USENIX ATC '24

Fast Inference for Probabilistic Graphical Models

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Outline



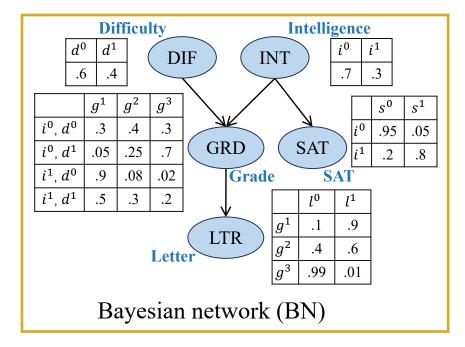
- Background and Motivation
- Objective I: Good Generality and Flexibility
- Objective II: High Efficiency
- Experimental Evaluation
- Conclusion

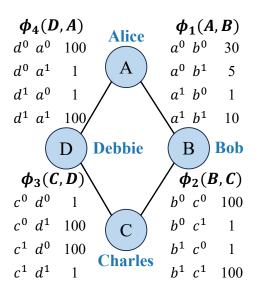


Background of PGMs



- Probabilistic graphical models (PGMs):
 - A graph: illustrates random variables and their relationships.
 - Parameters: quantify the strength of the relationships: a set of tables for discrete PGMs, e.g. *conditional probability tables (CPTs)* for BNs.
 - Joint distribution can be factorized into local CPTs of each node.



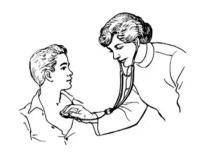




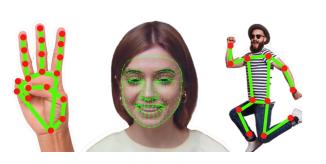
Background of PGMs



- Key advantages:
 - Transparent and intuitive graphical representation.
 - Solid theoretical foundations (probability theory).
- Applications:



PKC
PKA
Raf
PIP3
Mek
PIP3
Akt







Medical diagnosis

Biological informatics

Computer vision

Financial analysis

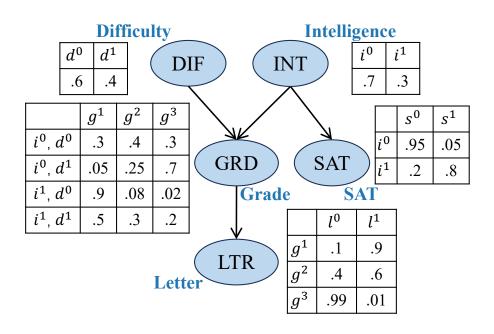
Social network analysis



Background of PGM Inference



- **Inference**: calculate the posterior probability distribution of *query* variables, given values of other *evidence* variables.
 - e.g. evidence: DIF = d¹, INT = i¹; query variable: LTR.
 -> P(LTR | DIF = d¹, INT = i¹).





Background of PGM Inference



- Approximate inference: less time but lower accuracy.
 - Importance sampling-based methods: use <u>importance function</u> to generate samples and estimate probability from the samples.
 - Importance function in PGMs: a probability distribution, can be decomposed into multiple *importance conditional probability tables (ICPTs)* of variables.
 - Widely used sampling-based algorithms:
 - Probabilistic logic sampling (PLS).
 - Likelihood weighting (LW).
 - Self-importance sampling (SIS).
 - AIS-BN.
 - EPIS-BN.



Motivation



- Major challenges:
 - NP-hardness of approximate inference problem.
 - Irregular nature of the graphical structure.
 - Stochastic nature of the sampling process.
 - Difficulty in abstracting and integrating various algorithm.
- We provide *Fast-PGM*, a system for importance sampling-based PGM inference. Main objectives:
 - Good generality and flexibility.
 - High efficiency.



