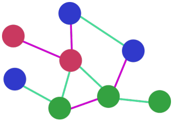
A Complete Characterization of Projectivity for Statistical Relational Models

Manfred Jaeger* and Oliver Schulte**

* Aalborg University
** Simon Fraser University

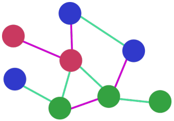
Possible Worlds

Heterogeneous relational structures that allow multiple types of relationships and nodes:



Possible Worlds

Heterogeneous relational structures that allow multiple types of relationships and nodes:



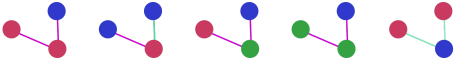
Generative probabilistic model

We are concerned with **families of distributions**:

$$P^{(n)} \qquad (n \in \mathbb{N})$$

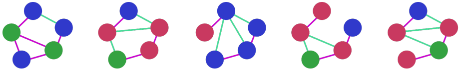
where $P^{(n)}$ is a distribution over n-worlds.

Size 3 worlds:



. . . ➡Distribution $P^{(3)}$

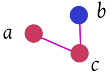
Size 5 worlds:

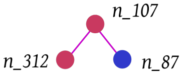


. . . ➡Distribution $P^{(5)}$

Exchangeability

We always assume that all distributions are **exchangeable**:

$P^{(3)}($ 

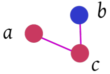
$) = P^{(3)}($ 

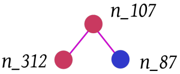
$)$

Isomorphic worlds have the same probability (names of nodes do not matter)!

Exchangeability

We always assume that all distributions are **exchangeable**:

$P^{(3)}($ 

$) = P^{(3)}($ 

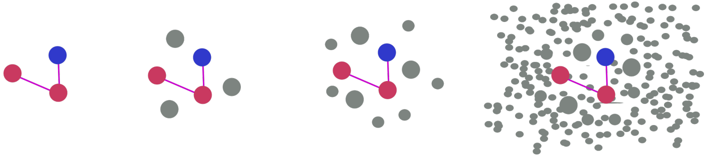
$)$

Isomorphic worlds have the same probability (names of nodes do not matter)!

Why statistical relational models?

- inherently **multi-relational**.
- **inductive:** learning from *training worlds* $\omega_1, \ldots, \omega_N$ (of different sizes); prediction for *query entities* embedded in a new world ω_q.
- **flexible inference:** computation of arbitrary conditional probabilities.

Projectivity



$P^{(3)} = 0.035$ $P^{(6)} = 0.035$ $P^{(12)} = 0.035$ $P^{(3000)} = 0.035$

The probability of a fixed substructure does not depend on the size of the domain it is embedded in.

Can be desirable, because:

- Exact size of domain may be unknown or changing over time.
- Inference complexity independent of domainsize (inference is *extremely lifted*!)
- Avoid *degeneracy:* extreme probabilities (0 or 1) for queries as $n \to \infty$

What we already know

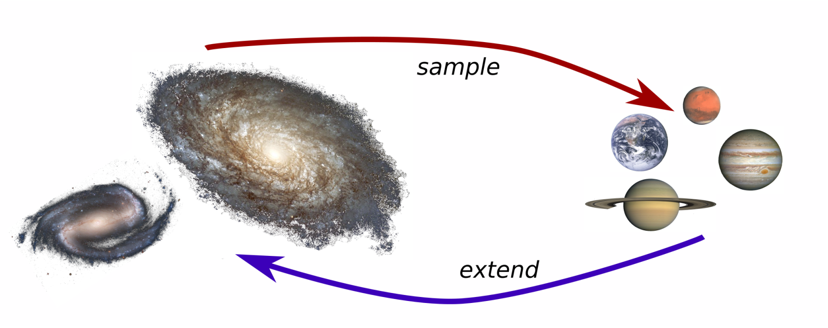
- Most SRL frameworks are not projective.
- Some syntactic fragments of SRL modeling languages identified as projective [Jaeger, Schulte, StarAI 2018].

