The wondrous world of credal and deep probabilistic circuits

SIPTA Seminar

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Eindhoven University of Technology

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$$1 + (2 \times 3)$$

Overview

Circuits, conceptually

Credal PCs

Probabilistic integral circuits

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Circuits, conceptually

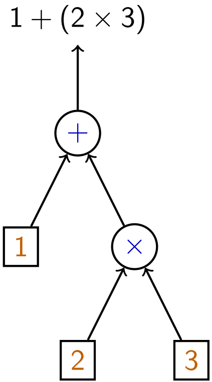
- From expression trees to circuits
- Probabilistic circuits

Credal PCs

Probabilistic integral circuits

Expression trees

- Graphical representation for *expressions*
- Edges show *composition* order
- Nodes show symbols for values and functions



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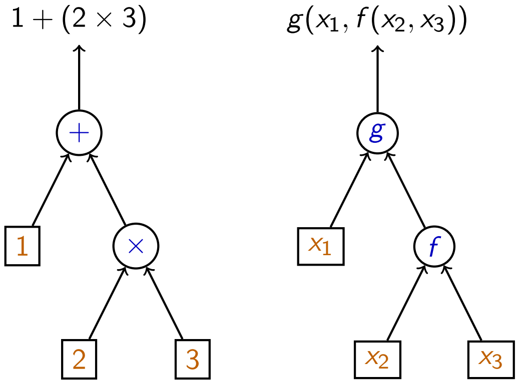

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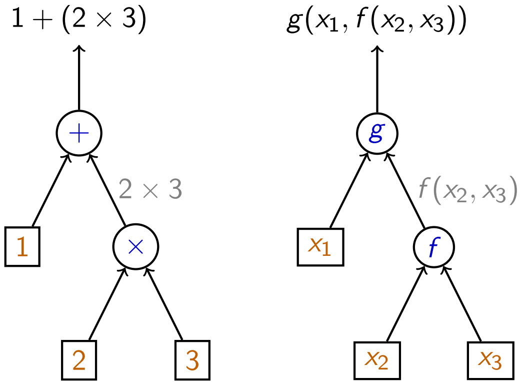
- Edges 'carry' partial *expressions*



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  Need not be a tree; often an SDAG
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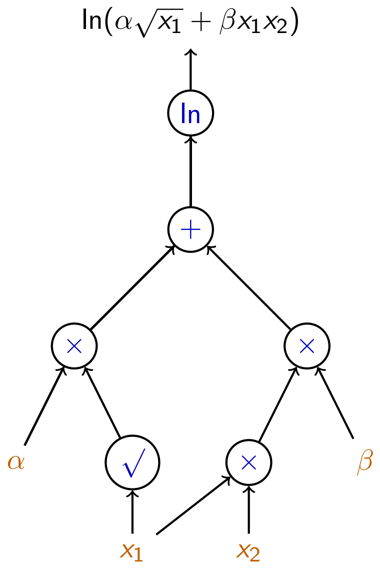

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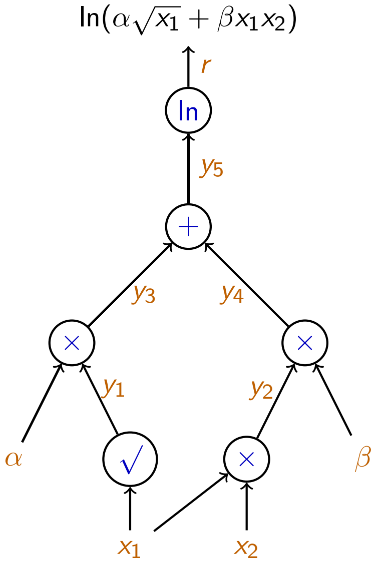

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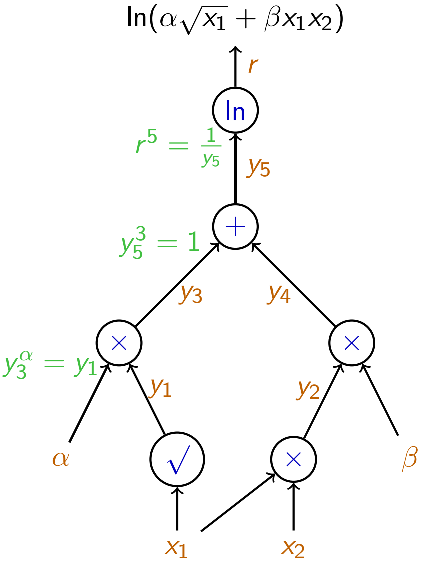

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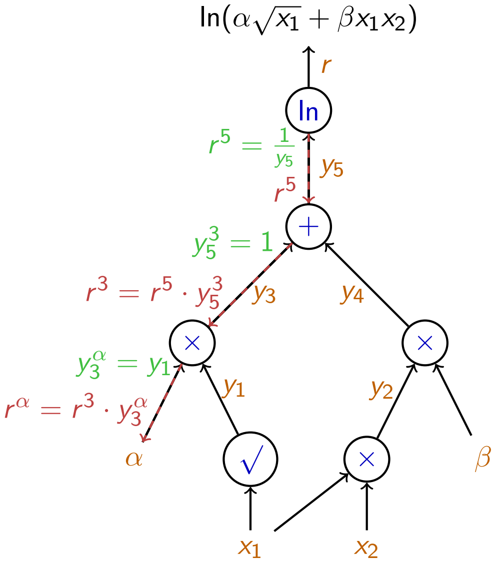

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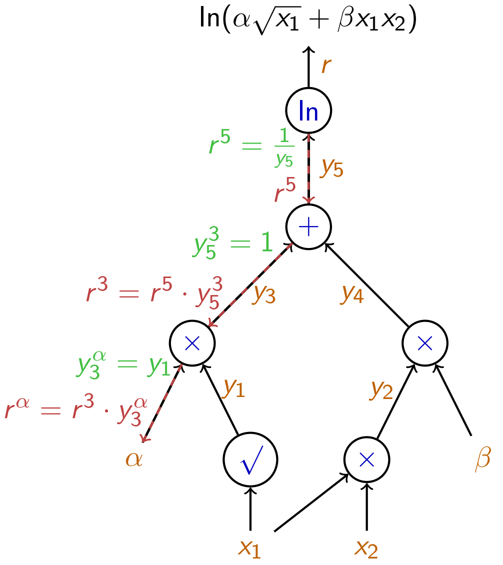
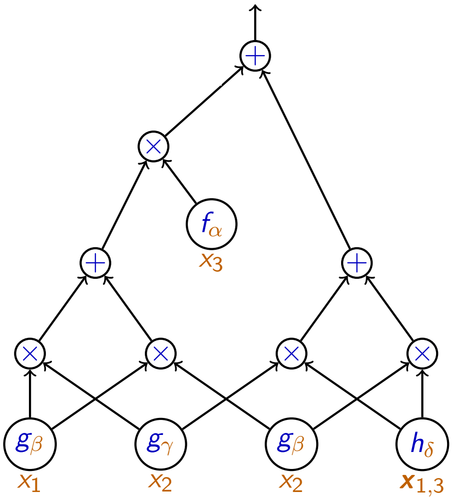
- 'Values' can be multidimensional arrays