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System Abstraction



 All the importance sampling-based algorithms can be abstracted into a general framework with four crucial modules.

```
Algorithm 3: Fast-PGM
  input: prior probability P(\mathcal{V}), weight v^0, # of samples required q, updating interval l
  output: estimated posterior marginal probability for all non-evidence variables
1 k \leftarrow 0, scrArr \leftarrow 0, \mathbf{w}_{curScr} \leftarrow 0, \mathbf{w}_{allScr} \leftarrow 0.
   /★ importance function initialization module
2 f^0(V) \leftarrow \text{initImpFunc}(P(V))
3 for i \leftarrow 1 to q do
       if i\%l == 0 then
             k \leftarrow k + 1
             /* importance function update module
             f^{k}(\mathcal{V}), v^{k} \leftarrow \text{updImpFunc}(\mathbf{w}_{curScr}, \mathbf{w}_{allScr})
            sample generation module
        s_i, w_{iScr} \leftarrow \text{genSamp}(f^k(\mathcal{V}), P(\mathcal{V}))
        /* importance score accumulation module
       \mathbf{w}_{curScr}, \mathbf{w}_{allScr}, \mathbf{scrArr} \leftarrow \operatorname{accScr}(s_i, w_{iScr}, v^k)
9 normalize scr Arr for each variable
```



System Abstraction

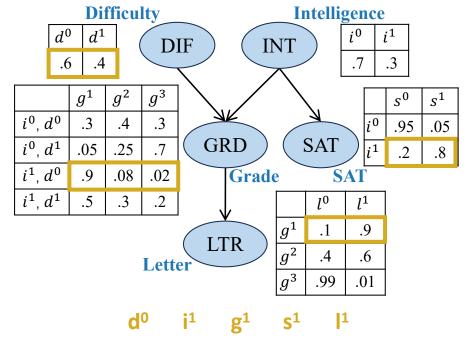


• Sample generation: generate a sample by sampling each variable (via topological order), and calculate its <u>importance score</u>. Distinguish variables

Steps to handle each variable V_j :

- 1. Get the instantiation of V_i 's parents.
- 2. Get the weight vector of V_j based on V_j 's ICPT and the instantiation of its parents.
- 3. Randomly pick a value of V_j based on the weight vector.
- 4. Compute the score and multiply it into the importance score.

Example: $INT = i^{1}$.



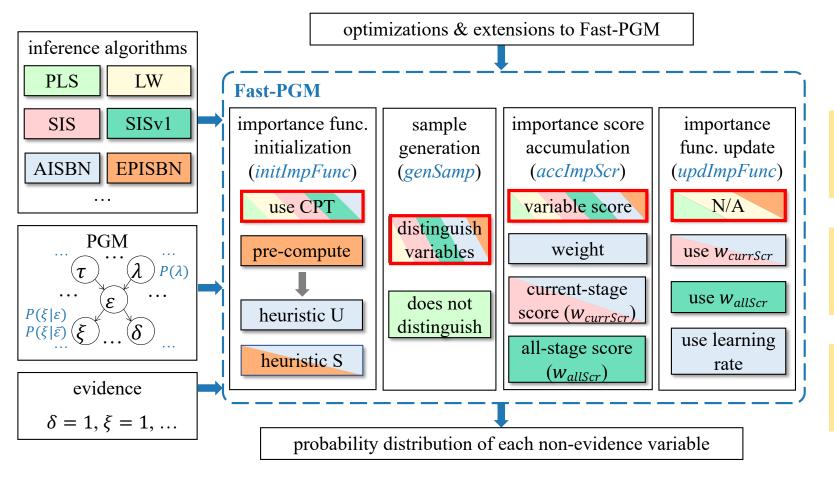
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Fast-PGM Overview



Fast-PGM enables good generality and flexibility.



Key features:

Versatile modules and functionalities support.

Quick new algorithm implementation.

Ease of optimization and extension.



