# Learning Sum-Product Networks

Martin Trapp

TU Graz

# Probabilistic Machine Learning

# Introduction

How can we make machines that learn from data using tools from probability theory?

Uncertainty is key to probabilistic machine learning and is expressed in all forms, e.g. noise in the data, uncertainty over the predictions, uncertainty over the model.

# Probabilistic Inference

**Challenge:** Probabilistic inference is often difficult for interesting models.

| | GANs | VAEs | Flows |
|---|---|---|---|
| Sampling | Y | Y | Y |
| Density | N | N/Y | Y |
| Marginals | N | N | ? |
| Conditionals | N | N | ? |
| Moments | N | N | ? |
| MAP | N | N | ? |

**Table 1:** Robert Peharz, Sum-Product Networks and Deep Learning: A Love Marriage. ICML workshop on TPM, 2019.

# Sum-Product Networks

# Sum-Product Networks

- Sum-product networks (SPNs)[1] are a sub-class of so-called tractable probabilistic models or probabilistic circuits[2], that admit tractable probabilistic inference.
- A class of queries $Q$ on a class of models $M$ is tractable, iff for any query $q \in Q$ and model $m \in M$ the computational complexity is at most polynomial.
- SPNs admit many probabilistic inference tasks, such as marginalisation, in linear time in their representation size.

---

[1] H. Poon & P. Domingos: Sum-product networks: A new deep architecture. In UAI, 2011.

[2] Van den Broeck et al.: Tractable probabilistic models: Representations, algorithms, learning and applications. Tutorial at UAI, 2019.

# Probabilistic Inference

| | GANs | VAEs | Flows | SPNs |
|---|---|---|---|---|
| Sampling | Y | Y | Y | Y |
| Density | N | N/Y | Y | Y |
| Marginals | N | N | ? | Y |
| Conditionals | N | N | ? | Y |
| Moments | N | N | ? | Y |
| MAP | N | N | ? | N/Y |

**Table 2:** Robert Peharz, Sum-Product Networks and Deep Learning: A Love Marriage. Talk at ICML, 2019.

# What is a Sum-Product Network?

Let $\mathbf{X} = \{X_1, \ldots, X_D\}$ be set of random variables.

A probabilistic circuit over $\mathbf{X}$ is a tuple $\mathcal{S} = (\mathcal{G}, \psi, \theta)$, where

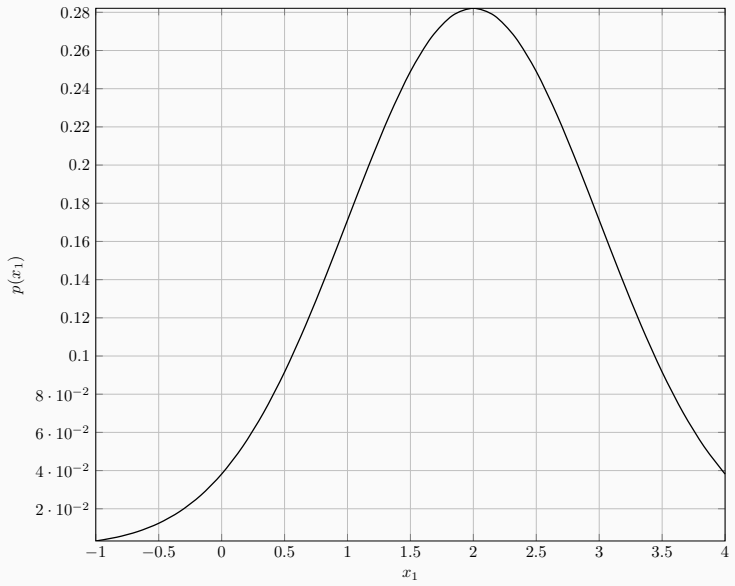
- $\mathcal{G}$ is a computational graph.
- $\psi$ is a scope function.
- $\theta$ is a set of parameters, e.g. sum-weights and leaf node parameters.

A Sum-Product Network (SPN) is a *smooth* (complete) and *decomposable* probabilistic circuit.

# Leaves L in $\mathcal{G}$

Leaf/input nodes are arbitrary (tractable) distributions, e.g. Gaussian, Multinomial, variational autoencoder.