Circuits

- Compact representation of computation graph
- Input variables shown to indicate input function arguments
- Parameters are 'attached' to functions



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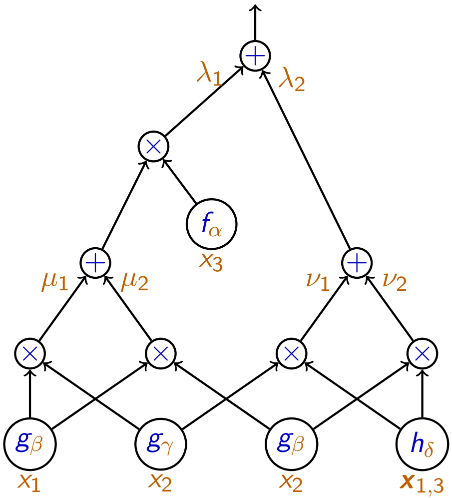

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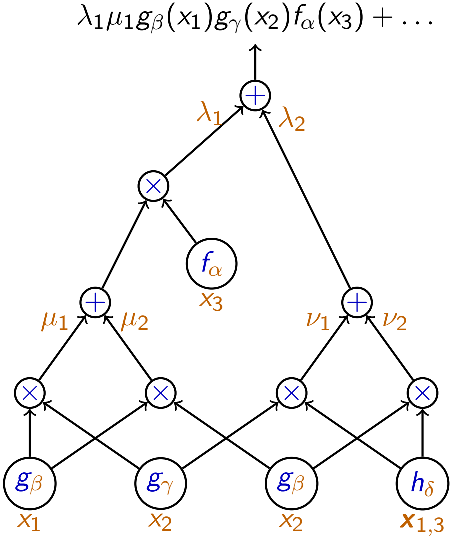

Probabilistic circuits (PCs)

- Circuits where
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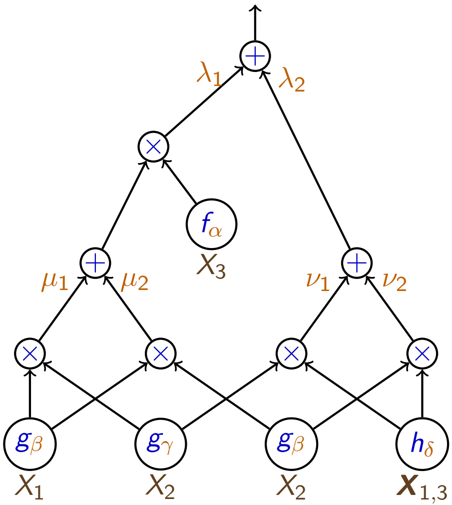
  - input functions are *probability mass functions/densities*
  - weighted sums are *convex mixtures*
  - products represent *independence*
- Output is 'likelihood' for represented joint probability distribution (normalization not always imposed)



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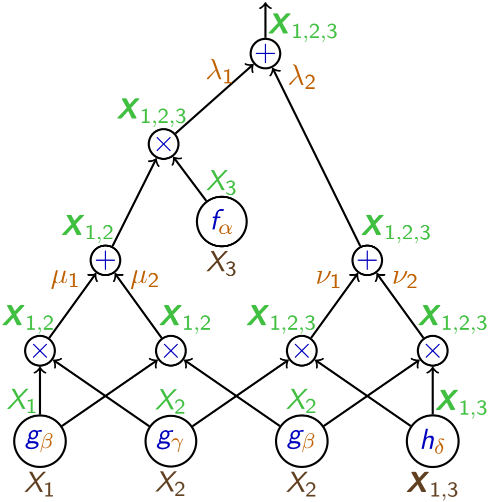
- Important properties: *smoothness, decomposability*



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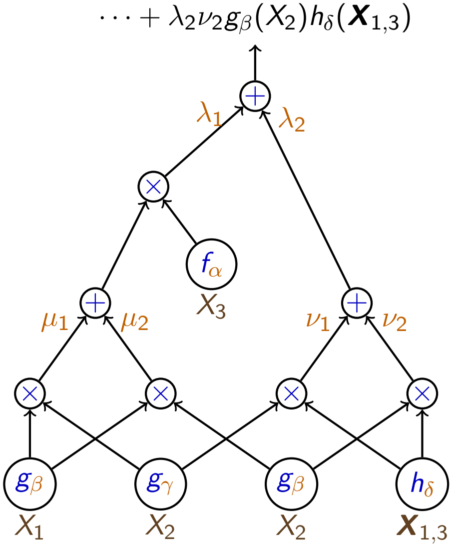
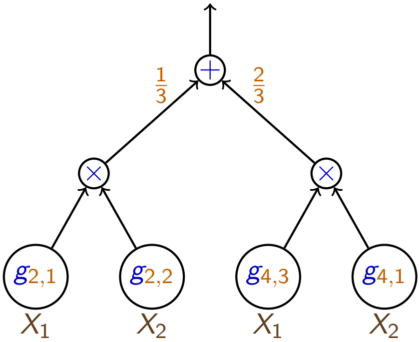


PCs are hierarchical mixture models



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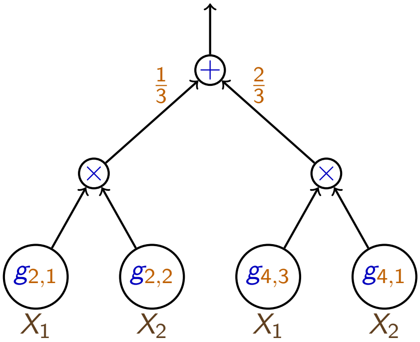