Outline



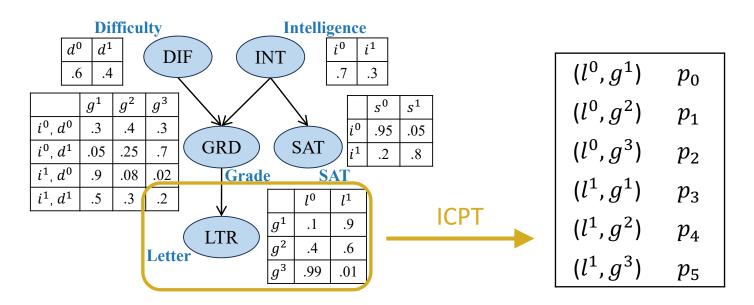
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 - Memory management
 - Computation simplification
 - Parallelization
- Experimental Evaluation
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Memory: Basic Data Structure



- Challenge 1: Large memory requirement for storing ICPTs.
 - The computations are done by maintaining an ICPT of each variable.



Related variables: LTR, GRD.

Keys: state configurations.

Values: probabilities.

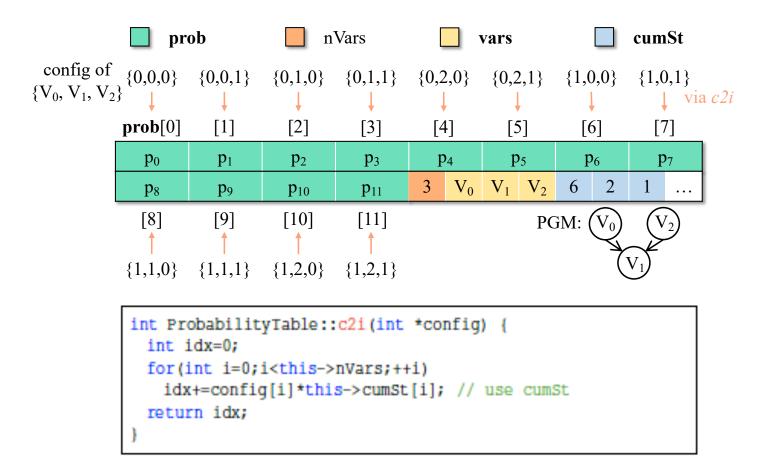
Number of entries = 2 * 3 = 6.



Memory: Basic Data Structure



Solution 1: Avoid storing state configurations for each entry.

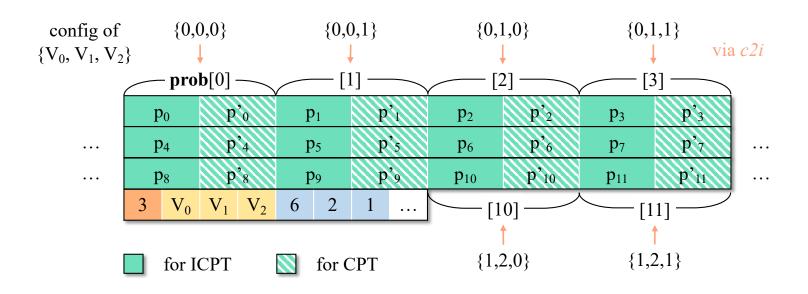




Memory: Data Fusion



- Challenge 2: Irregular memory accesses to ICPTs and CPTs caused by the stochastic nature of the sampling process.
- Solution 2: Fusing ICPT and CPT of each variable to enhance data locality.

