

Statistical Relational AI

Exploiting Symmetries

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Agenda

- ▶ Introduction [Tanya]
- ▶ Exploiting Symmetries
 - in Probabilistic Graphical Models [Marcel]

Focus Topic II

- ▶ Exploiting Symmetries
 - in Conditional Knowledge Bases [Marco]
 - Relational Probabilistic Conditionals
 - Principle of Maximum Entropy
 - Conditional Knowledge Compilation

- ▶ Summary [Tanya]

Relational Probabilistic Conditionals

Relational Background Theory

Definition (Function-free First-order Language)

$\mathcal{L}(\Sigma)$ is a **function-free first-order language** over a finite signature $\Sigma = (\text{Pred}, \text{Const})$.

- ▶ Sentences in $\mathcal{L}(\Sigma)$ interpreted based on **Herbrand semantics**.
 \rightsquigarrow Interpretations $\hat{=}$ truth assignment on ground atoms.
- ▶ Interpretations serve as **possible worlds** $\omega \in \Omega(\Sigma)$.
- ▶ Controlling **domain size** $k = |\text{Const}|$ crucial for tractable reasoning.

$\mathcal{L}(\Sigma) \hat{=}$ **relational language** with quantifiers; quantifiers do not extend expressivity but **convey symmetries**.

\rightsquigarrow Proper handling essential, esp. for efficient **model counting**.

Closed Conditionals

Definition (Closed Conditional)

$(B|A)[\xi]$ is a **closed conditional** if $A, B \in \mathcal{L}(\Sigma)$ are sentences and $\xi \in [0, 1]$.

- ▶ Informal meaning:

“If A holds, then B follows with probability ξ .”

- ▶ Formal interpretation via **conditional probabilities**.

Definition (Probabilistic Model)

$\mathcal{P}: \Omega(\Sigma) \rightarrow [0, 1]$ is a **probabilistic model** of a closed conditional $(B|A)[\xi]$, written

$$\mathcal{P} \models (B|A)[\xi] \quad \text{iff} \quad \mathcal{P}(A) > 0 \quad \text{and} \quad \mathcal{P}(B|A) = \xi.$$

$$(\mathcal{P}(A) = \sum_{\omega \models A} \mathcal{P}(\omega))$$

Open Conditionals

Definition (Open Conditional)

$(B|A)[\xi]$ is an **(open) conditional** if $A, B \in \mathcal{L}(\Sigma)$ are **formulas** and $\xi \in [0, 1]$.

Example

“Patients who show symptom s suffer from disease d with probability 0.6.”

- ▶ s, d as **nullary predicates**: closed conditional $(d|s)[0.6]$.
(no linkage to individuals)
- ▶ s, d as **unary predicates**: open conditional $(d(X)|s(X))[0.6]$.

Problem Open conditionals need **richer semantics** than conditional probabilities provide.

Grounding Semantics

Idea Understand open conditionals as **schemata** / **universally quantified**.

Definition (Grounding Semantics)

\mathcal{P} probability distribution, $r = (B|A)[\xi]$ (open) conditional, and $\text{grnd}_{\text{Const}}(r)$ set of proper groundings of r . Then,

$$\mathcal{P} \models_{\text{gs}} r \quad \text{iff} \quad \forall r' \in \text{grnd}_{\text{Const}}(r): \mathcal{P} \models r'.$$

Example

$(d(X)|s(X))[0.6]$ shortcut for $\{(d(p)|s(p))[0.6] \mid p \in \text{Const}\}$.

Problem Not compatible with **atypical individuals**
(e.g., if $\exists p \in \text{Const}: (d(p)|(s(p)))[0.3]$).

Averaging Semantics

Idea Understand probabilities as **arithmetic mean**.

Definition (Averaging Semantics [Kern-Isberner, Thimm 2010])

\mathcal{P} , r , $\text{grnd}_{\text{Const}}(r)$ as before. Then,

$$\mathcal{P} \models_{\text{as}} r \quad \text{iff} \quad \frac{\sum_{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r)} \mathcal{P}(B'|A')}{|\text{grnd}_{\text{Const}}(r)|} = \xi.$$

Example

$$\mathcal{P} \models_{\text{as}} ((d(X))|s(X))[0.6] \quad \text{iff} \quad \frac{\sum_{p \in \text{Const}} \mathcal{P}(d(p)|s(p))}{|\text{Const}|} = 0.6.$$

Problem In general, set of models **not convex**.