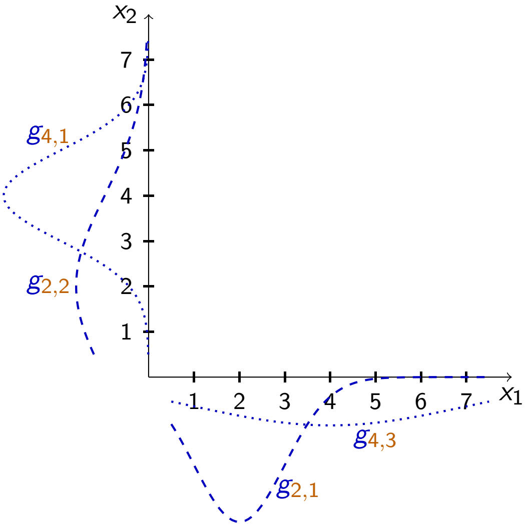

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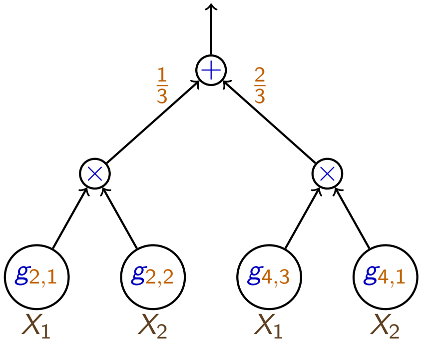

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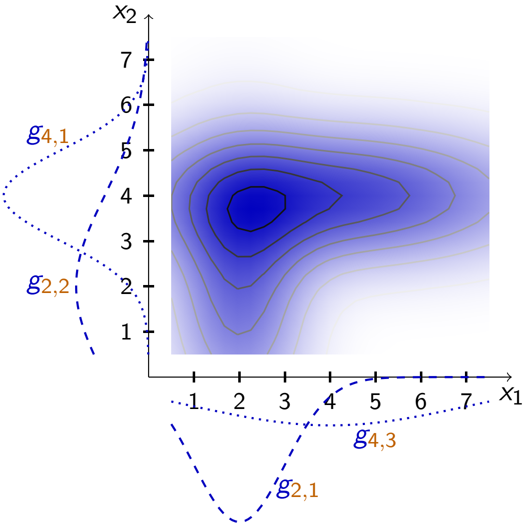

Latent variable interpretation for PCs

- *Latent* random variables
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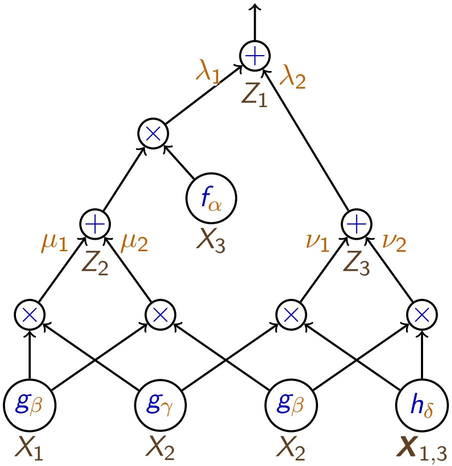

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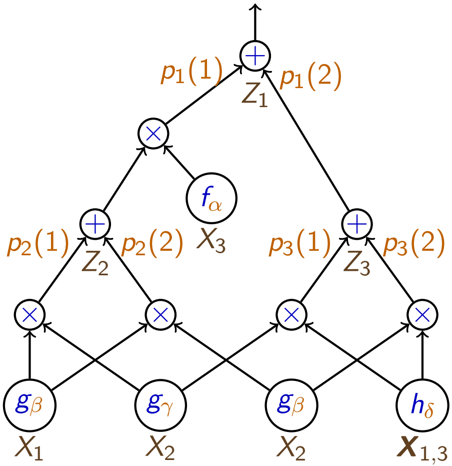

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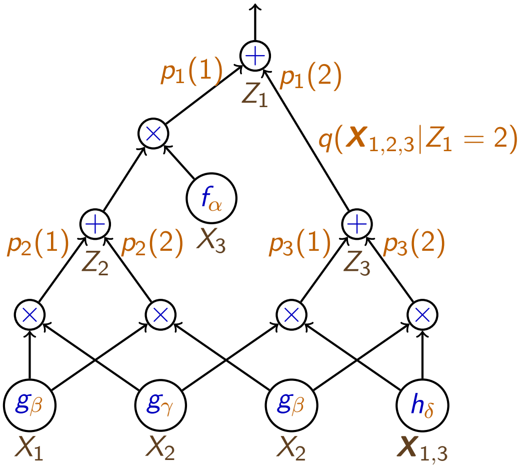

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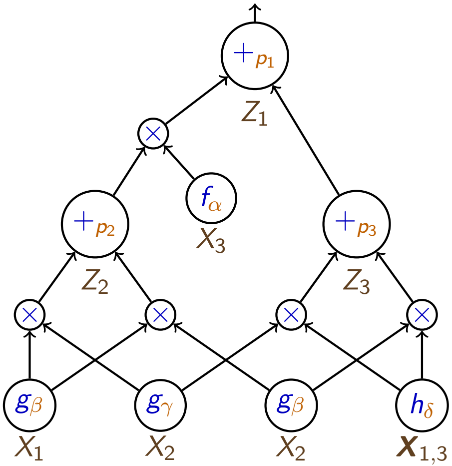

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- *Latent* random variables are associated to sum nodes
- Sum weights are interpreted as probability values
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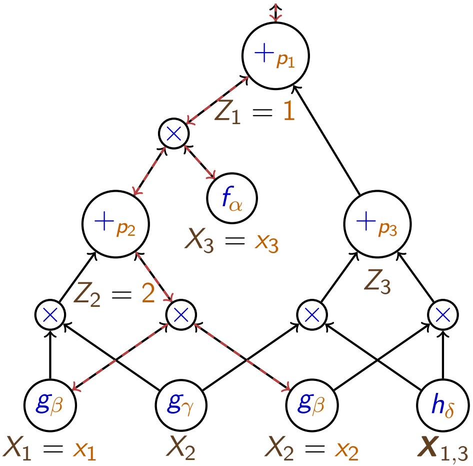
- Sampling the PC:
  - recursively sample the (latent) distributions from root to leaves
  - select single path at sum nodes
  - follow all paths at product nodes



Expectation circuits

- 'Sum' nodes compute *expectations* of functions defined by incoming edge values
- Replace input distributions by their *expectation* operators; input changed from variable values to functions
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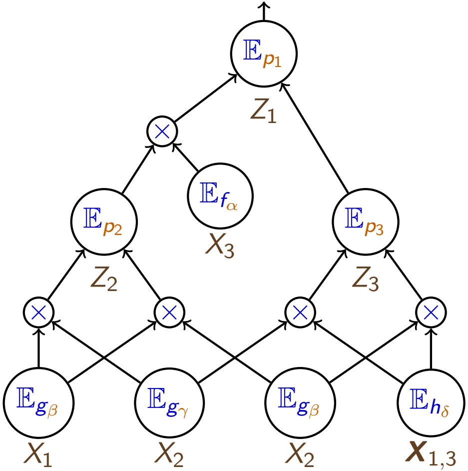

