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June 7th, 2020 - ICML 2020 - Virtual Vienna





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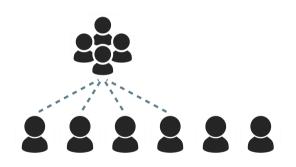


Each *player* has a certain skill



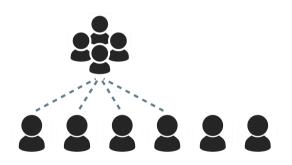
Each *player* has a certain skill continuous variables



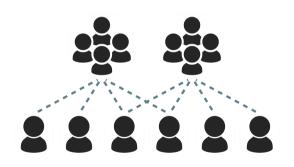


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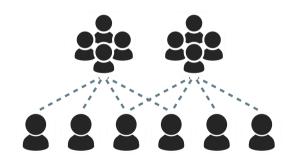
Players can form teams



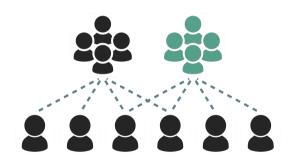
- Each *player* has a certain skill
- Players can form **teams**
 - intricate dependencies



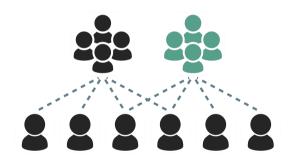
- Each *player* has a certain skill
- Players can form *teams*
- Each team's skill is bounded by its players' skills



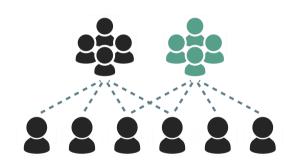
- Each *player* has a certain skill
- Players can form **teams**
- Each team's skill is bounded by its players' skills
 - complex constraints!



- Each *player* has a certain skill
- Players can form teams
- Each team's skill is bounded by its players' skills
- Good teams form a **squad**



- Each *player* has a certain skill
- Players can form **teams**
- Each team's skill is bounded by its players' skills
- Good teams form a **squad**
 - → discrete variables

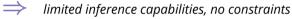


"What is the probability of team T_1 to outperform team T_2 , if T_1 is a squad but T_2 is not?"

Generative adversarial networks (GANs) [Goodfellow et al. 2014] Variational Autoencoders (VAEs) [Kingma et al. 2013]

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⇒ strong distributional assumptions

Generative adversarial networks (GANs) [Goodfellow et al. 2014] Variational Autoencoders (VAEs) [Kingma et al. 2013]

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Tractable Probabilistic Circuits (PCs) [Molina et al. 2018; Vergari et al. 2019]

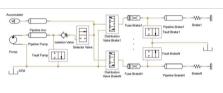
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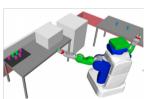
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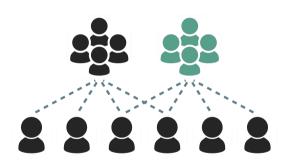
⇒ cannot deal with complex constraints



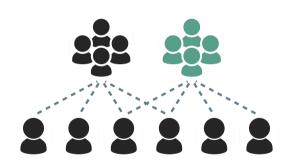


Satisfiability Modulo Theories of the linear arithmetic over the reals (SMT(\mathcal{LRA})) delivers all these ingredients by design!

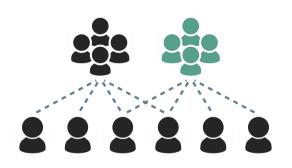
Widely used as a representation language for *robotics*, *verification* and *planning* [Barrett et al. 2010]



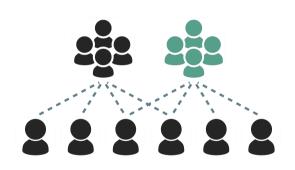
Each *player* has a certain skill



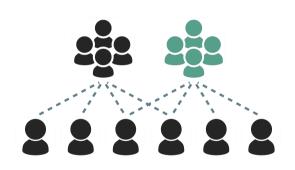
$$0 \le X_{P_i} \le 10$$
 for $i = 1, \dots, N$



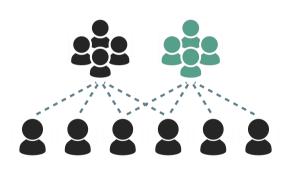
- $0 \le X_{P_i} \le 10$ for $i = 1, \dots, N$
- Each team's skill is bounded by its players' skills