\rightsquigarrow Maximum entropy model **not unique**.

Aggregating Semantics (I/IV)

Idea **Statistic** probabilities from a **subjective** point of view.

Definition (Aggregating Semantics [Kern-Isberner, Thimm 2010])

\mathcal{P} , r , $\text{grnd}_{\text{Const}}(r)$ as before. Then,

$$\mathcal{P} \models r \quad \text{iff} \quad \frac{\sum_{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r)} \mathcal{P}(A' \wedge B')}{\sum_{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r)} \mathcal{P}(A')} = \xi.$$

Example

$$\mathcal{P} \models ((d(X))|s(X))[0.6] \quad \text{iff} \quad \frac{\sum_{p \in \text{Const}} \mathcal{P}(s(p) \wedge d(p))}{\sum_{p \in \text{Const}} \mathcal{P}(s(p))} = 0.6.$$

possible worlds included multiple times \rightsquigarrow double sums

Aggregating Semantics (II/IV)

Definition (Aggregating Semantics [Kern-Isberner, Thimm 2010])

\mathcal{P} , r , $\text{grnd}_{\text{Const}}(r)$ as before. Then,

$$\mathcal{P} \models r \quad \text{iff} \quad \frac{\sum_{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r)} \sum_{\omega \models A' \wedge B'} \mathcal{P}(\omega)}{\sum_{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r)} \sum_{\omega \models A'} \mathcal{P}(\omega)} = \xi.$$

For each ground instance, WFOMC tasks with weights that have to be calculated. (here, \mathcal{P} will be inferred from a knowledge base)

Problem Can this be done efficiently?

\rightsquigarrow Only if WFOMC tasks are **symmetric**.

(to some extent)

Aggregating Semantics (III/IV)

Definition (Conditional Structure (I/II) [Kern-Isberner 2004])

$r = (B|A)[\xi]$ conditional, ω possible world. Then,

$$\text{ver}_r(\omega) = |\{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r) \mid \omega \models A' \wedge B'\}|,$$

$$\text{fal}_r(\omega) = |\{(B'|A')[\xi] \in \text{grnd}_{\text{Const}}(r) \mid \omega \models A' \wedge \neg B'\}|.$$

Definition (Aggregating Semantics [Kern-Isberner, Thimm 2010])

Let \mathcal{P} , r , $\text{grnd}_{\text{Const}}(r)$ as before. Then,

$$\mathcal{P} \models r \quad \text{iff} \quad \frac{\sum_{\omega \in \Omega(\Sigma)} \text{ver}_r(\omega) \cdot \mathcal{P}(\omega)}{\sum_{\omega \in \Omega(\Sigma)} (\text{ver}_r(\omega) + \text{fal}_r(\omega)) \cdot \mathcal{P}(\omega)} = \xi.$$

Aggregating Semantics (IV/IV)

Justification of Aggregating Semantics

Statistic probabilities in extreme cases,
otherwise statistics weighted by subjective beliefs.

Case 1 Reasoner is certain about model of real world
 $\rightsquigarrow \mathcal{P}(\omega') = 1$ for a single possible world ω' . Then,

$$\mathcal{P} \models r \quad \text{iff} \quad \frac{\text{ver}_r(\omega')}{\text{ver}_r(\omega') + \text{fal}_r(\omega')} = \xi.$$

Case 2 Reasoner is maximally uncertain

$\rightsquigarrow \mathcal{P}(\omega) = \frac{1}{|\Omega(\Sigma)|}$ for $\omega \in \Omega(\Sigma)$. Then,

$$\mathcal{P} \models r \quad \text{iff} \quad \frac{\sum_{\omega \in \Omega(\Sigma)} \text{ver}_r(\omega)}{\sum_{\omega \in \Omega(\Sigma)} (\text{ver}_r(\omega) + \text{fal}_r(\omega))} = \xi.$$

Probabilistic Inference Task

Definition (Knowledge Base)

$\mathcal{R} = (\mathcal{F}, \mathcal{B})$ is a **knowledge base** if \mathcal{F} is finite set of sentences and \mathcal{B} finite set of non-deterministic conditionals ($\xi \notin \{0, 1\}$).