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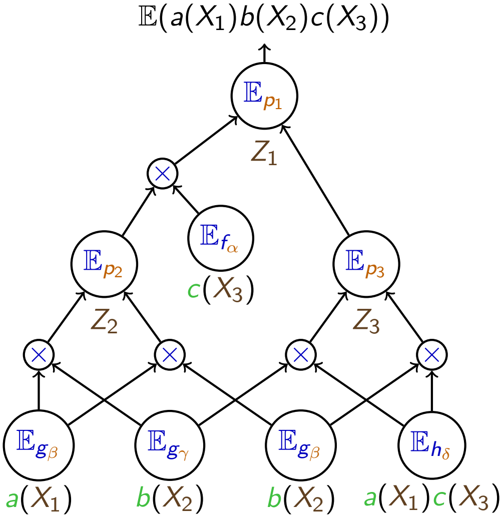
- Joint function must *factorize* for single-pass computation
- Otherwise: use algorithm with only factorizable functions



PCs are often efficient

(Which is why they are popular)

- Class of PCs;
  - each characterized by *size* (number of edges)
  - leaf computation assumed 'efficient'
- Classes of queries:
  - EVI: $\mathbb{E}(a(X_1)b(X_2)c(X_3))$
  - MAR: $\mathbb{E}(a(X_1)b(X_2))$
  - CON: $\mathbb{E}(a(X_1)b(X_2)|X_3 = x_3)$
  - MAP: $\text{argmax}_{\boldsymbol{x}_{1,2}} \mathbb{E}(a(x_1)b(x_2)|X_3 = x_3)$
  - ...

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*A query class is **tractable** for a model class if the computational cost of running such a query on such a model is polynomial in the model's size.*

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- Tractability of PCs:
  - EVI: ✔(single pass, linear)
  - MAR: ✔(single pass, linear)
  - CON: ✔(double pass, linear)
  - MAP: ✘($\geq$ NP-hard)

Overview

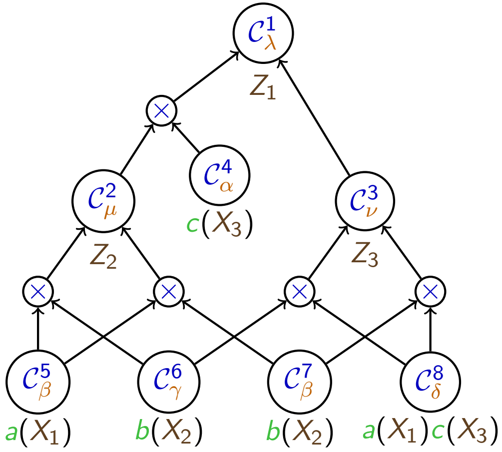
Circuits, conceptually

Credal PCs

- Definition
- Propagation
- Opportunities

Probabilistic integral circuits

Credal PCs (aka credal sum-product networks)



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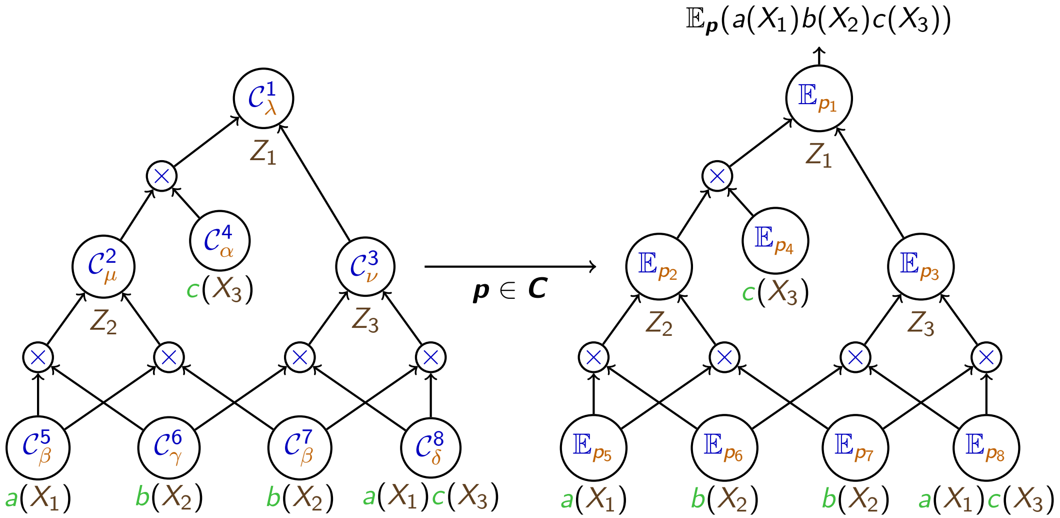
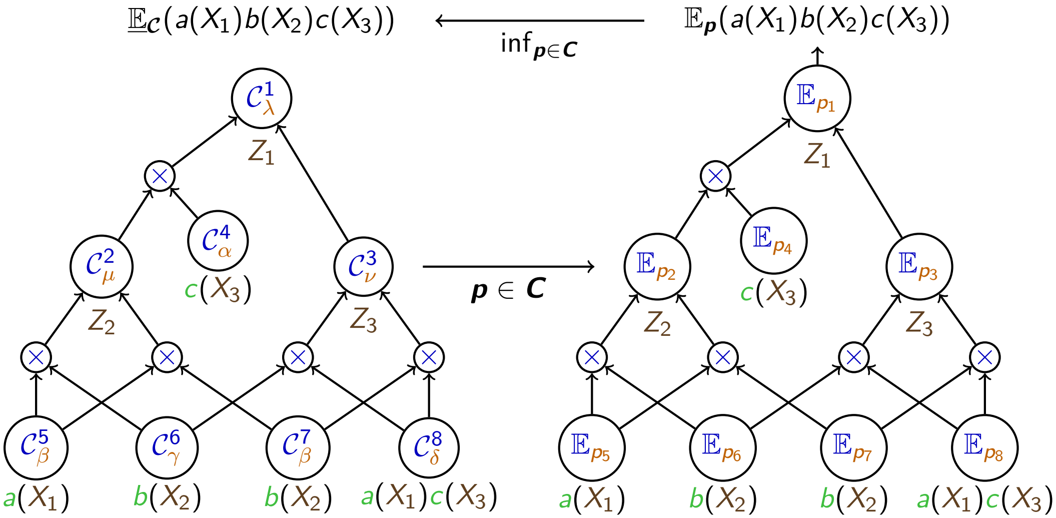


Credal PCs *are defined as lower envelopes of PCs*



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- Assumed that local credal sets are
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  - 'efficient' to work with (linear-vacuous, 2-monotone, simple LP, etc.)