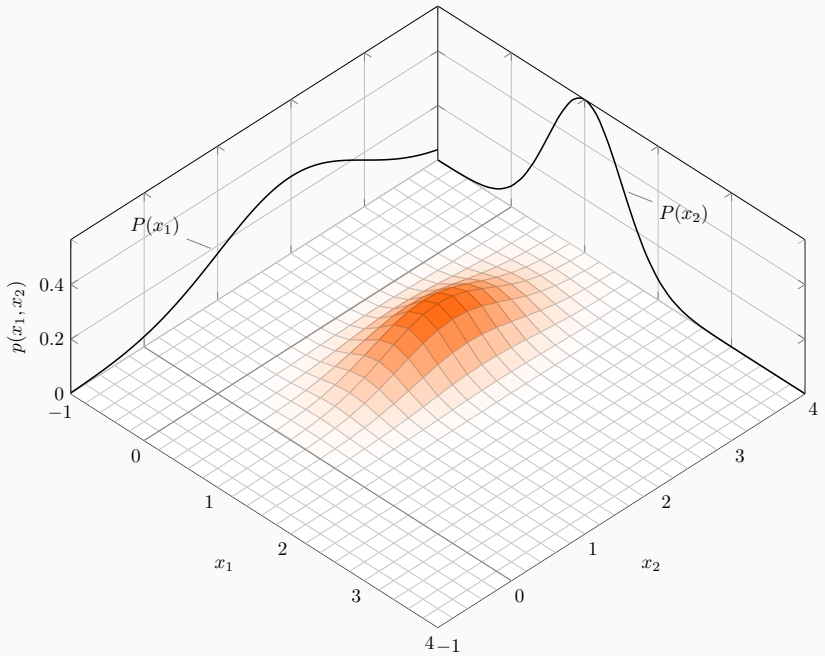
$$\mathrm{L}(x) = p(x \mid \theta_{\mathrm{L}})$$



# Product Nodes $\mathsf{P}$ in $\mathcal{G}$

Product nodes encode independence assumptions between sets of random variables.

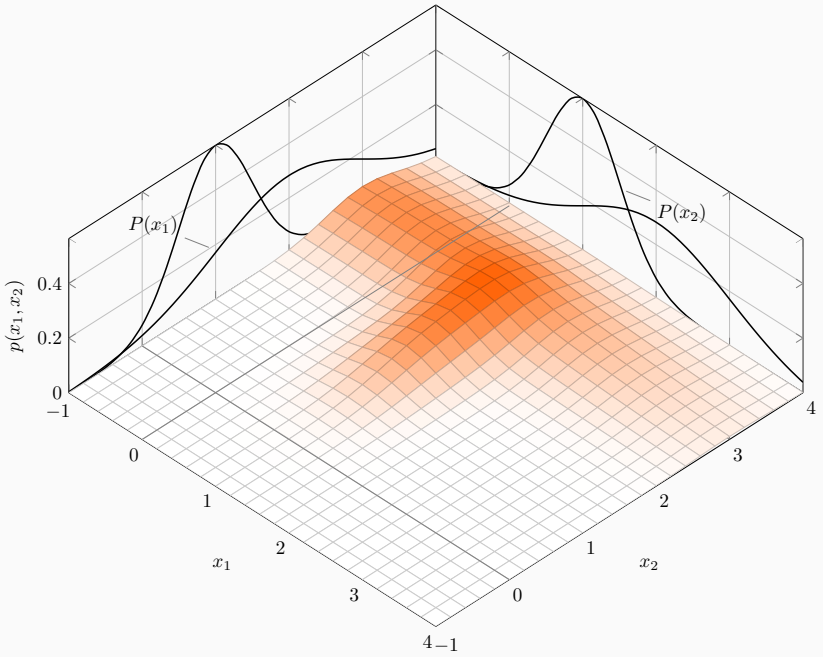
$$\mathsf{P}(x) = \prod_{\mathsf{C} \in \mathbf{ch}(\mathsf{P})} \mathsf{C}(x)$$



# Sum Nodes $\mathsf{S}$ in $\mathcal{G}$

Sum nodes[3] replace independence with conditional independence within the network.

$$\mathsf{S}(x) = \sum_{\mathsf{C} \in \mathbf{ch}(\mathsf{P})} w_{\mathsf{S},\mathsf{C}} \mathsf{C}(x)$$




[3] $\sum_{\mathsf{C} \in \mathbf{ch}(\mathsf{S})} w_{\mathsf{S},\mathsf{C}} = 1$ and $w_{\mathsf{S},\mathsf{C}} \geq 0$.

# Computational Graph $\mathcal{G}$

$\mathcal{G}$ is a rooted connected directed acyclic graph (DAG), containing: sum (S), product (P) and leaf nodes (L).

