, *variables*, $\mathcal{MB}$, *neighbors*)

Implementation

- Implemented using *C++* and *MPI* (conforms to *C++14* and *MPI 3.1*)
  Available at https://github.com/asrivast28/ramBLe

- Optimizations for fast execution in practice
  - Algorithm specific optimizations – *GS* work reduction
  - Experimented with different statistic computation strategies for CI tests
  - Dynamic load balancing scheme

Experiments and Results

- Experimental setup
  - 64 nodes of the *Hive* cluster, 16 MPI processes per node – **1024 processes**
  - *RHEL* 7.6, *gcc* v9.2.0, *MVAPICH2* v2.3.3
- Used real gene-expression data sets to learn gene networks

Name	Organism	Genes (n)	Observations (m)
D1	*S. cerevisiae*	5,716	2,577
D2	*A. thaliana*	18,373	5,102
D3	*A. thaliana*	18,380	16,838

- Used three simulated data sets ($S1$, $S2$, and $S3$) to show scalability
  - $n = 30{,}000$; $m = 10{,}000$; edge addition probabilities: $5e-5$, $1e-4$, and $5e-4$

Experiments and Results

- Sequential comparison with prior state-of-the-art – *bnlearn*
  - Popular library for learning BNs; *C* implementation interfaces with *R*

Algorithm	Data set	Run-time (s) *bnlearn*	Run-time (s) *Ours*	Speedup
GS	*D1*	8 720.0	240.1	36.3
	D2	×	6 760.3	N/A
	D3	×	18 695.0	N/A
IAMB	*D1*	975.9	624.6	1.6
	D2	40 605.7	14 529.8	2.8
	D3	84 403.1	46 603.2	1.8
Inter-IAMB	*D1*	992.0	624.1	1.6
	D2	40 819.0	14 559.0	2.8
	D3	89 839.7	48 442.4	1.9

Experiments and Results

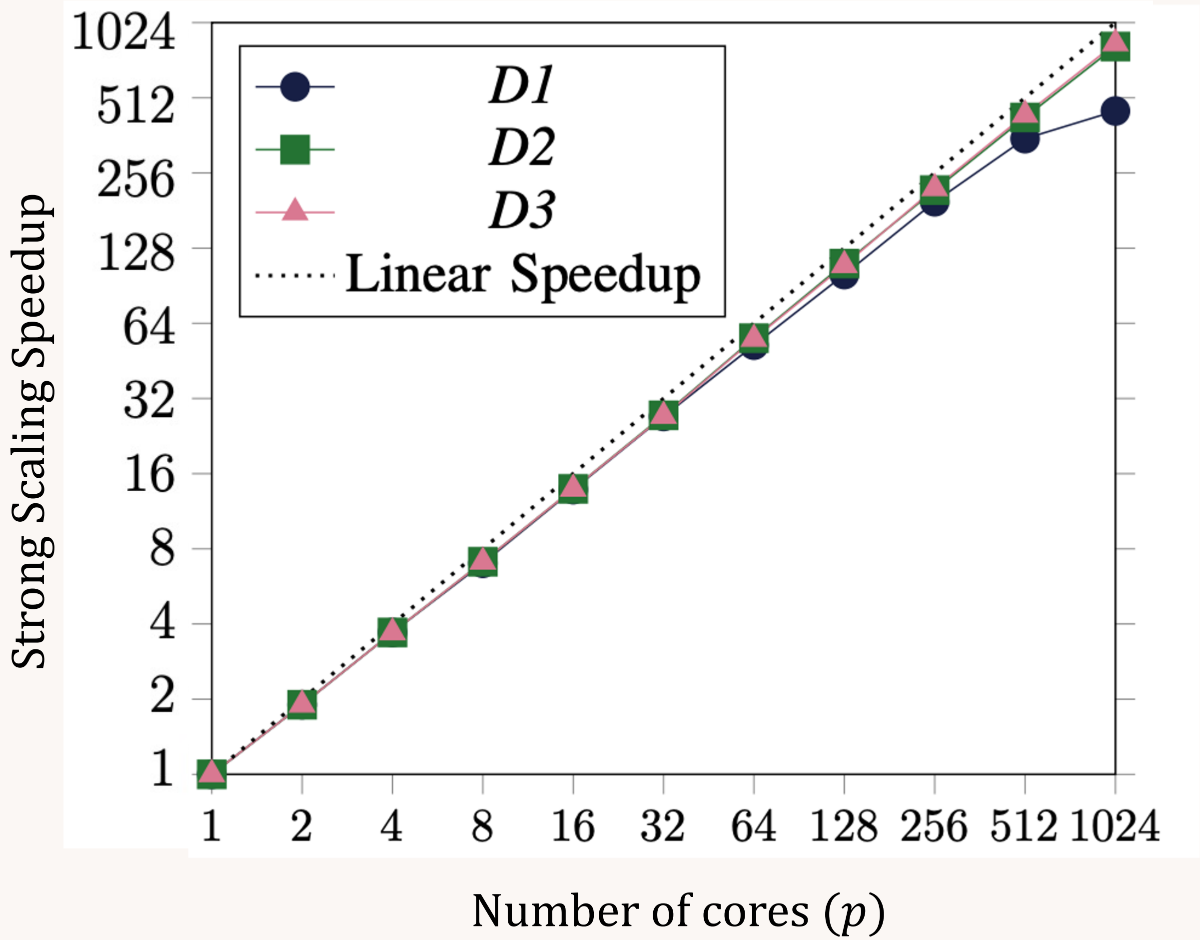
- Sequential comparison with prior state-of-the-art – *bnlearn*
  - Popular library for learning BNs; *C* implementation interfaces with *R*
- BNs learned by our implementations are similar to those by *bnlearn*
  - Recalled 99.84% edges with a precision of 99.92% for $D1$ data set
  - Changes in the ordering of the variables caused the differences
- Parallelism in *bnlearn* yields diminishing returns beyond a single node
  - e.g., *IAMB* shows a self-speedup of 3.4X on 16 cores for $D3$ data set while the self-speedup using 64 cores on four nodes is 3.9X