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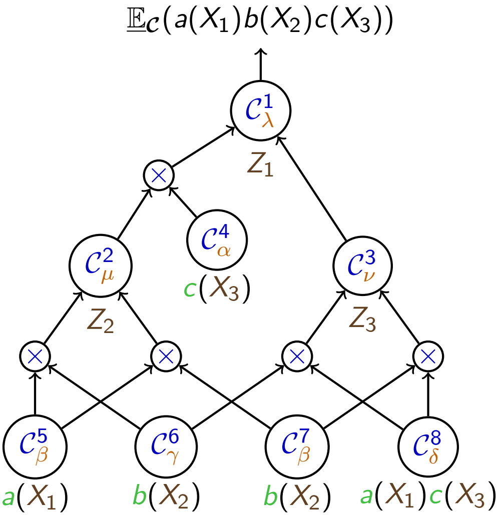
- How to calculate the lower envelope?
  - Gradient descent on PC parameters using backpropagation (likely inefficient, to be combined with constrained optimization in local credal sets)
  - Work directly with lower and upper expectations?

Lower–upper expectation circuits



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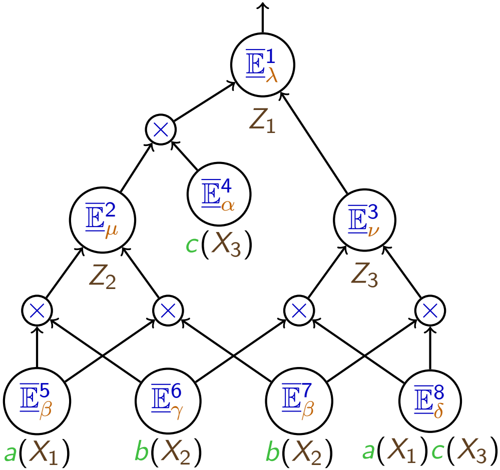

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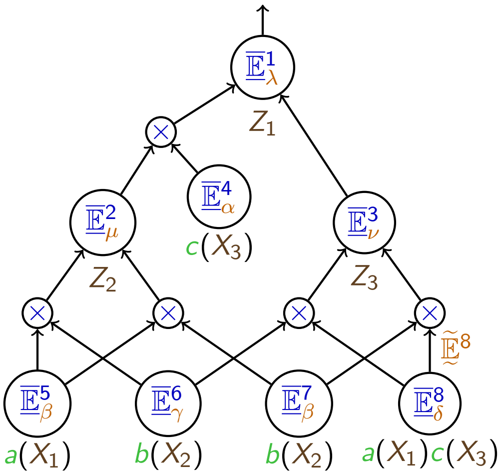

Propagation calculation rules

- Leaf expectation nodes with incoming function d^i:

$$\underset{\sim}{\mathbb{E}}^i = \underline{\mathbb{E}}^i(d^i) \qquad \widetilde{\mathbb{E}}^i = \overline{\mathbb{E}}^i(d^i)$$

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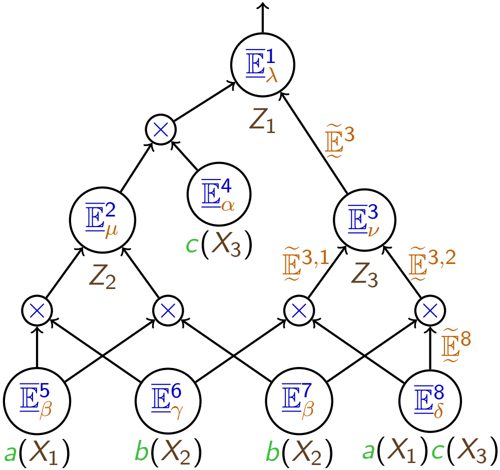

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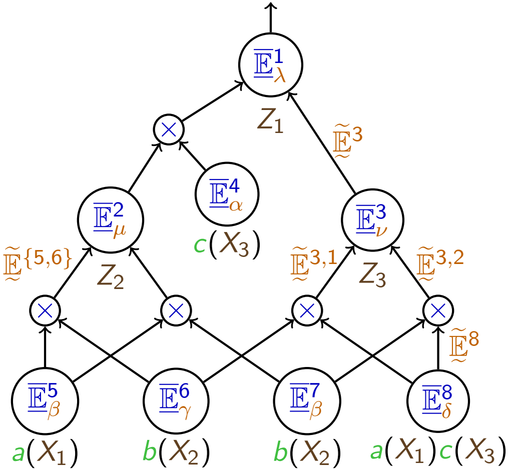

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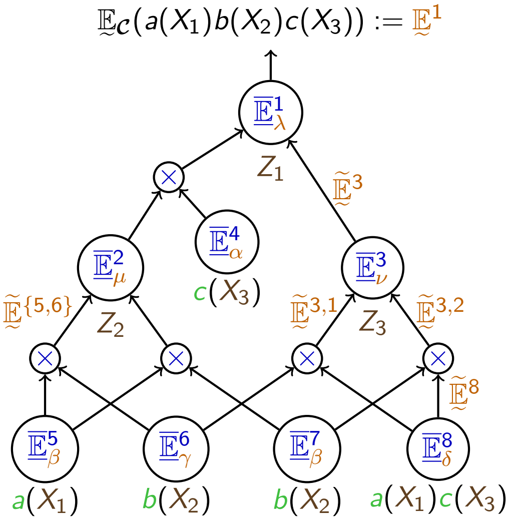

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Using propagation to compute credal PC lower expectations[1]

Exact inference

It sometimes holds that $\underline{\mathbb{E}}_{\mathcal{C}}(f) = \underset{\sim}{\mathbb{E}}_{\mathcal{C}}(f)$:

- For *tree* topologies, this holds for *any factorizing f*
- For *SDAG* topologies, this holds for *any nonnegative factorizing f*

[1] All credal PC results from Montalvan, Centen, Krak, Quaeghebeur & De Campos's "Beyond tree-shaped credal probabilistic circuits", *IJAR* 171:109047 (2024).

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A single propagation pass is linear in the size of the circuit, so for the cases above

- EVI: ✔
- MAR: ✔

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Approximate inference: outer approximation

It always holds that $\underset{\sim}{\mathbb{E}}_{\mathcal{C}}(f) \leq \underline{\mathbb{E}}_{\mathcal{C}}(f)$ for any factorizing f.