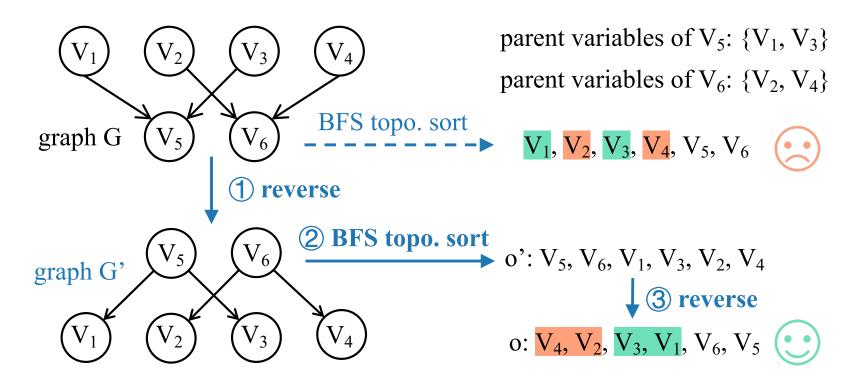




Memory: Data Reordering



- Challenge 3: Irregular memory accesses caused by the graphical structure.
- Solution 3: Data reordering to maximize proximity of each node's parents.

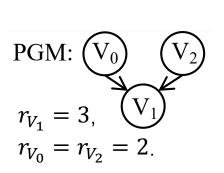




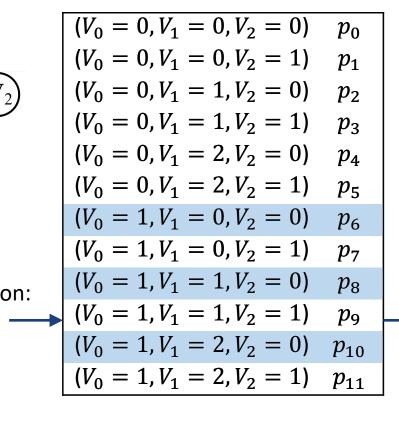
Computation: Table Reorganization



- Most expensive operation: Get the weight vector of variables.
 - By reducing the ICPT of each variable based on the instantiation of its parents.



Parent instantiation:
$$V_0 = 1, V_2 = 0.$$



Size of ICPT:
$$r_{V_j} \times \prod_{V_i \in Par(V_j)} r_{V_i}$$
 (exponential in $|Par(V_j)| + 1$)!

Overall Complexity: $O(q \times \sum_{V_j \notin E} (|Par(V_j)| \times r_{V_j} \times \prod_{V_i \in Par(V_j)} r_{V_i})).$

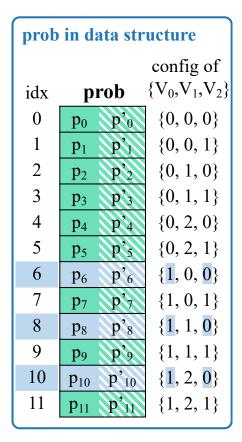
Weight vector: p_6 p_8 p_{10}

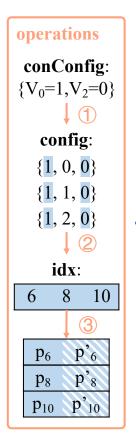


Computation: Table Reorganization

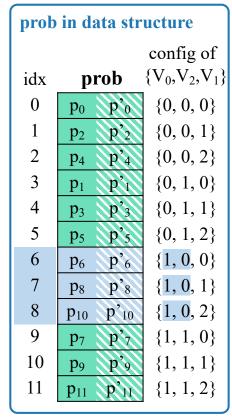


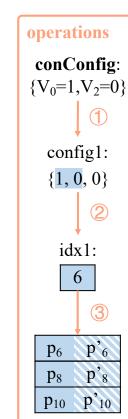
• Table reorganization optimization to simplify computations.

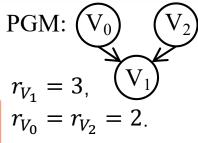




Variable itself is in the rightmost.







$$O(q \times \sum_{V_j \notin E} (r_{V_j} \times (|Par(V_j)| + 1))$$

$$O(q \times \sum_{V_j \notin E} (|Par(V_j)| + 1))$$



Parallelization



- Case-level parallelism (coarse-grained parallelism):
 - Load unbalancing due to different evidence variables.
- Variable-level parallelism (fine-grained parallelism):
 - Requirement of graph partitioning that relies on PGM structures.
 - Small workloads but high parallel overhead.

Sample-level parallelism:

• Parallelize the generation of samples within each importance updating stage.