- ▶ Sentences ($\hat{=}$ facts) force specific possible worlds to have **probability zero** / **restrict probability space**.

$$\rightsquigarrow \Omega_{\mathcal{F}}(\Sigma) = \{\omega \in \Omega(\Sigma) \mid \omega \models \mathcal{F}\}.$$

Definition (Probabilistic Inference Task)

\mathcal{R} consistent knowledge base. Then,

- 1 Calculate model \mathcal{P} of \mathcal{R} . (model selection task)
- 2
 - a Given conditional r , **decide** $\mathcal{R} \models_{\mathcal{P}} r$?
 - b Given formulas A, B , **calculate** ξ such that $\mathcal{R} \models_{\mathcal{P}} (B|A)[\xi]$.

Principle of Maximum Entropy

Maximum Entropy Model (I/III)

Model selection $\hat{=}$ from knowledge base to belief state.

In principal not necessary. E.g., also possible:

$$\mathcal{R} \models_{\mathcal{P}} r \quad \text{if} \quad \mathcal{P} \models r \quad \text{for all models } \mathcal{P} \text{ of } \mathcal{R}.$$

Problem Leads to few / uninformative inferences.

Idea Select model which infers conditionals with **most expected probability** / which adds **least information**.

Definition (Maximum Entropy Model [cf. Paris 1994])

\mathcal{R} consistent knowledge base. Then,

$$ME_{\mathcal{R}} = \arg \max_{\mathcal{P} \models \mathcal{R}} - \sum_{\omega \in \Omega_{\mathcal{F}}(\Sigma)} \mathcal{P}(\omega) \cdot \log \mathcal{P}(\omega).$$

Maximum Entropy Model (II/III)

Proposition

\mathcal{R} consistent knowledge base. Then,

$$\text{ME}_{\mathcal{R}} \models \mathcal{R}. \quad (\text{i.e., } \text{ME}_{\mathcal{R}} \models r \forall r \in \mathcal{R})$$

- ▶ $\text{ME}_{\mathcal{R}}$ **unique solution** of convex optimization problem.
↪ Dual optimization problem [cf. Boyd, Vandenberghe 2004].

Product Representation

$$r_i = (B_i | A_i)[\xi_i]$$

\mathcal{R} p-consistent*, $\mathcal{B} = \{r_1, \dots, r_n\}$. Then, there is $\vec{\alpha} \in \mathbb{R}_{>0}^n$ s.t.

$$\text{ME}_{\mathcal{R}}(\omega) = \alpha_0 \cdot \prod_{i=1}^n \alpha_i^{\text{ver}_{r_i}(\omega) - \xi_i \cdot (\text{ver}_{r_i}(\omega) + \text{fal}_{r_i}(\omega))}, \quad \omega \in \Omega_{\mathcal{F}}(\Sigma).$$

(α_0 normalization constant)

*) has positive model on $\Omega_{\mathcal{F}}(\Sigma)$, i.e., 0-1-probabilities forced by sentences only

Maximum Entropy Model (III/III)

$$\text{ME}_{\mathcal{R}}(\omega) = \alpha_0 \cdot \prod_{i=1}^n \alpha_i^{\text{ver}_{r_i}(\omega) - \xi_i \cdot (\text{ver}_{r_i}(\omega) + \text{fal}_{r_i}(\omega))}$$

- ▶ Optimize for $\vec{\alpha}$ (n -many values; constant in k)
instead of $\text{ME}_{\mathcal{R}}$. ($|\Omega(\Sigma)|$ -many values; exponential in k)

Definition (Conditional Structure (II/II) [Kern-Isberner 2004])

\mathcal{R} knowledge base, $\omega, \omega' \in \Omega_{\mathcal{F}}(\Sigma)$. Then,

$$\sigma_{\mathcal{R}}(\omega) = ((\text{ver}_{r_i}(\omega), \text{fal}_{r_i}(\omega)))_{i=1}^n, \quad (\text{conditional structure})$$

$$\omega \sim_{\sigma_{\mathcal{R}}} \omega' \quad \text{iff} \quad \sigma_{\mathcal{R}}(\omega) = \sigma_{\mathcal{R}}(\omega'). \quad (\text{conditional equivalence})$$