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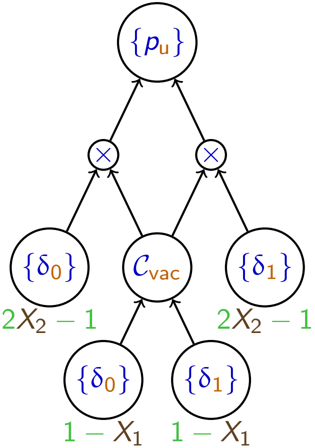

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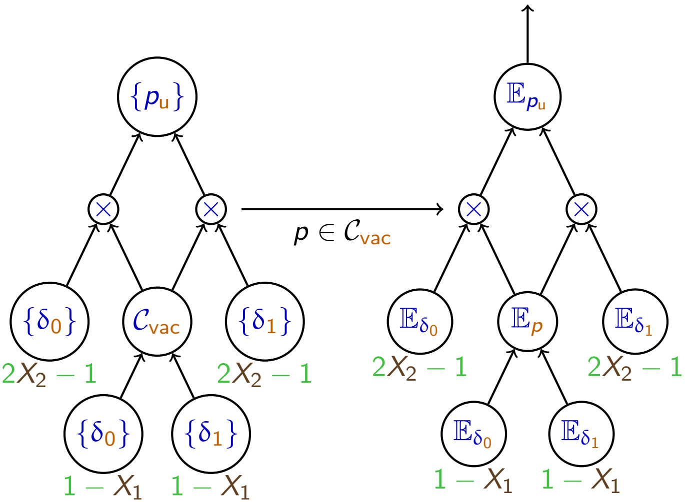

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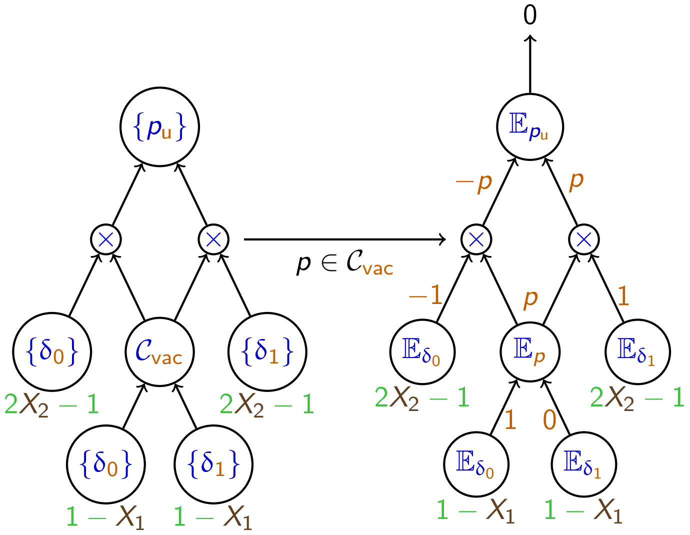

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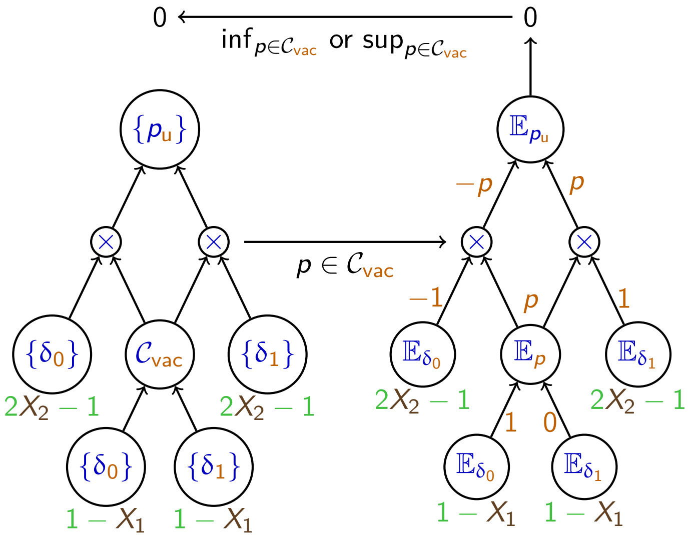

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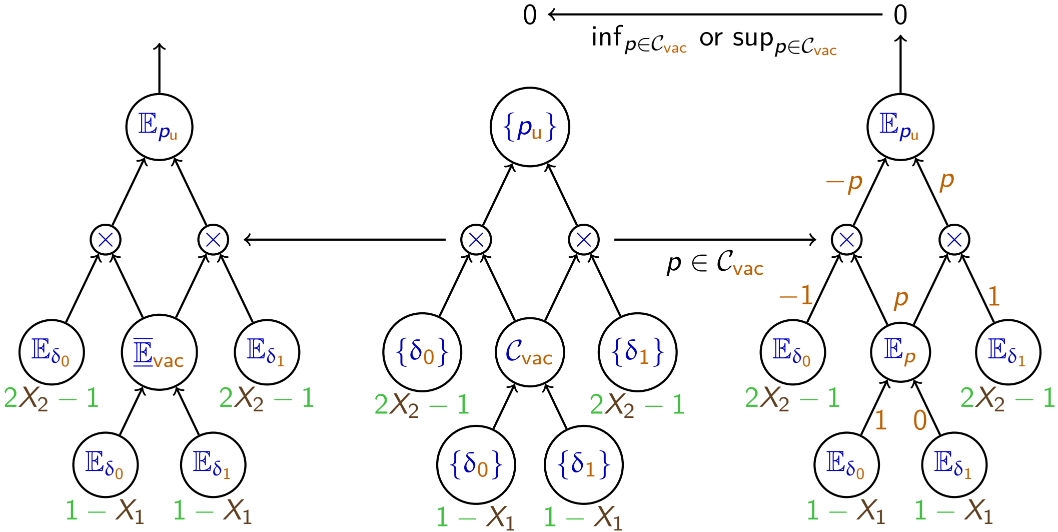

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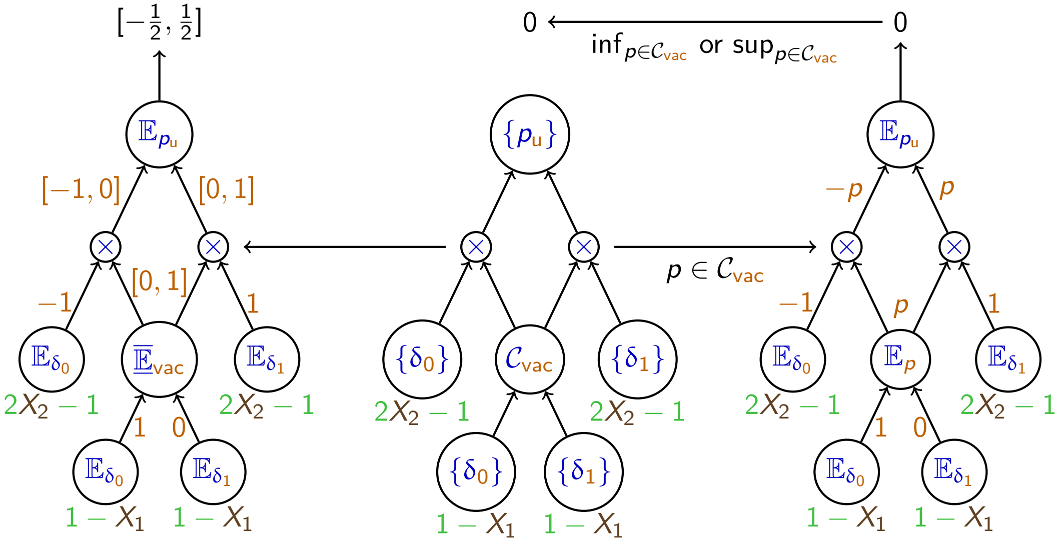
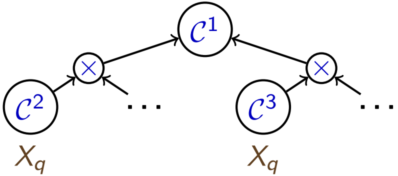