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Overall comparison with existing work:

Table 2: Execution time comparison of Fast-PGM ("Ours") with SMILE ("S") and BNJ ("B") on 1000 test cases. Speedups of Fast-PGM over SMILE and BNJ are also reported. "N/A" means that the library does not support the corresponding algorithm.

	PLS					LW					SIS				
PGM	Time (sec)			Speedup		Time (sec)			Speedup		Time (sec)			Speedup	
	S	В	Ours	S	В	S	В	Ours	S	BNJ	S	В	Ours	S	В
Alarm	0.39	1.59	0.13	3.0	12.0	0.42	1.50	0.11	3.7	13.2	N/A	3.0	0.14	N/A	20.7
Hailfinder	0.76	5.7	0.26	3.0	22.1	0.66	2.7	0.21	3.1	13.1	N/A	15.8	0.26	N/A	60.0
Pathfinder	5.0	76.0	1.1	4.4	66.8	6.1	88.0	1.0	5.8	84.2	N/A	1.1k	1.3	N/A	850
Pigs	21.4	1.2k	1.4	15.0	841	14.6	1.2k	1.5	10.1	854	N/A	4.9k	1.8	N/A	2.8k
Munin2	68.4	6.2k	4.5	15.1	1.4k	48.9	6.0k	4.5	10.8	1.3k	N/A	27k	5.9	N/A	4.5k
Munin4	67.8	6.1k	5.1	13.4	1.2k	47.7	7.6k	5.2	9.2	1.5k	N/A	32k	6.9	N/A	4.6k
			SISv1					AIS-BN]	EPIS-BN	1	
PGM	Т	ime (se		Spec	edup	Т	ime (se			edup	Т	ime (se			edup
PGM	S	ime (se		Spec	edup B	S				edup B	S				edup B
PGM Alarm			c)				ime (se	c)	Spec			ime (se	c)	Spec	
	S	В	c) Ours	S	B	S	ime (se	c) Ours	Spec S	B	S	ime (se	Ours	Spec S	B
Alarm	S 0.46	B N/A	Ours 0.15	S 3.2	B N/A	S 0.77	ime (se B	Ours	Spec S	B 69.3	S 0.65	ime (se	Ours 0.14	Spec S 4.5	B N/A
Alarm Hailfinder	S 0.46 0.83	B N/A N/A	Ours 0.15 0.27	3.2 3.1	B N/A N/A	S 0.77 1.3	ime (se B 10.2 27.7	Ours 0.15 0.27	Spec S 5.2 4.9	69.3 104	S 0.65 0.83	ime (se B N/A N/A	Ours 0.14 0.26	Spec S 4.5 3.2	B N/A N/A
Alarm Hailfinder Pathfinder	S 0.46 0.83 13.0	N/A N/A N/A	Ours 0.15 0.27 1.3	3.2 3.1 10.0	N/A N/A N/A	S 0.77 1.3 11.5	ime (se B 10.2 27.7 2.7k	Ours 0.15 0.27 1.3	Spec S 5.2 4.9 8.8	69.3 104 2.1k	S 0.65 0.83 6.0	ime (se B N/A N/A N/A	Ours 0.14 0.26 1.3	Spec S 4.5 3.2 4.5	B N/A N/A N/A

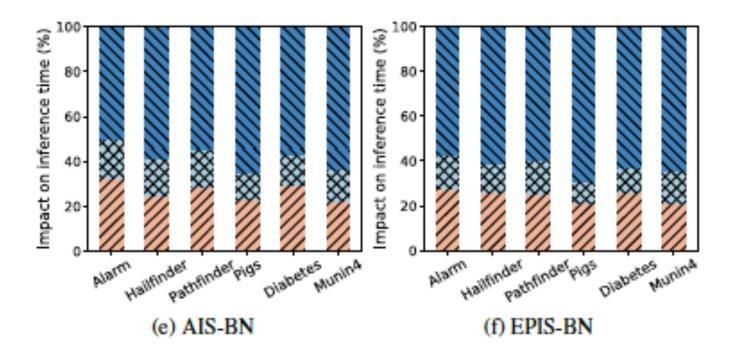
Our solution support more algorithms.