- $0 \le X_{P_i} \le 10$ for $i = 1, \dots, N$
- $\mid X_{T_j} X_{P_i} \mid < 1$ for $j = 1, \ldots, M, i = 1, \ldots, |T_j|$



- $0 \le X_{P_i} \le 10$ for $i = 1, \dots, N$
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- Good teams form a **squad**

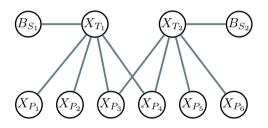


- $0 \le X_{P_i} \le 10$ for $i = 1, \dots, N$
- $\mid X_{T_j} X_{P_i} \mid < 1$ for $j = 1, \ldots, M, i = 1, \ldots, |T_j|$
- $B_{S_j} \Rightarrow X_{T_j} > 2$ for $j = 1, \dots, M, i = 1$

$$\Delta = \bigwedge_{i} 0 \le X_{P_i} \le 10 \bigwedge_{j} \bigwedge_{i \in T_j} |X_{T_j} - X_{P_i}| < 1 \bigwedge_{j} (B_{S_j} \Rightarrow X_{T_j} > 2)$$

a single CNF SMT(\mathcal{LRA}) formula Δ ...





a single CNF SMT(\mathcal{LRA}) formula Δ ...and its **primal graph**

SMT + weights

$$\bigwedge_{i} 0 \le X_{P_{i}} \le 10$$

$$\bigwedge_{j} \bigwedge_{i \in T_{j}} |X_{T_{j}} - X_{P_{i}}| < 1$$

$$\bigwedge_{j} (B_{S_{j}} \Rightarrow X_{T_{j}} > 2)$$

$$\downarrow^{w(X_{P_{i}}), \text{ if } 0 \le X_{P_{i}} \le 10$$

$$w(X_{T_{j}}, X_{P_{i}}), \text{ if } |X_{T_{j}} - X_{P_{i}}| < 1$$

$$w(B_{S_{j}}, X_{T_{j}}), \text{ if } B_{S_{j}} \Rightarrow X_{T_{j}} > 2$$

SMT formula Δ

weight functions $\,\mathcal{W}\,$

SMT + weights = Weighted Model Integration

$$\bigwedge_{i} 0 \le X_{P_{i}} \le 10$$

$$\bigwedge_{j} \bigwedge_{i \in T_{j}} |X_{T_{j}} - X_{P_{i}}| < 1$$

$$\bigwedge_{j} (B_{S_{j}} \Rightarrow X_{T_{j}} > 2)$$

complex support

densities

(unnormalized)

 $\mathsf{Pr}_{\Delta}(\mathbf{X}, \mathbf{B})$

SMT + densities = Weighted Model Integration

Given an SMT(\mathcal{LRA}) formula Δ over continuous vars $\mathbf X$ and discrete ones $\mathbf B$, and weight function $\mathcal W$, the **weighted model integral** (WMI) is

$$\mathsf{WMI}(\Delta, \mathcal{W}; \mathbf{X}, \mathbf{B}) \triangleq \sum_{\boldsymbol{b} \in \mathbb{B}^{|\mathbf{B}|}} \int_{(\mathbf{x}, \boldsymbol{b}) \models \Delta} w(\mathbf{x}, \boldsymbol{b}) \, d\mathbf{x}.$$

i.e., computing the **partition function** of the unnormalized distribution \Pr_{Δ} \implies i.e., integrating the weighted volumes of the feasible regions of $\Delta!$

Belle et al., "Probabilistic inference in hybrid domains by weighted model integration", 2015



"What is the probability of team T_1 to outperform team T_2 , if T_1 is a squad but T_2 is not?"