SDAGs designed for tractable inference

Setup

- *General focused query function*:
  $f(\boldsymbol{X}) = g(X_q)h(\boldsymbol{X}_{\neq q})$, with
  - g any function
  - h nonnegative factorizing

- *X_q-queried structure*:
  no path between the root and any input node with scope X_q contains edges that are part of a cycle



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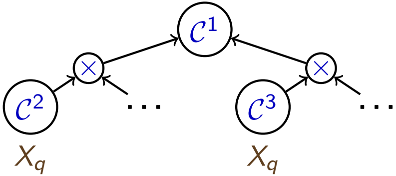

Results

- In this setup $\underline{\mathbb{E}}_{\mathcal{C}}(f) = \utilde{\mathbb{E}}_{\mathcal{C}}(f)$

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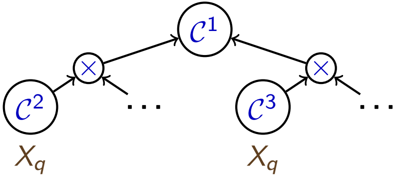

Results

- In this setup $\mathbb{E}_{\mathcal{C}}(f) = \mathbb{E}_{\tilde{\mathcal{C}}}(f)$
- Also $\mathbb{E}_{\mathcal{C}}(g(X_q)|\boldsymbol{X}_e = \boldsymbol{x}_e)$ with $\boldsymbol{X}_e \subseteq \boldsymbol{X}_{\neg q}$ can be computed exactly by propagation, as the solution ζ of

$$\mathbb{E}_{\mathcal{C}}\left(\mathbb{I}_{\boldsymbol{x}_e}(\boldsymbol{X}_e)(g(X_q) - \zeta)\right) = 0$$

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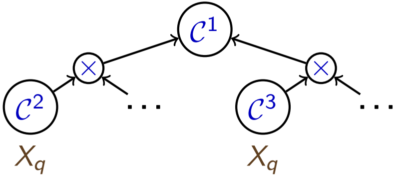

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- Determining *credal dominance* between decision options $\hat{o}$ and $\check{o}$ is a special case if this, as it requires investigating

$$\underline{\mathbb{E}}_{\mathcal{C}}\Big(\mathbb{I}_{\hat{o}}(X_q) - \mathbb{I}_{\check{o}}(X_q) \Big| \boldsymbol{X}_{\mathrm{e}} = \boldsymbol{x}_{\mathrm{e}}\Big) > 0$$

Opportunities in the area of imprecise-probabilistic PCs

- Embracing lower–upper expectation circuits fully by considering SDAGs as a compact notation for trees?
- Other ‘product’ operators?
- Learning from data beyond adding ‘imprecision’ to sum nodes?

Overview

Circuits, conceptually

Credal PCs

Probabilistic integral circuits

- From deep PCs to PICs
- Training PICs
- Opportunities

Evolution and characteristics of deep PCs

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- Tendency to overparameterize and tensorize structures (making it well-adapted to deep-learning implementation)
- Cycles seem to have a positive effect on expressiveness (reuse of components)
- Training seems harder than in neural-based deep learning models

Probabilistic integral circuits (PICs)[2]

Observation Other classes of deep generative models are easier to train (VAEs, Flows)

Hypothesis Their intertwined use of *continuous* latent variables and *neural networks* play an important role in this

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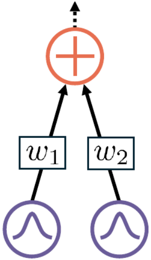

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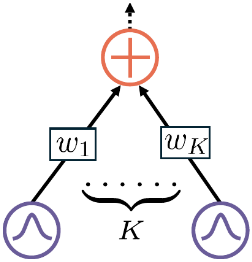

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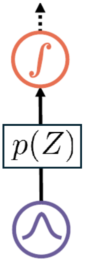

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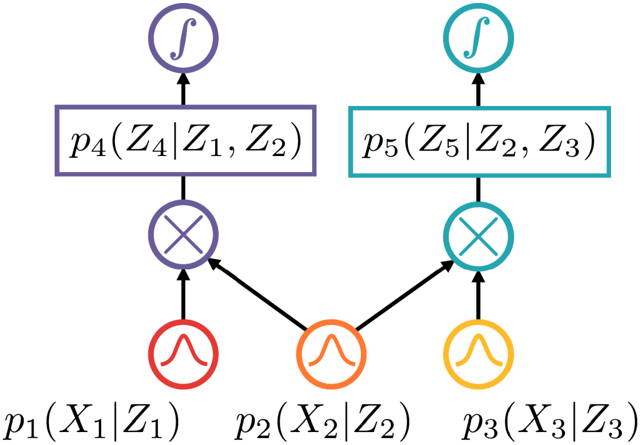
PICs are 'symbolic' circuits



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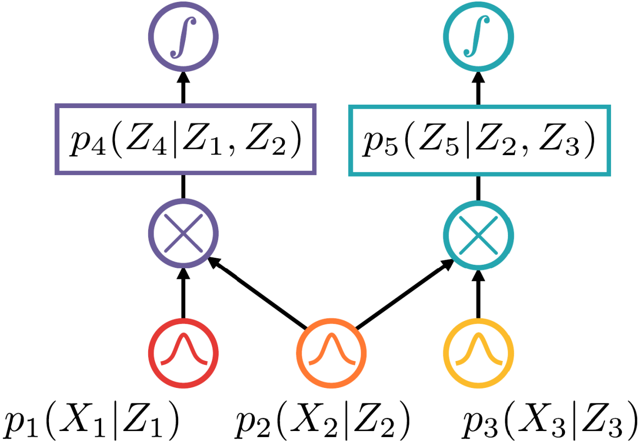