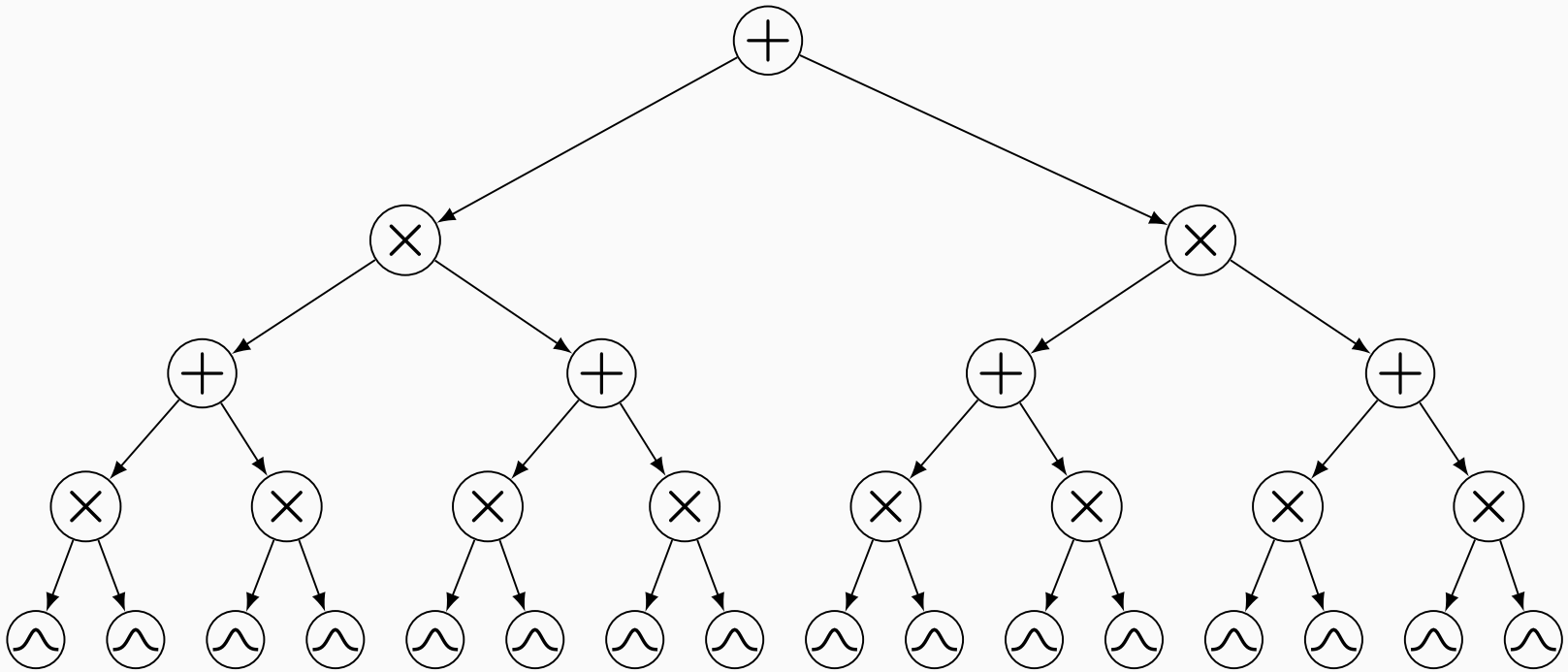


**Figure 1:** Example of a tree-shaped computational graph.

# Scope Function $\psi$

The scope function assigning each node N in a sub-set of **X**,[4] and has to fulfil the following properties:

1. If N is the root node, then $\psi(\mathsf{N}) = \mathbf{X}$.
2. If N is a sum or product, then $\psi(\mathsf{N}) = \bigcup_{\mathsf{N}' \in \mathbf{ch}(\mathsf{N})} \psi(\mathsf{N}')$.

[4] This sub-set is often referred to as the scope of a node.