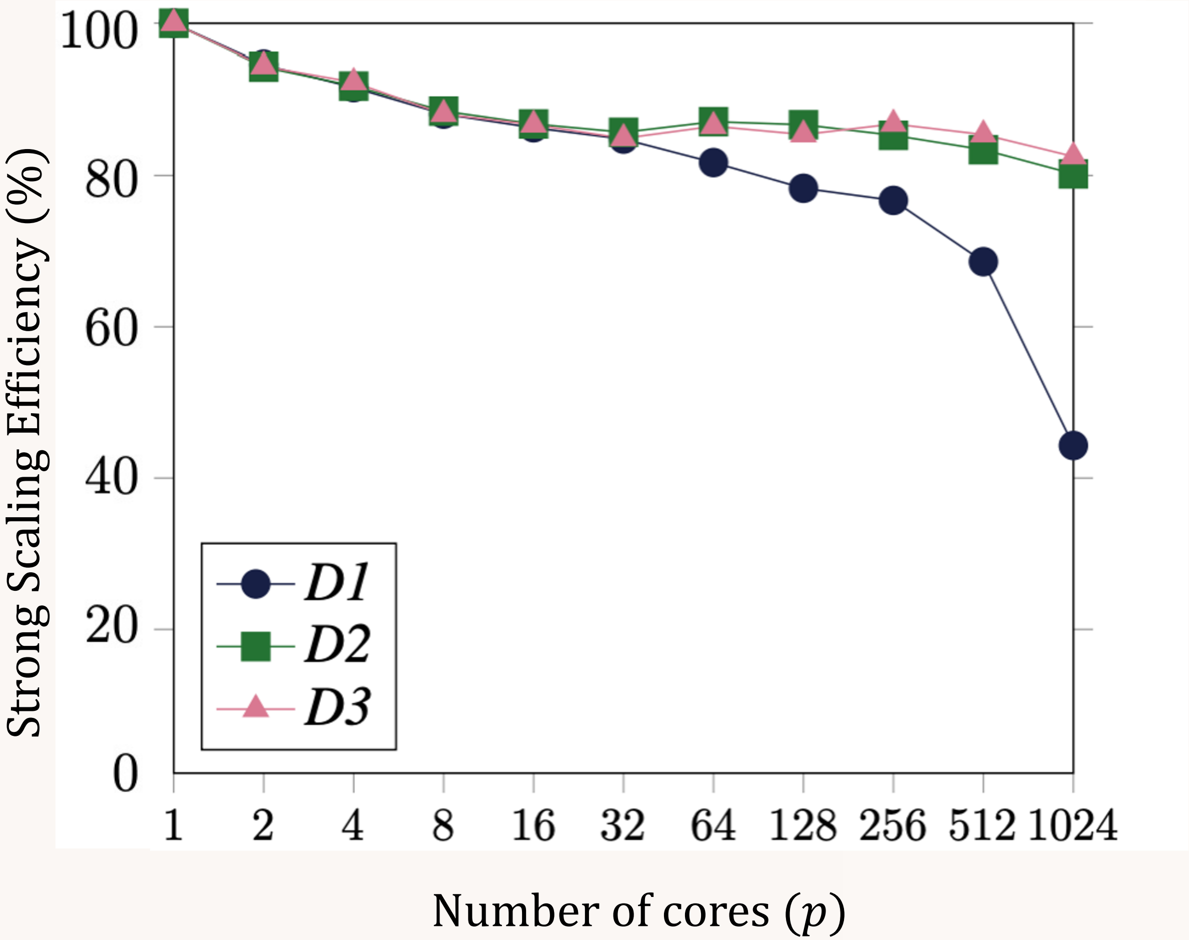
Experiments and Results

- Parallel performance of our framework – notions of scalability
- **Strong Scaling**
  - Fixed total work; how does the run-time scale with increasing parallelism? (n is kept constant as p increases)
- **Weak Scaling**
  - Fixed work per processor; how does the run-time scale with increasing parallelism? (n is increased as p increases)
- Speedup and efficiency are measured
  - Perfect parallel algorithm shows **linear speedup** and **100% efficiency**