3 – 20 x faster than SMILE; two – four orders of magnitude speedup than BNJ.





• Impact of individual optimizations:



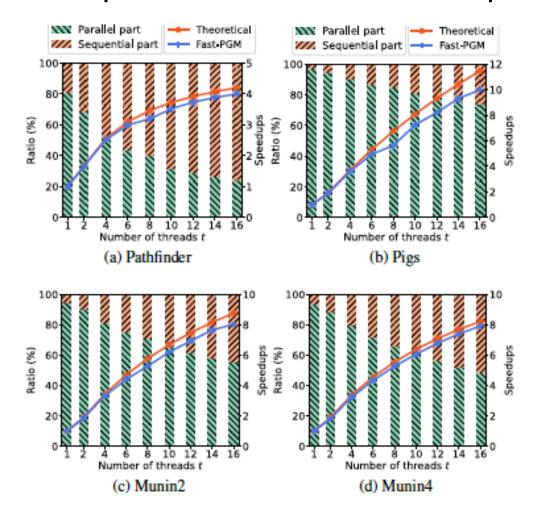
Overall: 25% from memory management, 14% from computation simplification, 61% from parallelization.

Learning-based algorithms benefit more from memory management and computation simplification compared to non-learning-based algorithms.





Comparison with theoretical speedup:



Theoretical speedup is computed by Amdahl's law:

$$Speedup(t) = \frac{1}{(1 - rp) + \frac{rp}{t}}$$

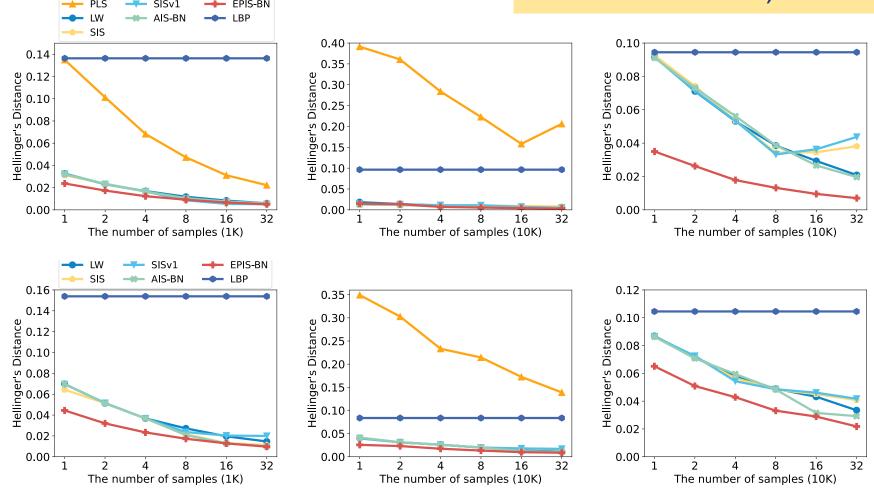
Our practical speedups approach the theoretical speedups.





Accuracy of approximation:

EPIS-BN is the best, PLS is the worst.





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Conclusion



- We propose Fast-PGM, a system for PGM inference. Through systematic abstraction, Fast-PGM provides a general framework with rich interfaces, enabling fast and easy optimization, extension, and customization.
- We incorporate memory management, computation simplification, and parallelization techniques, which are applicable to other PGM topics and can inspire acceleration for a broader class of graph-based algorithms.
- We conduct experiments to study the effectiveness of Fast-PGM and the impact of our optimizations.
- Future work could extend Fast-PGM to distributed environment and incorporate additional inference algorithms.

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Thank you for listening! Q & A

Fast Inference for Probabilistic Graphical Models

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