# Scope Function $\psi$

The scope function assigning each node N in a sub-set of **X**,[4] and has to fulfil the following properties:

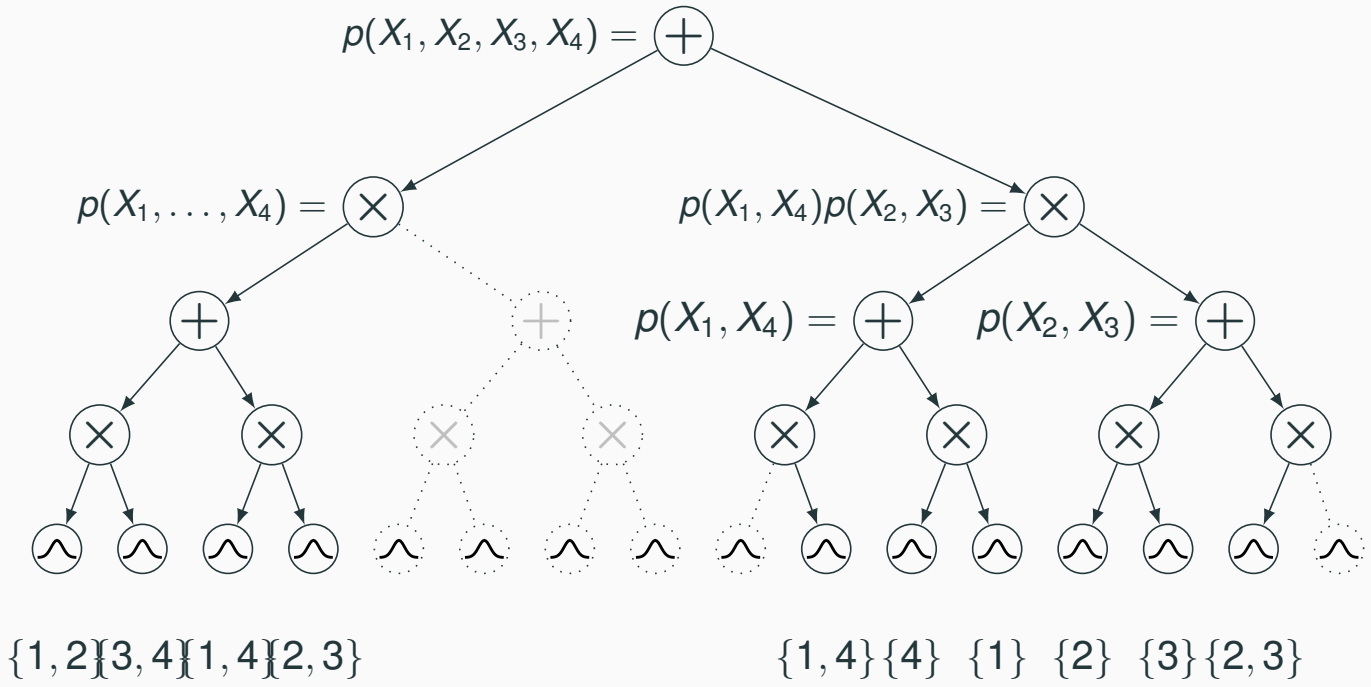
1. If N is the root node, then $\psi(\mathrm{N}) = \mathbf{X}$.
2. If N is a sum or product, then $\psi(\mathrm{N}) = \bigcup_{\mathrm{N}' \in \mathbf{ch}(\mathrm{N})} \psi(\mathrm{N}')$.

In case of SPNs we also assume that:

1. For each $\mathrm{S} \in \mathbf{S}$ we have $\forall \mathrm{N}, \mathrm{N}' \in \mathbf{ch}(\mathrm{S}) \colon \psi(\mathrm{N}) = \psi(\mathrm{N}')$ (*smoothness*)
2. For each $\mathrm{P} \in \mathbf{P}$ we have $\forall \mathrm{N}, \mathrm{N}' \in \mathbf{ch}(\mathrm{P}) \colon \psi(\mathrm{N}) \cap \psi(\mathrm{N}') = \emptyset$ (*decomposability*).

[4] This sub-set is often referred to as the scope of a node.

# Example SPN $\mathcal{S} = (\mathcal{G}, \psi, \theta)$




Note that we define $\mathsf{L}(x) := 1$ for every $x$ if and only if $\psi(\mathsf{L}) = \emptyset$.

# Interpretations of SPNs

What is an SPN?

- Multi-linear feed-forward Neural Network (NN) with non-linear inputs.
- Deep structured mixture model with exponentially many components.
- Hierarchical tensor decomposition.

# Parameter Learning

# Parameter Learning in SPNs

SPNs are differentiable multi-linear NNs with non-linear inputs, thus common parameter learning for NNs can be applied.