Experiments and Results

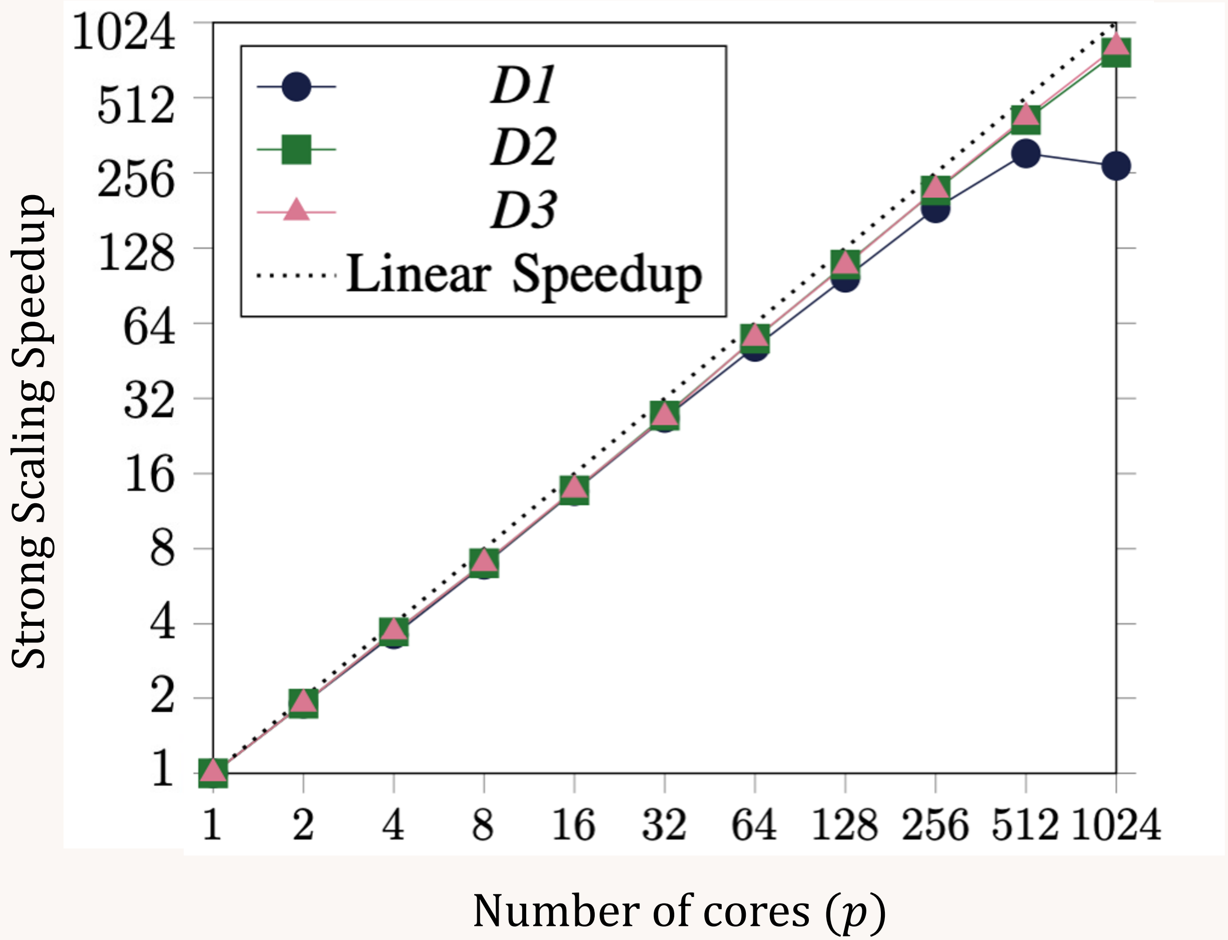
- Strong scaling of our framework – *IAMB*