Advanced probabilistic reasoning

$$\Phi_S: (B_{S_1}=1 \wedge B_{S_2}=0) \implies T_1 \text{ is a squad}, \ T_2 \text{ is not}$$
 $\Phi_T: (X_{T_1}>X_{T_2}) \implies T_1 \text{ outperforms } T_2$



Advanced probabilistic reasoning

$$\Phi_S: (B_{S_1}=1 \land B_{S_2}=0) \qquad \Longrightarrow \quad T_1 \text{ is a squad}, \ T_2 \text{ is not}$$

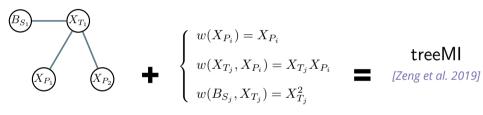
$$\Phi_T: (X_{T_1}>X_{T_2}) \qquad \Longrightarrow \quad T_1 \text{ outperforms } T_2$$

$$\mathsf{Pr}_{\Delta}(\Phi_T \mid \Phi_S) = \frac{\mathsf{WMI}(\Delta \land \Phi_T \land \Phi_S, \mathcal{W})}{\mathsf{WMI}(\Delta \land \Phi_S, \mathcal{W})} = \frac{4,206}{7,225} \approx 58.22\%$$

conditional probabilities as a ratio of two weighted model integrals



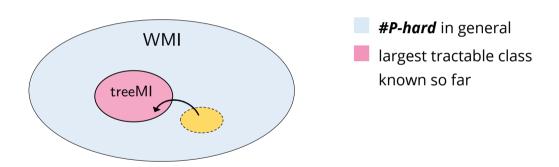
treeMI

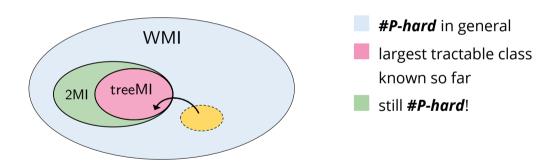


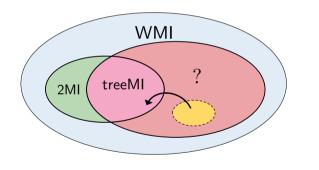
tree-shaped primal graph

constrained monomials ${\cal W}$

polytime WMI inference

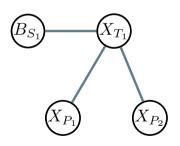






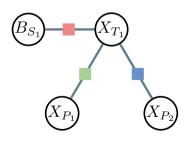
- #**P-hard** in general
- largest tractable class known so far
 - still #P-hard!
- can we do better?

We frame tractable WMI inference at scale as a *message passing* scheme...



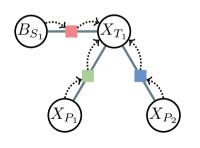
...on primal graphs...

We frame tractable WMI inference at scale as a *message passing* scheme...



...on primal graphs turned into *factor graphs*

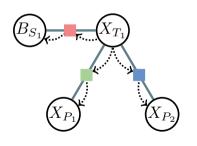
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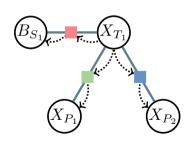
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...on primal graphs turned into *factor graphs*

comprising an *upward* and a *downward* pass

We frame tractable WMI inference at scale as a *message passing* scheme...

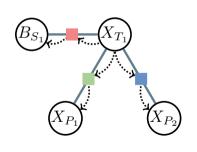


...on primal graphs turned into *factor graphs*

- comprising an *upward* and a *downward* pass
- exchanging messages from *node to factors*

$$\mathbf{m}_{x_i \to f_{\mathcal{S}}}(x_i) = \prod\nolimits_{f_{\mathcal{S}'} \in \mathsf{neigh}(x_i) \backslash f_{\mathcal{S}}} \mathbf{m}_{f_{\mathcal{S}'} \to x_i}(x_i)$$

We frame tractable WMI inference at scale as a *message passing* scheme...



...on primal graphs turned into *factor graphs*

- comprising an *upward* and a *downward* pass
- exchanging messages from *node to factors*
- and from *factors to nodes*

$$\mathbf{m}_{f_{ij} \rightarrow x_i}(x_i) = \int f_{ij}(x_i, x_j) \cdot \mathbf{m}_{x_j \rightarrow f_{ij}}(x_j) \ dx_j$$

Which parametric family Ω for weights to **guarantee tractable WMI inference**?