Approaches that go beyond NN techniques:

- Expectation Maximisation [R. Peharz et al.: On the latent variable interpretation of sum-product networks. TPAMI, 2017.]
- Variational Inference [H. Zhao et al.: Collapsed variational inference for sum-product networks. In ICML, 2016.]
- Bayesian moment matching [A. Rashwan et al.: Online and distributed Bayesian moment matching for parameter learning in sum-product networks. In AISTATS, 2016.]
- **Safe Semi-Supervised Learning** [M. Trapp et al.: Safe semi-supervised learning of sum-product networks. In UAI, 2017.]

# Safe Semi-Supervised Learning

## Contrastive Pessimistic Likelihood Estimation (CPLE)

- $\mathcal{X} = \{\boldsymbol{x}_n, \lambda_n\}_{n=1}^{N}$, $\lambda_n \in \mathcal{R}^K$ = labelled data points
- $\mathcal{U} = \{\boldsymbol{u}_m\}_{m=1}^{M}$ = unlabelled data points
- $\boldsymbol{q}_m \in \Delta_{K-1}$ = soft labels
- $\theta^+$ = SPN trained only on $\mathcal{X}$
- $\theta$ = SPN trained using CPLE on all data points
- $\mathcal{L}(\theta|\mathcal{X}, \mathcal{U}, \boldsymbol{q})$ = likelihood or conditional likelihood

# Safe Semi-Supervised Learning

## Contrastive Pessimistic Likelihood Estimation (CPLE)

- $\mathcal{X} = \{\boldsymbol{x}_n, \lambda_n\}_{n=1}^N$, $\lambda_n \in \mathcal{R}^K$ = labelled data points
- $\mathcal{U} = \{\boldsymbol{u}_m\}_{m=1}^M$ = unlabelled data points
- $\boldsymbol{q}_m \in \Delta_{K-1}$ = soft labels
- $\theta^+$ = SPN trained only on $\mathcal{X}$
- $\theta$ = SPN trained using CPLE on all data points
- $\mathcal{L}(\theta|\mathcal{X}, \mathcal{U}, \boldsymbol{q})$ = likelihood or conditional likelihood

Training:

1. Update soft labels so that $\mathcal{L}(\theta^+|\mathcal{X}, \mathcal{U}, \boldsymbol{q}) > \mathcal{L}(\theta|\mathcal{X}, \mathcal{U}, \boldsymbol{q})$.
2. Update $\theta$ so that $\mathcal{L}(\theta^+|\mathcal{X}, \mathcal{U}, \boldsymbol{q}) < \mathcal{L}(\theta|\mathcal{X}, \mathcal{U}, \boldsymbol{q})$.
3. If not converged, move to step 1.