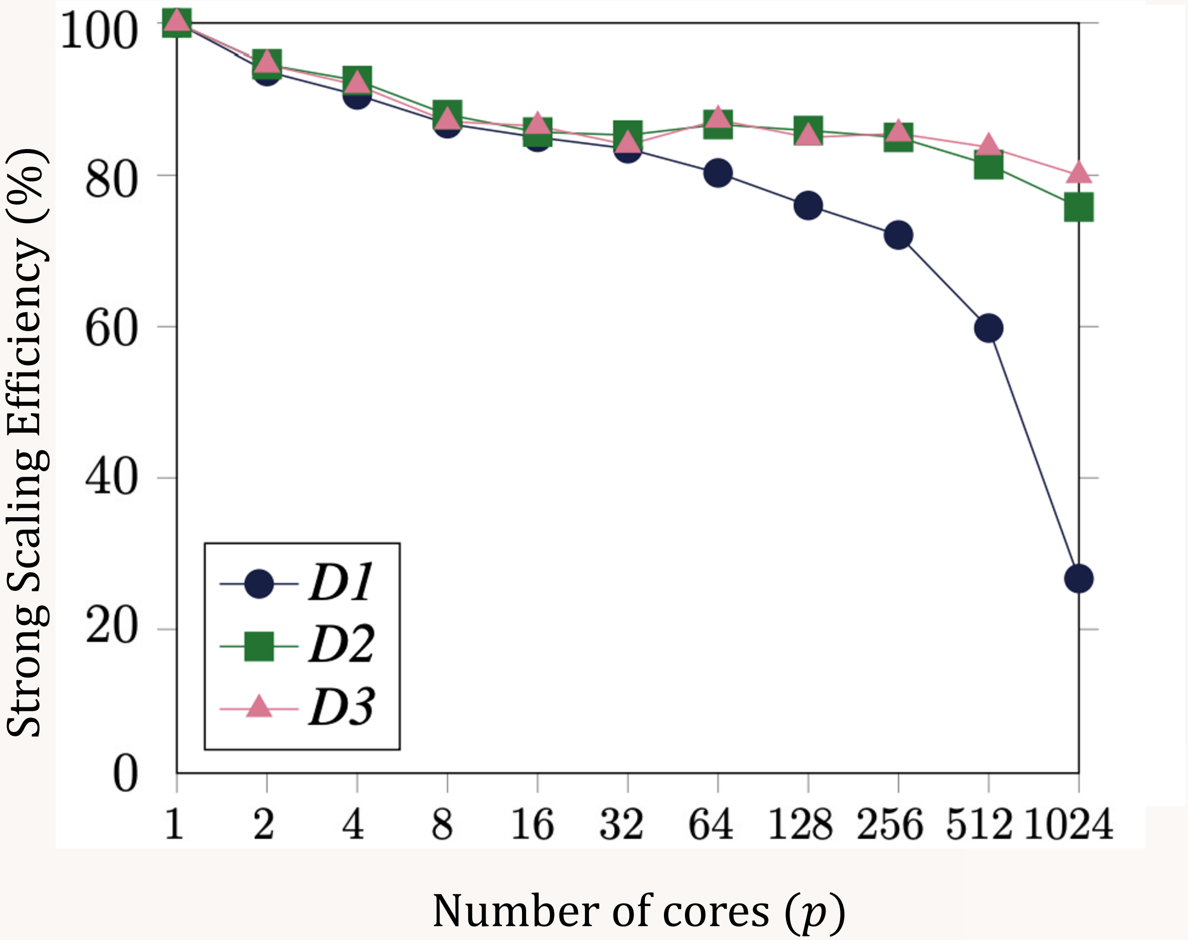




Experiments and Results