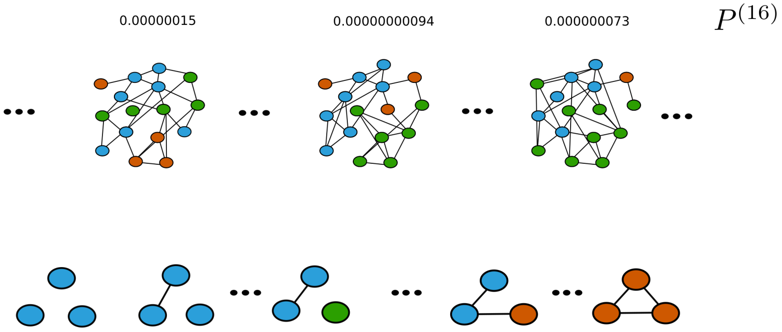
Our question

- What exactly are projective models?
- Can we identify a representation language that can represent **all** projective models, and **only** projective models?

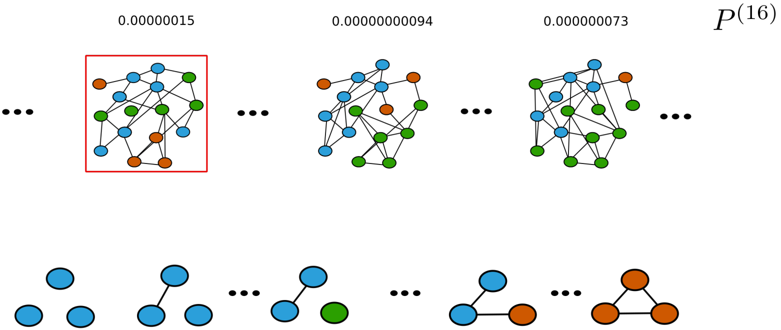
➥On our way towards the answer to these questions, we clarify relationships with several other structural properties of generative families $(P^{(n)})_{n\in\mathbb{N}}$.

Sampling and Extending


sample
extend

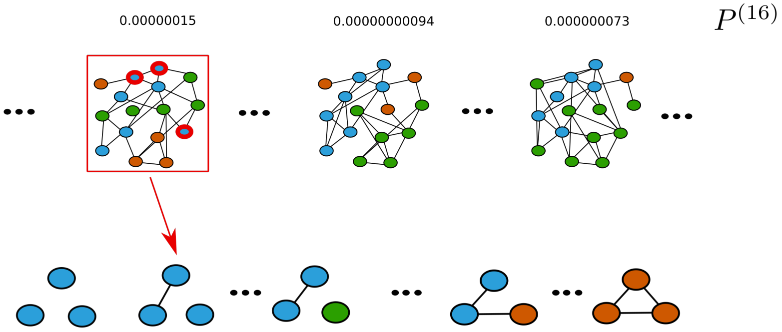


Given: $P^{(n)}$, k<n



Given: $P^{(n)}$, k<n

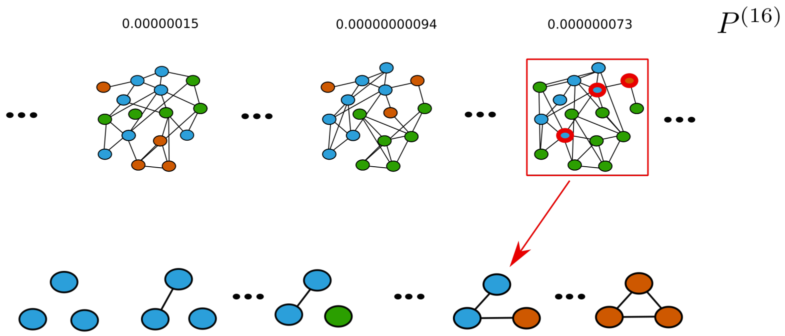
...pick n-world according to $P^{(n)}$



Given: $P^{(n)}$, k<n

. . . pick n-world according to $P^{(n)}$

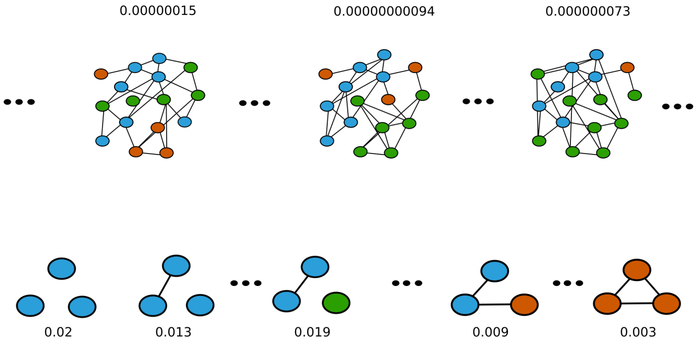
. . . select ordered k-tuple of elements $\rightsquigarrow$ sampled k-world