Principle of Conditional Indifference [Kern-Isberner 2004]

$$\omega \sim_{\sigma_{\mathcal{R}}} \omega' \implies \text{ME}_{\mathcal{R}}(\omega) = \text{ME}_{\mathcal{R}}(\omega'), \quad \omega, \omega' \in \Omega_{\mathcal{F}}(\Sigma).$$

Maximum Entropy Inference

Definition (Maximum Entropy Inference Relation)

\mathcal{R} consistent knowledge base, r conditional. Then,

$$\mathcal{R} \sim_{\text{ME}} r \quad \text{iff} \quad \text{ME}_{\mathcal{R}} \models r.$$

Task 1 Given \mathcal{R} , approximate $\vec{\alpha}$.

Task 2 Given approximation $\vec{\alpha}^*$ and r , decide $\text{ME}_{\mathcal{R}}^* \models r$.

Evolution of Iterative Scaling Methods for Task 1

- ▶ Generalized iterative scaling (approx. $\text{ME}_{\mathcal{R}}$) [Darroch, Ratcliff 1972]
- ▶ Improved iterative scaling (approx. $\vec{\alpha}$)
[Berger, Della Pietra, Della Pietra 1996]
- ▶ Iterative scaling + conditional equivalence [Finthammer, Beierle 2014]
- ▶ **Condensed iterative scaling** [W, Kern-Isberner, Finthammer, Beierle 2019]

Excursion: Maximum Entropy and MLNs

Definition (Markov Logic Network [Richardson, Domingos 2006])

$\mathcal{N} = \{(F_i, \nu_i) \mid i = 1, \dots, m\}$ is a **Markov logic network (MLN)** if $F_i \in \mathcal{L}(\Sigma)$ are formulas and $\nu_i \in \mathcal{R} \cup \{\infty, -\infty\}$ are weights.

\mathcal{N} specifies probability distribution \nwarrow
for hard constraints

$$\mathcal{P}_{\mathcal{N}}(\omega) = \frac{1}{\eta} \cdot \exp\left(\sum_{i=1}^m \nu_i \cdot \text{cnt}_i(\omega)\right), \quad \omega \in \Omega(\Sigma),$$

with $\text{cnt}_i(\omega) = |\{F'_i \in \text{grnd}_{\text{Const}}(F_i) \mid \omega \models F'_i\}|$. (η normalization constant)

Proposition [W, Kern-Isberner, Finthammer, Beierle 2019]

$\mathcal{R} = (\mathcal{F}, \mathcal{B})$ p-consistent knowledge base (with $r_i = (B_i|A_i)[\xi] \in \mathcal{B}$) and MLN

$$\mathcal{N} = \bigcup_{i=1}^n (\{(A_i \wedge B_i, (1 - \xi_i) \cdot \log \alpha_i)\} \cup \{(A_i \wedge \neg B_i, -\xi_i \cdot \log \alpha_i)\}) \\ \cup \{(\neg F, -\infty) \mid F \in \mathcal{F}\}.$$

Then, $\text{ME}_{\mathcal{R}} = \mathcal{P}_{\mathcal{N}}$.

Conditional Knowledge Compilation

Starting Point/Motivation: Condensed Iterative Scaling

Input: ρ -Consistent knowledge base \mathcal{R}
Output: Approximation $\vec{\alpha}^*$, normalization α_0^*

```
1   $G = \sum_{i=1}^n |\text{grnd}_{\text{Const}}(r_i)|$ 
2   $k = 0$ 
3  FOR  $i = 1, \dots, n$ :  $\alpha_i^k = 1$ 
4  UNTIL  $\langle \text{termination condition} \rangle$  DO :
5       $k \leftarrow k + 1$ 
6  FOR  $i = 1, \dots, n$ :  $\alpha_i^k = \alpha_i^{k-1} \cdot \left( 1 + \frac{\Phi_{\mathcal{R}}^{i,k-1}}{\xi_i \cdot |\text{grnd}_{\text{Const}}(r_i)| \cdot \Phi_{\mathcal{R}}^{k-1}} \right)^{-1/G}$ 
7   $\alpha_0^k = (\Phi_{\mathcal{R}}^k)^{-1}$ 
8  RETURN  $(\alpha_1^k, \dots, \alpha_n^k), \alpha_0^k$ 
```