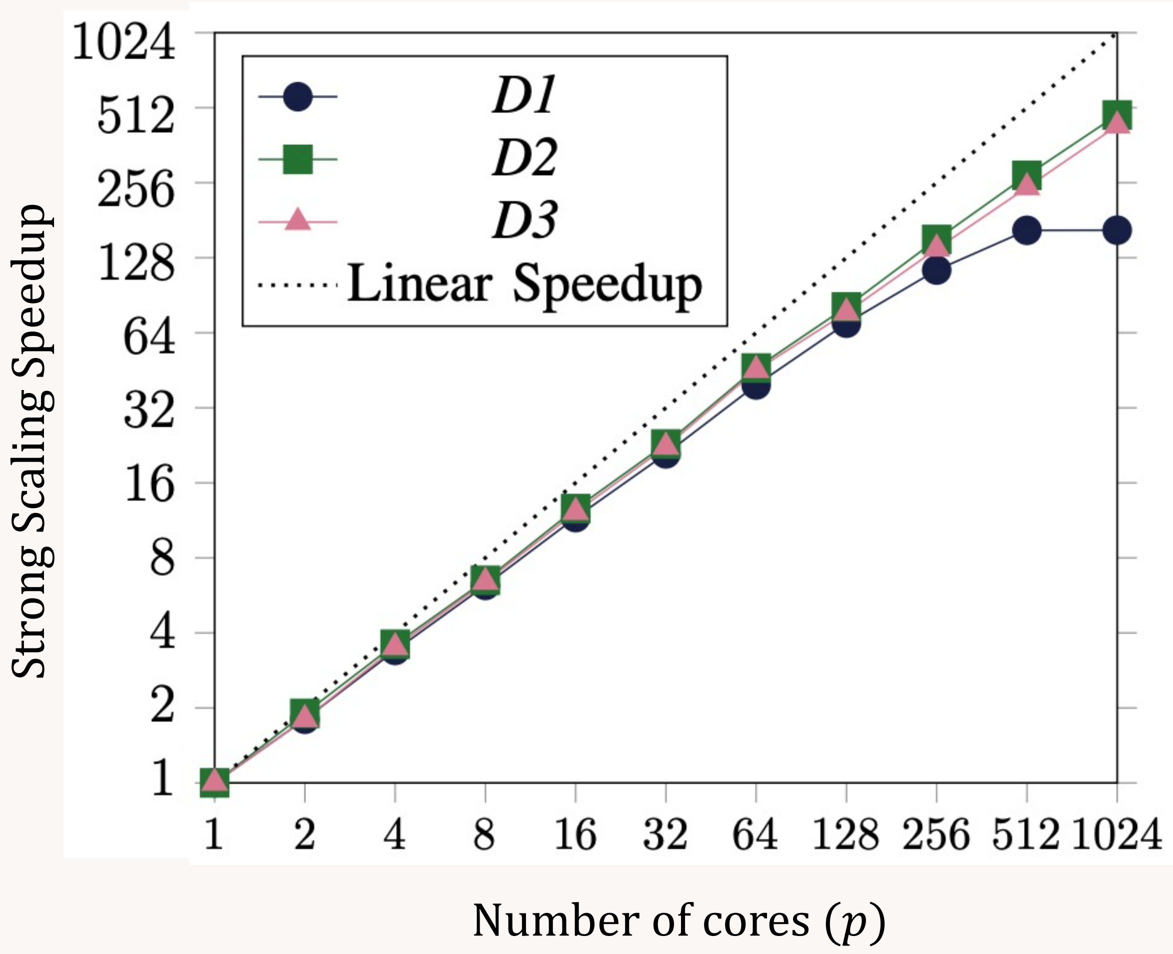
- Strong scaling of our framework – *Inter-IAMB*