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  - *integrates out* latent variables
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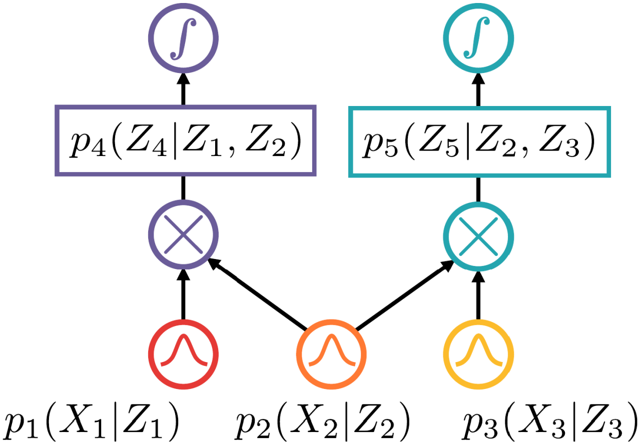
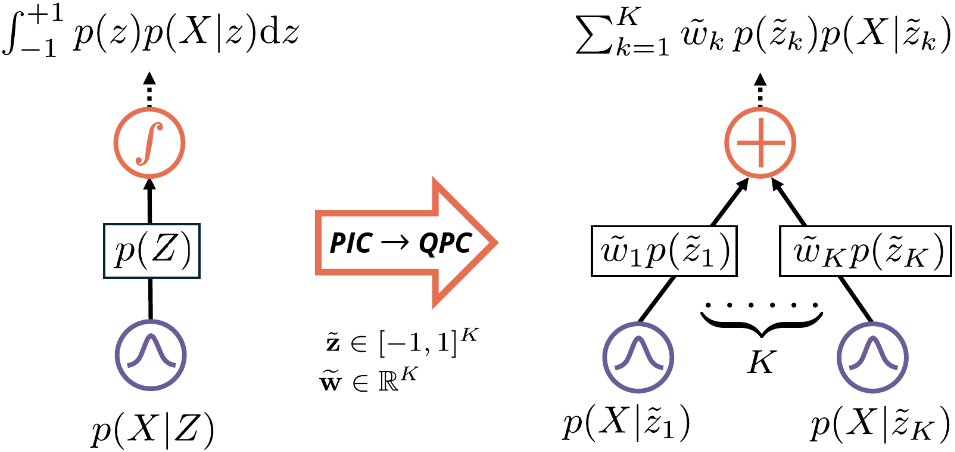


- Integral node:
  - *integrates out* latent variables
  - *leaves unaffected* non-latent variables
  - *introduces* new latent variable
  - parameterized with a *neural network*
- *Edges carry functions*, not values!
- Generally not tractable as such

Approximating PICs with PCs by numerical quadrature



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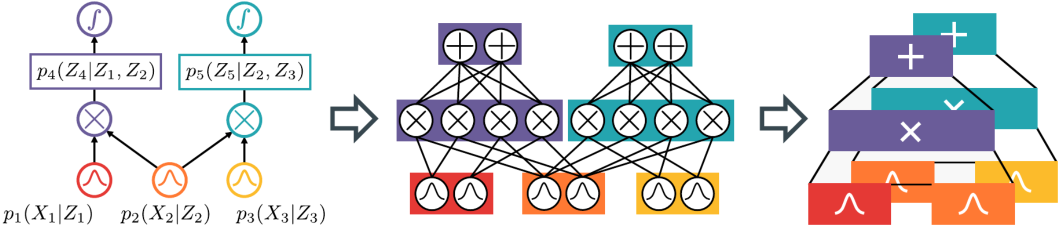
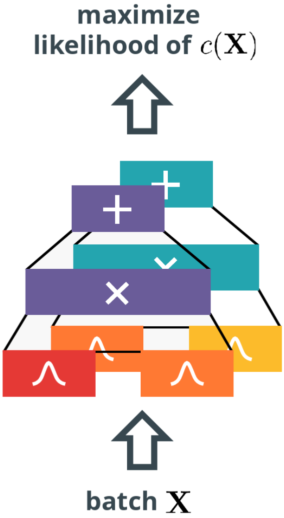


- tensorization and overparameterization is applied
- locally dense
- *folding* to exploit parallel computation

Training a PIC via its QPC



- Training QPC:
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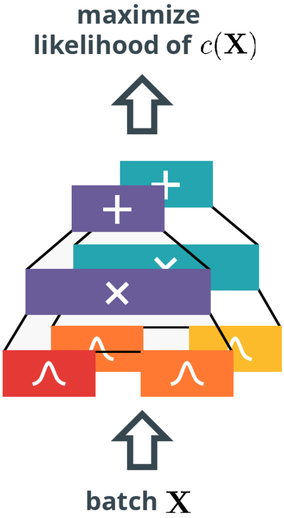

- Training QPC:
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  - use random batches of data
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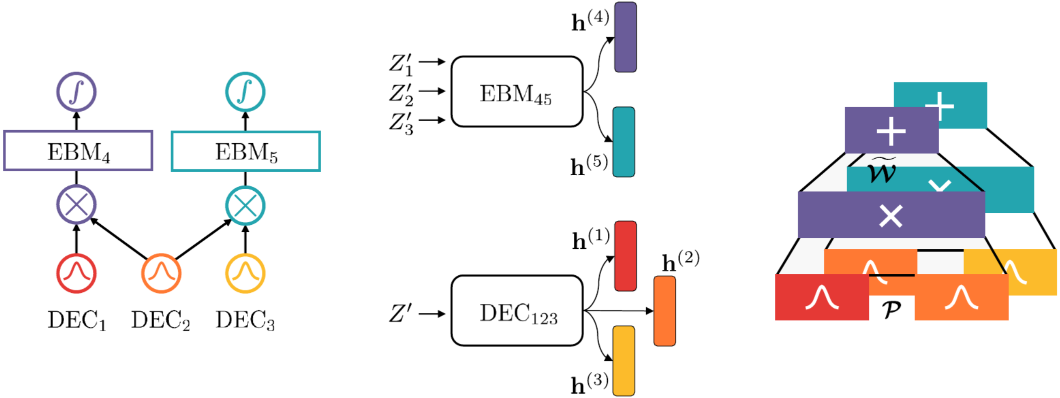
- Training PIC:
  - as above, but
  - propagate gradients to neural network parameters
  - take maximizing step *for neural network parameters* per batch

Making training practical using neural functional sharing



Takeaway & opportunities in the area of deep PCs

- State-of-the-art deep PCs (PICs) combine ideas from various fields and require ML engineering to design.
- Methods to directly train PICs without generating QPCs?
- Create imprecise-probabilistic PIC variants?

The wondrous world of credal and deep probabilistic circuits

SIPTA Seminar

Erik Quaeghebeur

Eindhoven University of Technology

22 January 2025, 15:00 CET