- ▶ $\lim_{k \rightarrow \infty} (\alpha_1^k, \dots, \alpha_n^k) = \vec{\alpha}$, $\lim_{k \rightarrow \infty} \alpha_0^k = \alpha_0$
- ▶ No expensive iterations ($n = |\mathcal{B}|$ constant in k)

Problem Oracle needed for

$$\Phi_{\mathcal{R}}^{i,k} = \sum_{\omega \in \Omega_{\mathcal{F}}(\Sigma)} (\text{ver}_{r_i}(\omega) + \xi_i \cdot (\text{ver}_{r_i}(\omega) + \text{fal}_{r_i}(\omega))) \cdot \Pi_{\mathcal{R}}^k$$

$$\Phi_{\mathcal{R}}^k = \sum_{\omega \in \Omega_{\mathcal{F}}(\Sigma)} \Pi_{\mathcal{R}}^k, \quad \Pi_{\mathcal{R}}^k = \prod_{j=1}^n (\alpha_j^k)^{\text{ver}_{r_j}(\omega)} \cdot ((\alpha_j^k) - \xi_j)^{(\text{ver}_{r_j}(\omega) + \text{fal}_{r_j}(\omega))}$$

conditional knowledge
compilation is needed
to stay tractable

Conditional Knowledge Compilation (I/III)

- In this tutorial: Focus on

$$\Phi_{\mathcal{R}}^k = \sum_{\omega \in \Omega_{\mathcal{F}}(\Sigma)} \prod_{j=1}^n (\alpha_j^k)^{\text{ver}_{r_j}(\omega)} \cdot ((\alpha_j^k)^{-\xi_j})^{(\text{ver}_{r_j}(\omega) + \text{fal}_{r_j}(\omega))}.$$

$\hat{=}$ normalization (the expensive task in probabilistic reasoning)

- Calculating $\Phi_{\mathcal{R}}^{i,k}$ and answering queries work analogously.

[W, Kern-Isberner, Finthammer, Beierle 2019]

Task: Calculate polynomial and factorize whenever possible:

$$(\Sigma \Pi \rightarrow \Pi \Sigma)$$

$$\phi_{\mathcal{R}}(\vec{x}, \vec{y}) = \sum_{\omega \in \Omega_{\mathcal{F}}(\Sigma)} \prod_{j=1}^n (x_j)^{\text{ver}_{r_j}(\omega)} \cdot (y_j)^{(\text{ver}_{r_j}(\omega) + \text{fal}_{r_j}(\omega))}$$

Example

$$\mathcal{R} = (\emptyset, \{(d(X)|s(X))[0.6]\})$$

► **Naïve approach:**

For each $\omega \in \Omega(\Sigma)$, calculate $\sigma_{\mathcal{R}}(\omega)$. ($4^{|\text{Const}|}$ -many possible worlds)

► **Combinatorial arguments:**

$j = \#$ patients with symptom s , $m = \#$ patients with s and d :

$$\phi_{\mathcal{R}} = \sum_{j=0}^{|\text{Const}|} \sum_{m=0}^j \binom{|\text{Const}|}{j} \binom{j}{m} \cdot x_1^m \cdot y_1^j \cdot 2^{|\text{Const}|-j}$$

► **Exploiting symmetries:**

Impact of all patients the same (treat independently):

$$\phi_{\mathcal{R}} = (x_1 \cdot y_1 + y_1 + 2)^{|\text{Const}|}$$

Conditional Knowledge Compilation (III/III)

Proposition [W, Kern-Isberner, Ecke 2017]

$\mathcal{R} = (\emptyset, \mathcal{B})$ where conditionals are built upon **boolean combinations of unary predicates** (e.g., $(d(X)|_{s_1(X)} \wedge \neg s_2(X))$), $c \in \text{Const}$. Then,

$$\mathcal{R} \sim_{\text{ME}} (B|A)[\xi] \quad \text{iff} \quad \mathcal{R}\langle c \rangle \sim_{\text{ME}} (B\langle c \rangle|A\langle c \rangle)[\xi]$$

independent of $|\text{Const}|$! ($A\langle c \rangle = A$ grounded by constant c)

Is there a general framework?