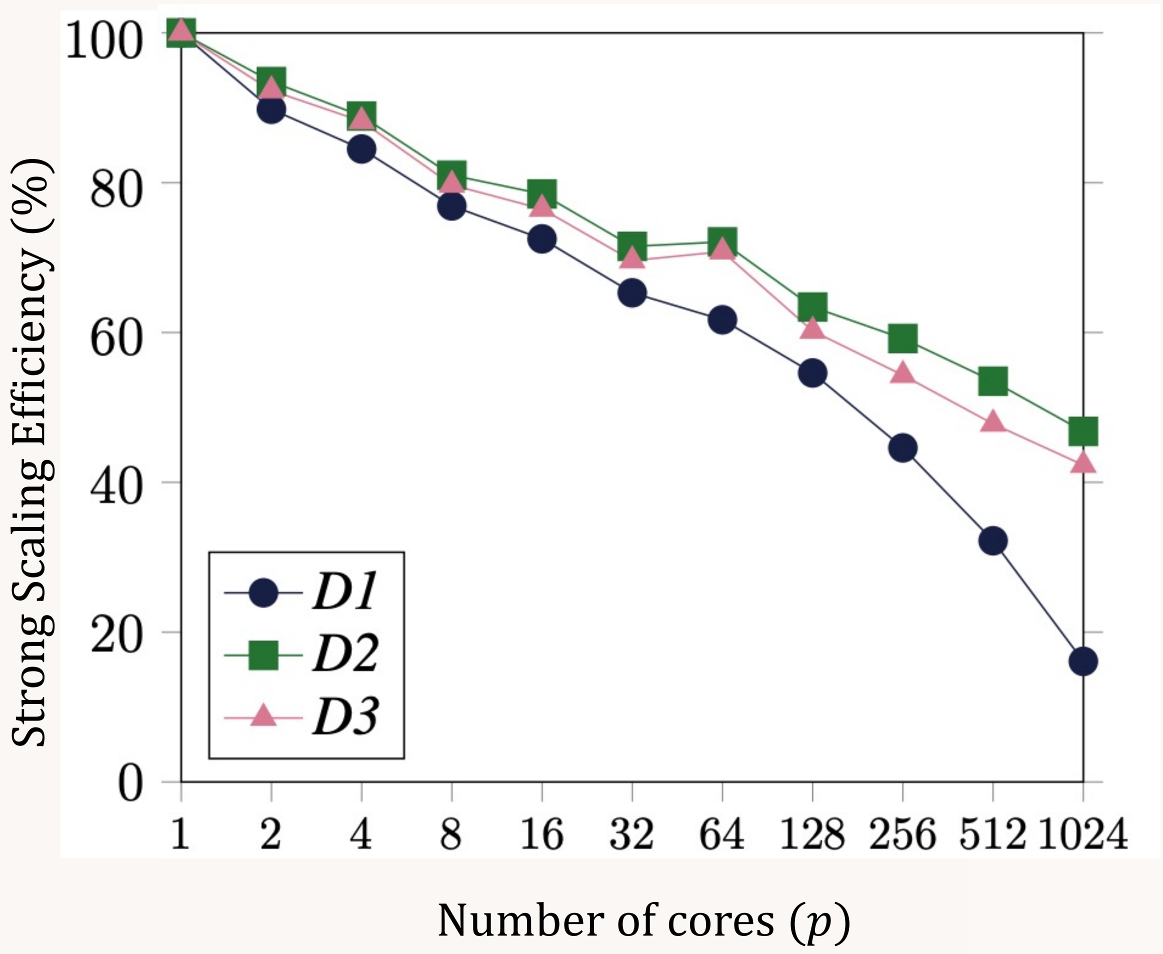




Experiments and Results

- Strong scaling of our framework – *GS*

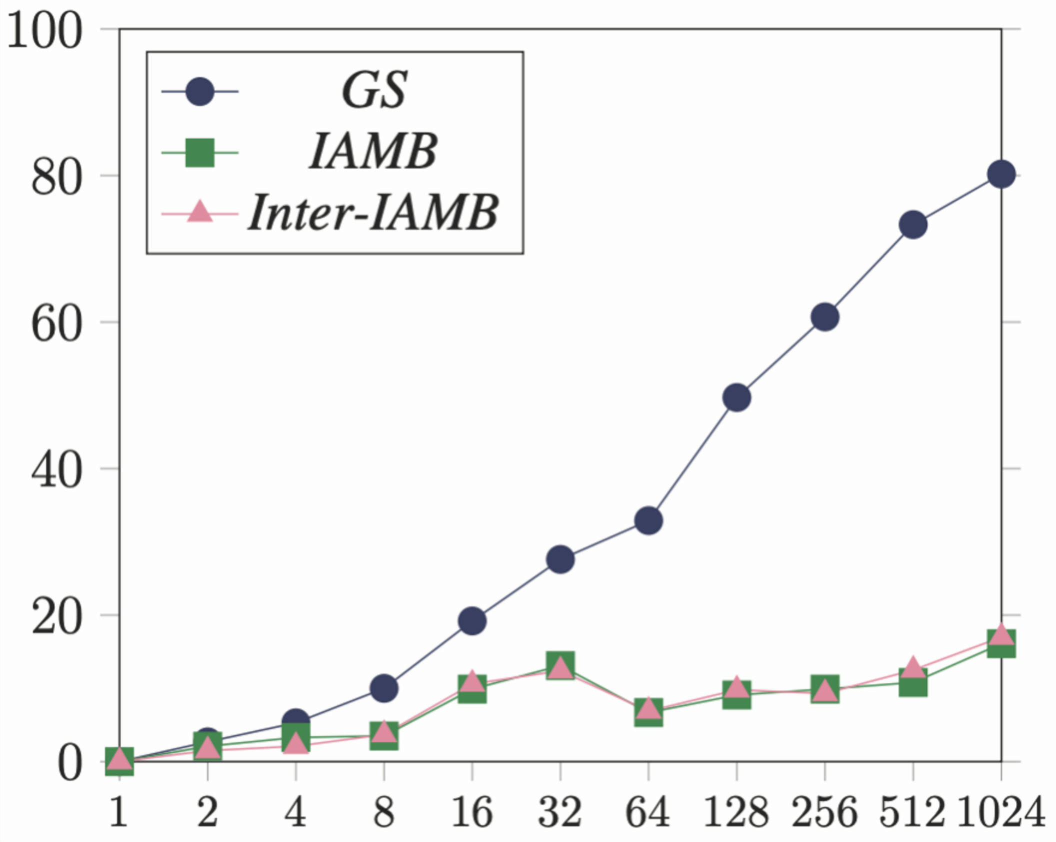




Experiments and Results

- Investigating the scaling performance of *GS*
  - High communication overhead due to lower total work?