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$$\begin{split} \mathbf{m}_{f_{ij} \to x_i}(x_i) &= \int \prod_{\Gamma \in \Delta_{\mathcal{S}}} [\![\mathbf{x}_{\mathcal{S}} \models \Gamma]\!] \prod_{\ell \in \mathcal{L}_{\Gamma}} w_{\ell}(\mathbf{x}_{\mathcal{S}})^{[\![\mathbf{x}_{\mathcal{S}} \models \ell]\!]} \cdot \mathbf{m}_{x_j \to f_{ij}}(x_j) \, dx_j \\ \mathbf{m}_{x_i \to f_{\mathcal{S}}}(x_i) &= \prod_{f_{\mathcal{S}'} \in \mathsf{neigh}(x_i) \backslash f_{\mathcal{S}}} \mathbf{m}_{f_{\mathcal{S}'} \to x_i}(x_i) \end{split}$$

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Weights $\mathcal{W} \in \Omega$ should be *closed under product*...

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Weights $\mathcal{W} \in \Omega$ should be *closed under product*, *closed under integration*, *and tractable for symbolic integration*

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Weights $\mathcal{W} \in \Omega$ should be *closed under product, closed under integration, and tractable for symbolic integration*

⇒ e.g., arbitrary polynomials, exponentiated linear polynomials, etc.



An SMT formulation induces a piecewise weight representation

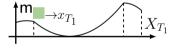
⇒ strikingly different from message passing for classical PGMs!

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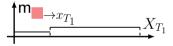


An SMT formulation induces a *piecewise weight representation*

⇒ strikingly different from message passing for classical PGMs!







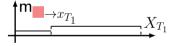


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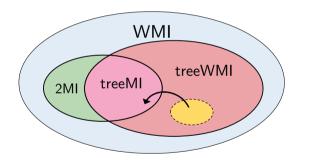
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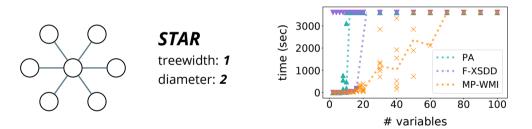
The number of all pieces in MP-WMI is $\mathcal{O}(4nc)^{2d+2}$, where d is the graph diameter \implies the primal graph should have a **bounded diameter!**



- #P-hard in general
- the largest tractable class known before
 - still #P-hard
- new largest class!

Scaling-up inference

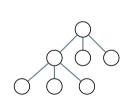
Large set of synthetic benchmarks up to **N** = **100** vars, 5 trials, different primal graphs



MP-WMI takes a *fraction of the time* of other exact WMI solvers like PA [Morettin et al. 2017] and F-XSDD [Zuidberg Dos Martires et al. 2019]

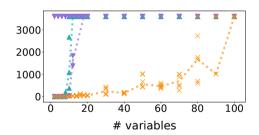
Scaling-up inference

Large set of synthetic benchmarks up to **N** = **100** vars, 5 trials, different primal graphs



SNOW

treewidth: 1 diameter: log(N)



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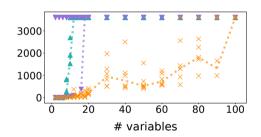
Scaling-up inference

Large set of synthetic benchmarks up to **N** = **100** vars, 5 trials, **different primal graphs**



PATH

treewidth: **1** diameter: **N**

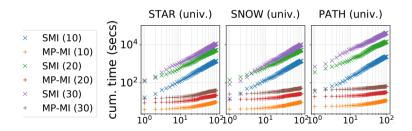


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Query amortization

A single message exchange allows to amortize univariate and bivariate queries

⇒ also all marginals and all moments!



MP-WMI answers 100 WMI queries faster than competitors solving 10 [Zeng et al. 2019]

Real-world data is *noisy*...

Real-world data is *noisy*, *complex*...

Real-world data is *noisy*, *complex* and *mixed continuous-discrete*...

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The WMI framework is very appealing for probabilistic inference in the real-world!

Real-world data is *noisy*, *complex* and *mixed continuous-discrete*...

The WMI framework is very appealing for probabilistic inference in the real-world! MP-WMI delivers fast inference and defines the **largest class of tractable WMI models**

Real-world data is *noisy*, *complex* and *mixed continuous-discrete*...

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Next

However, MP-WMI requires tree-shaped bounded diameter primal graphs



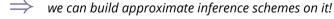
we can build approximate inference schemes on it!

Real-world data is *noisy*, *complex* and *mixed continuous-discrete*...

The WMI framework is very appealing for probabilistic inference in the real-world! MP-WMI delivers fast inference and defines the **largest class of tractable WMI models**

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However, MP-WMI requires tree-shaped bounded diameter primal graphs





github.com/UCLA-StarAI/mpwmi

References I

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