Idea: Translate knowledge base into **structured sentence**,
count **typed models** of structured sentence.

(types reflect conditional structures of models)

\rightsquigarrow **First-order typed model counting**

[W, Finthammer, Kern-Isberner, Beierle 2017]

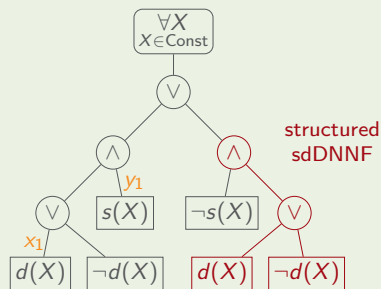
Typed Model Counting (I/III)

Example

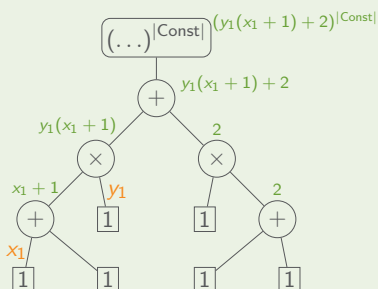
$$\mathcal{R} = (\emptyset, \{(d(X)|s(X))[0.6]\})$$

$$\phi_{\mathcal{R}}^s = \forall X. [y_1 \circ s(X) \wedge (x_1 \circ d(X) \vee \neg d(X)) \vee \neg s(X)]$$

Typed first-order circuit



Algebraic circuit



Typed Model Counting (II/III)

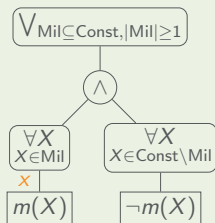
- ▶ Typed model counting works for arbitrary structured sentences as long as no structure elements are in scope of negations. (1)
- ▶ Same model counting techniques as in WFOMC of sentences in sdDNNF can be applied as long as (1) is guaranteed.

Example

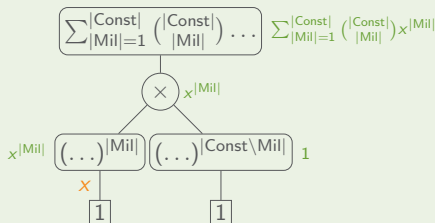
$$\phi^s = \exists X.x \circ m(X)$$

(m = millionaire)

Typed first-order circuit



Algebraic circuit



Typed Model Counting (III/III)

Algebraic Model Counting [Kimmig, Van den Broeck, De Raedt 2017]

- ▶ (Symmetric) WFOMC of sentences.
- ▶ Ground atoms are interpreted by weights.
- ▶ Weights are elements of an algebraic semiring.

Typed Model Counting [W, Finthammer, Kern-Isberner, Beierle 2017]

- ▶ Elements of semiring are written directly into sentence.
- ▶ Ground atoms are interpreted by 1.
- ▶ **Disadvantage:** Structured background language necessary.
- ▶ **Advantage:** No external processing of weights.
↪ Symmetry between weights easy to handle.

Proposition

Typed model counting problems can be transformed into algebraic model counting problems.

Closing Remarks

Summary of Focus Topic II

- ▶ (Only) **open conditionals** make full use of relational language.
- ▶ **Aggregating semantics** gives open conditionals a sophisticated meaning. [Kern-Isberner, Thimm 2010; Thimm, Kern-Isberner 2012]
- ▶ **Principle of maximum entropy** provides a model of conditional knowledge bases which is preferable from an information theoretically point of view, [Jayes 1957; Shannon 1948] and also from a **commonsense** point of view. [Paris, Vencovská 1990; Paris 1994; Paris 1998]
- ▶ Concepts from **symmetric WFOMC** can be transferred to conditional maximum entropy reasoning via **typed model counting / algebraic model counting**. [Van den Broeck 2013; Kimmig, Van den Broeck, De Raedt 2017; W, Finthammer, Kern-Isberner, Beierle 2017]
 \rightsquigarrow In specific cases, drawing **lifted inferences** possible.

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- ▶ Discussion [all]
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