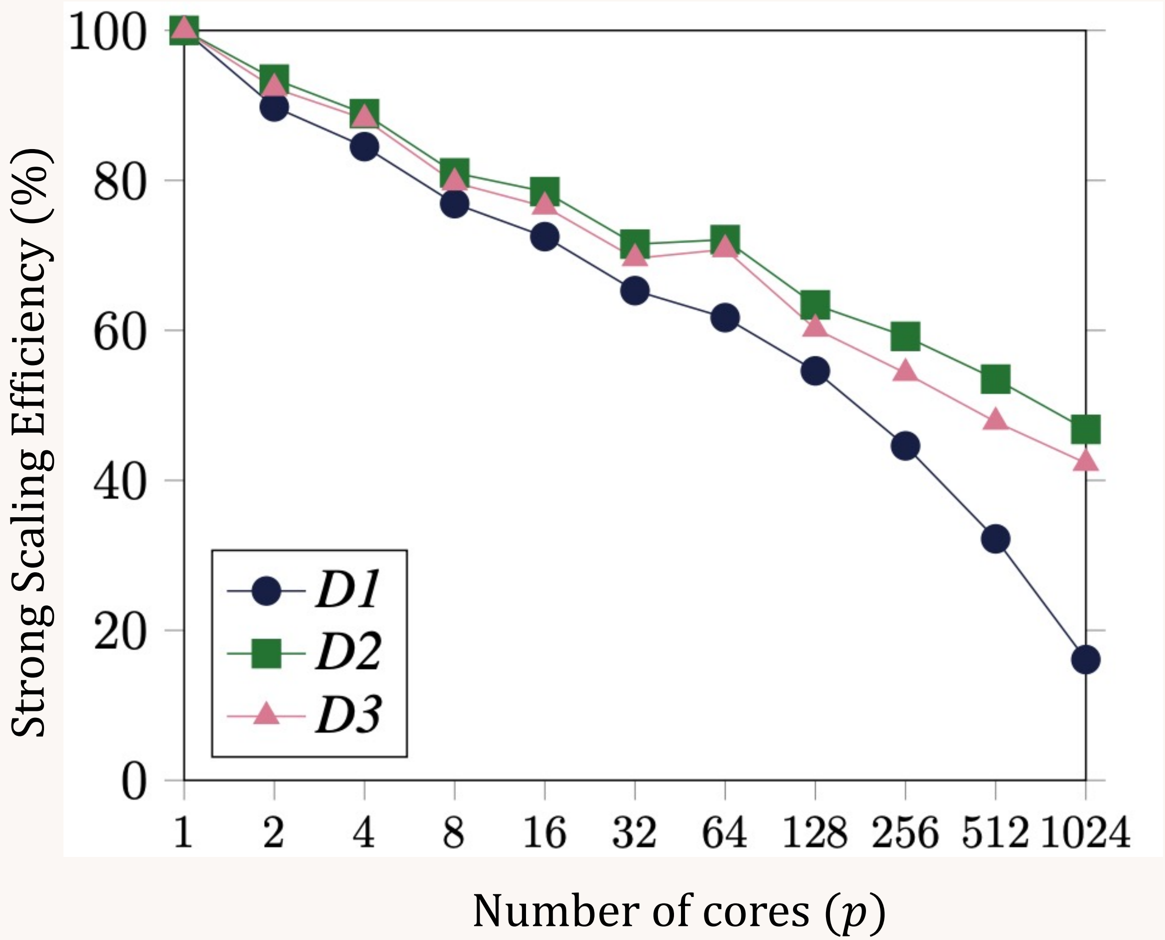
Fraction of total run – time spent in communication (%)

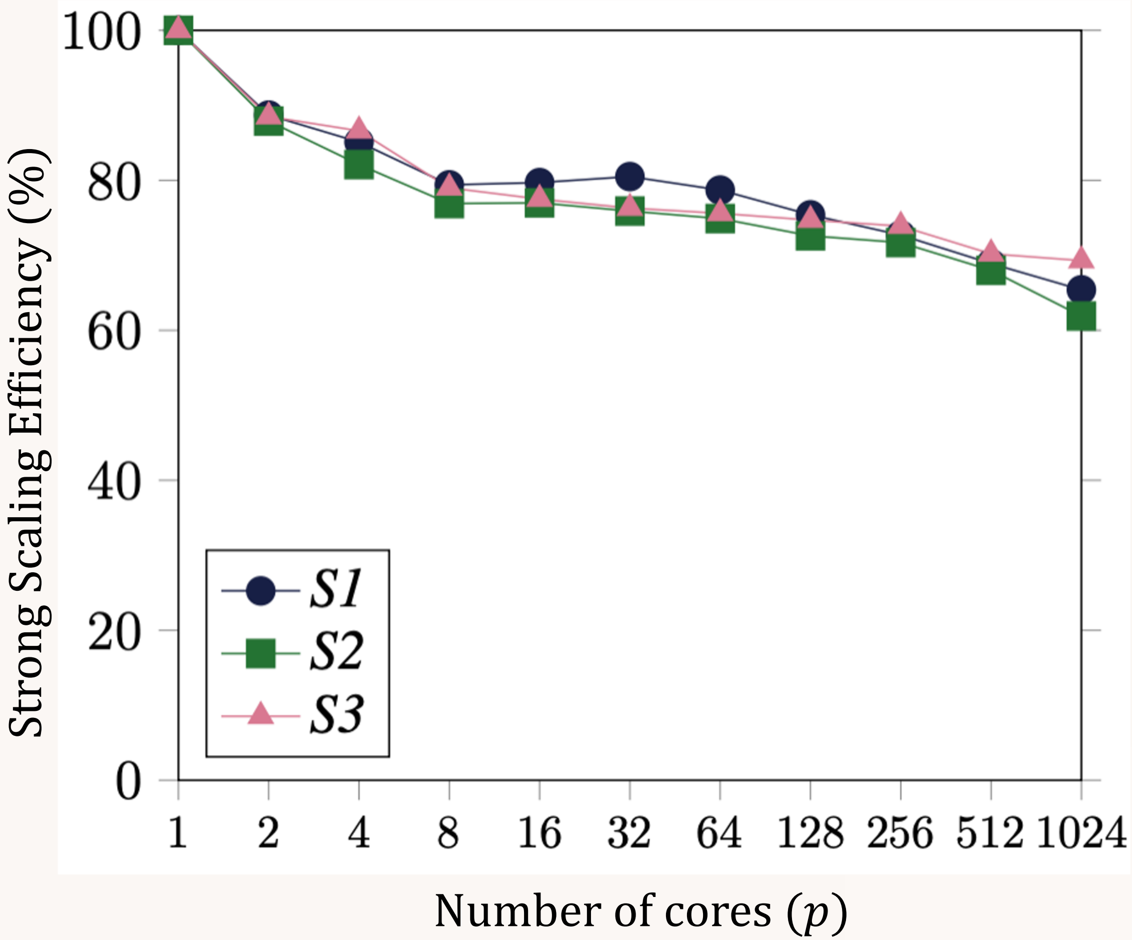


Number of cores (p)