Given: $P^{(n)}$, k<n

...pick n-world according to $P^{(n)}$

...select ordered k-tuple of elements $\rightsquigarrow$ sampled k-world



$P^{(16)}$

$P^{(16)} \downarrow [3]$

Given: $P^{(n)}$, k<n

... pick n-world according to $P^{(n)}$

... select ordered k-tuple of elements $\rightsquigarrow$ sampled k-world

➥ Obtain sampling/marginal distribution $P^{(n)} \downarrow [k]$

Projectivity: precise

The family $(P^{(n)})_n$ is **projective**, if for all $k < n$:

$$P^{(n)} \downarrow [k] = P^{(k)}.$$

Extendability

$P^{(k)}$ is (projective) **extendable** if for every n there exists $P^{(n)}$ such that

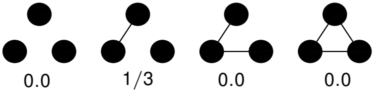
$$P^{(n)} \downarrow [k] = P^{(k)}$$

and the $P^{(n)}$ form a projective family.

Why care about extendability?

- Often use weights/probabilities for small sub-structures (“features”, “motifs”) as the basis for defining a model:
  - *Exponential random graph models, Markov logic networks*
  - Halpern, Bacchus, Grove, Koller: *random worlds approach*
  - Kuželka, Wang, Davis, Schockaert (AAAI 2018): *relational marginals*
- A distribution $P^{(k)}$ (small k) can be seen as prototypical example for such specifications
- Question then: given a specific $P^{(k)}$, can it be consistently generalized to arbitrary $n > k$?

Counterexample



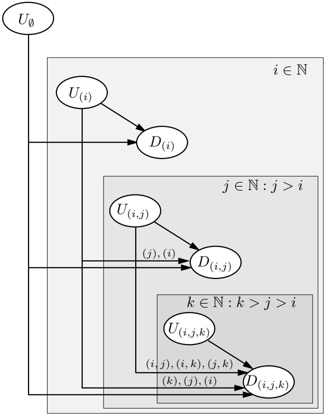
is not extendable (not the marginal of any $P^{(n)}$ with $n \geq 5$).

[related example: Kuželka et al., AAAI 18]

AHK Representations and Representation Theorem

Adaptation of representation of infinite exchangeable arrays by Aldous (1981), Hoover (1979), Kallenberg (2006).

Plate representation for a given *relational signature S* with relations of *maximal arity a*.

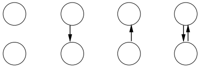


Model components:

D-variables: encode possible world by collecting for $m = 1, \ldots a$ all the m-arity data.

Example $S = \{red/1, edge/2\}$. State space for $D_{(i)}$ variables:

State space for $D_{(i,j)}$ variables:



U-variables: i.i.d., uniform on $[0, 1]$

Conditional distribution of *D*'s given *U*'s defined by deterministic functions $f^{(m)}$ $m = 1, \ldots, a$.

We obtain characterizations of projectivity and extendability:

...for a given $P^{(k)}$:

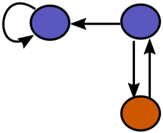
$$P^{(k)} \text{ extendable } \Leftrightarrow P^{(k)} \text{ projective extendable } \Leftrightarrow P^{(k)} \text{ has AHK representation}$$

...for a family $(P^{(n)})_n$:

$$(P^{(n)})_n \text{ projective } \Leftrightarrow (P^{(n)})_n \text{ has AHK representation}$$

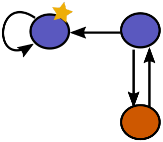
➥AHK models are a maximally expressive framework for “very well behaved” families

The AHK characterization leads to insights into the structure of projective families:



Take a world with positive probability according to $P^{(n)}$,

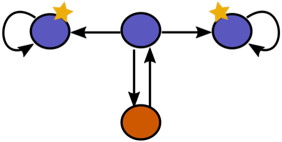
The AHK characterization leads to insights into the structure of projective families:



Take a world with positive probability according to $P^{(n)}$,

...select an arbitrary entity

The AHK characterization leads to insights into the structure of projective families:

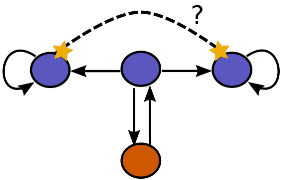


Take a world with positive probability according to $P^{(n)}$,

...select an arbitrary entity

...create a clone of that entity

The AHK characterization leads to insights into the structure of projective families:



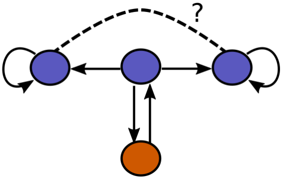
Take a world with positive probability according to $P^{(n)}$,

...select an arbitrary entity

...create a clone of that entity

...relations between clone and original are unspecified

The AHK characterization leads to insights into the structure of projective families:



Take a world with positive probability according to $P^{(n)}$,

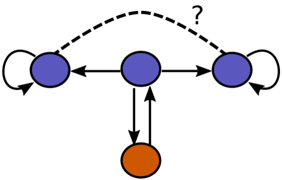
...select an arbitrary entity

...create a clone of that entity

...relations between clone and original are unspecified

➥The resulting *set of* $n+1$-worlds then has a nonzero probability in $P^{(n+1)}$

The AHK characterization leads to insights into the structure of projective families:



Take a world with positive probability according to $P^{(n)}$,

. . . select an arbitrary entity

. . . create a clone of that entity

. . . relations between clone and original are unspecified

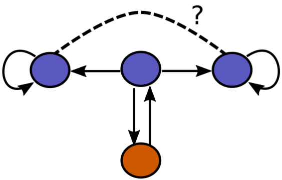
➥ The resulting *set of* $n + 1$-worlds then has a nonzero probability in $P^{(n+1)}$

Counterexample revisited

If $(P^{(n)})_n$ projective:

$P^{(3)}($  $) > 0$

The AHK characterization leads to insights into the structure of projective families:



Take a world with positive probability according to $P^{(n)}$,

...select an arbitrary entity

...create a clone of that entity

...relations between clone and original are unspecified

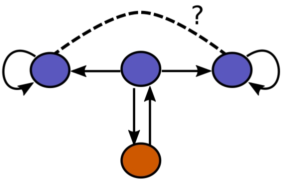
➥ The resulting *set of* $n+1$-worlds then has a nonzero probability in $P^{(n+1)}$

Counterexample revisited

If $(P^{(n)})_n$ projective:

$P^{(3)}($  $) > 0 \Rightarrow P^{(2)}($  $) > 0$

The AHK characterization leads to insights into the structure of projective families:



Take a world with positive probability according to $P^{(n)}$,

. . . select an arbitrary entity

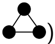
. . . create a clone of that entity

. . . relations between clone and original are unspecified

➥The resulting *set of* $n+1$-worlds then has a nonzero probability in $P^{(n+1)}$

Counterexample revisited

If $(P^{(n)})_n$ projective:

$P^{(3)}($  $) > 0 \Rightarrow P^{(2)}($  $) > 0 \Rightarrow P^{(3)}($ ,  $) > 0$

Done:

- Comprehensive characterization of projectivity and related properties
- In the paper: also analysis of *domain sampling distribution*
- Extended version with proofs: `https://arxiv.org/abs/2004.10984`

Todo:

- Fuller understanding of tradeoff for projective models:
  - Benefits: computational, statistical tractability. Semantic robustness.
  - Drawbacks: limits of expressivity
- Practical implementation of AHK models:
  - how to represent and learn the deterministic functions that map U-variables to D-variables?

Done:

- Comprehensive characterization of projectivity and related properties
- In the paper: also analysis of *domain sampling distribution*
- Extended version with proofs: `https://arxiv.org/abs/2004.10984`

Todo:

- Fuller understanding of tradeoff for projective models:
  - Benefits: computational, statistical tractability. Semantic robustness.
  - Drawbacks: limits of expressivity
- Practical implementation of AHK models:
  - how to represent and learn the deterministic functions that map U-variables to D-variables?

Thanks for watching!