Experiments and Results

- Scaling performance of *GS* – real data versus simulated data



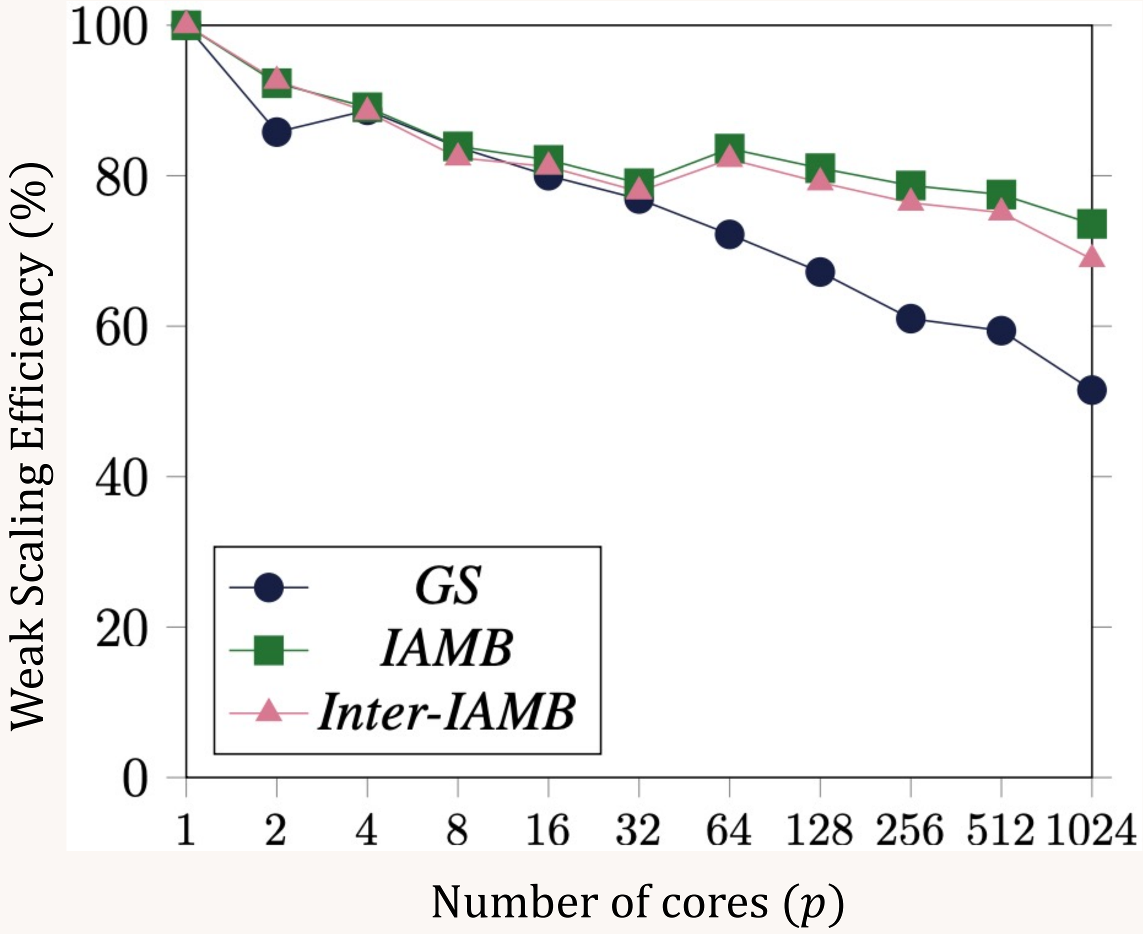


Experiments and Results

- Weak scaling of our framework
- Fixed work per processor – how do we vary n with increasing p?
  - Choose all the variables when using the largest p, a subset of variables for smaller p
- Estimated work per processor = n^2/p
  - Chosen number of variables scale as $\sqrt{p}$, i.e., $n_p = n\sqrt{p/p_{max}}$
  - We chose the first n_p variables in the data sets for our experiments

Experiments and Results

- Weak scaling of our framework – *D2*



Experiments and Results

- Our parallel algorithms learn genome-scale BNs in < 1 minute on 1024 cores, down from more than 13 hours sequentially
  - Maximum speedup of 844.8X and 82.5% scaling efficiency on 1024 cores
  - *IAMB* and *Inter-IAMB* show a sustained efficiency of > 75% for $D2$ and $D3$
- Learning BNs from simulated data sets takes < 2 minutes on 1024 cores, as compared to more than a day sequentially
  - Maximum speedup of 845X and 82.5% scaling efficiency on 1024 cores
  - GS shows an improved efficiency of > 60% for all the data sets

Thanks! Questions?