# Semi-Supervised Learning

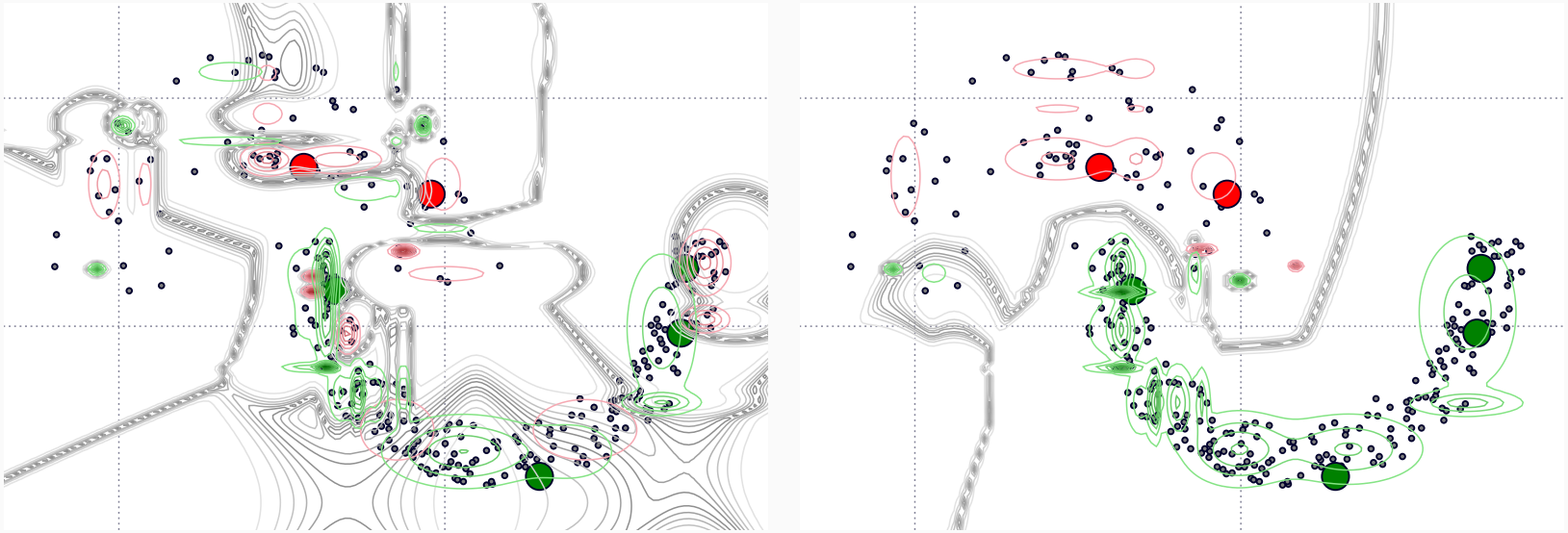
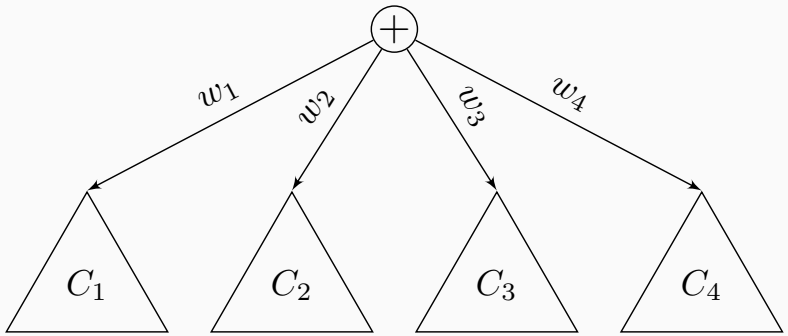
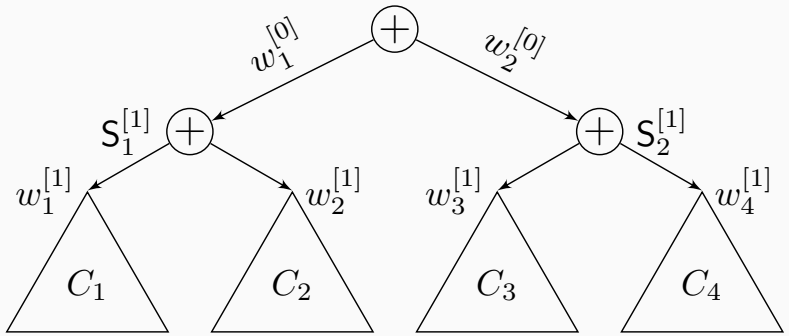


**Figure 2:** Decision boundary of a semi-supervised SPN at iteration 1 (left) and after convergence (right).

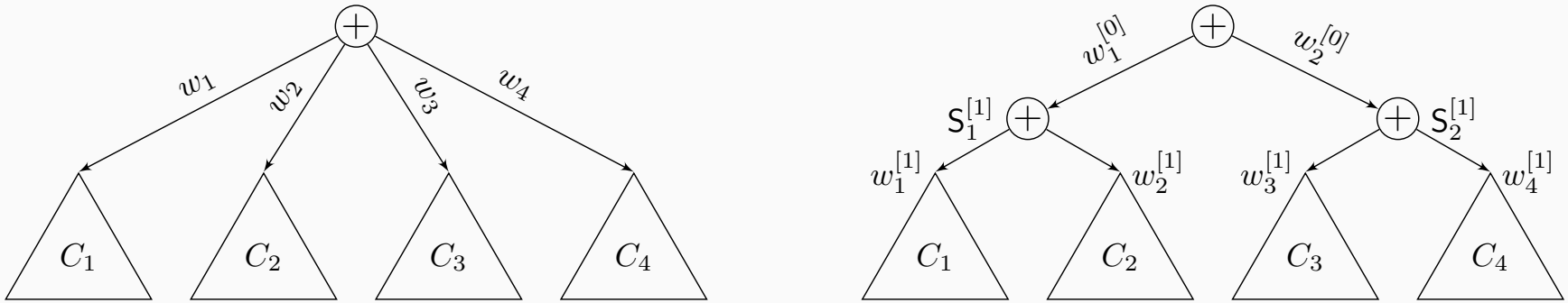
# Over-parametrization in SPNs[5]




[5] M. Trapp et al.: Optimisation of Overparametrized Sum-Product Networks. ICML Workshop on Tractable Probabilistic Models, 2019.

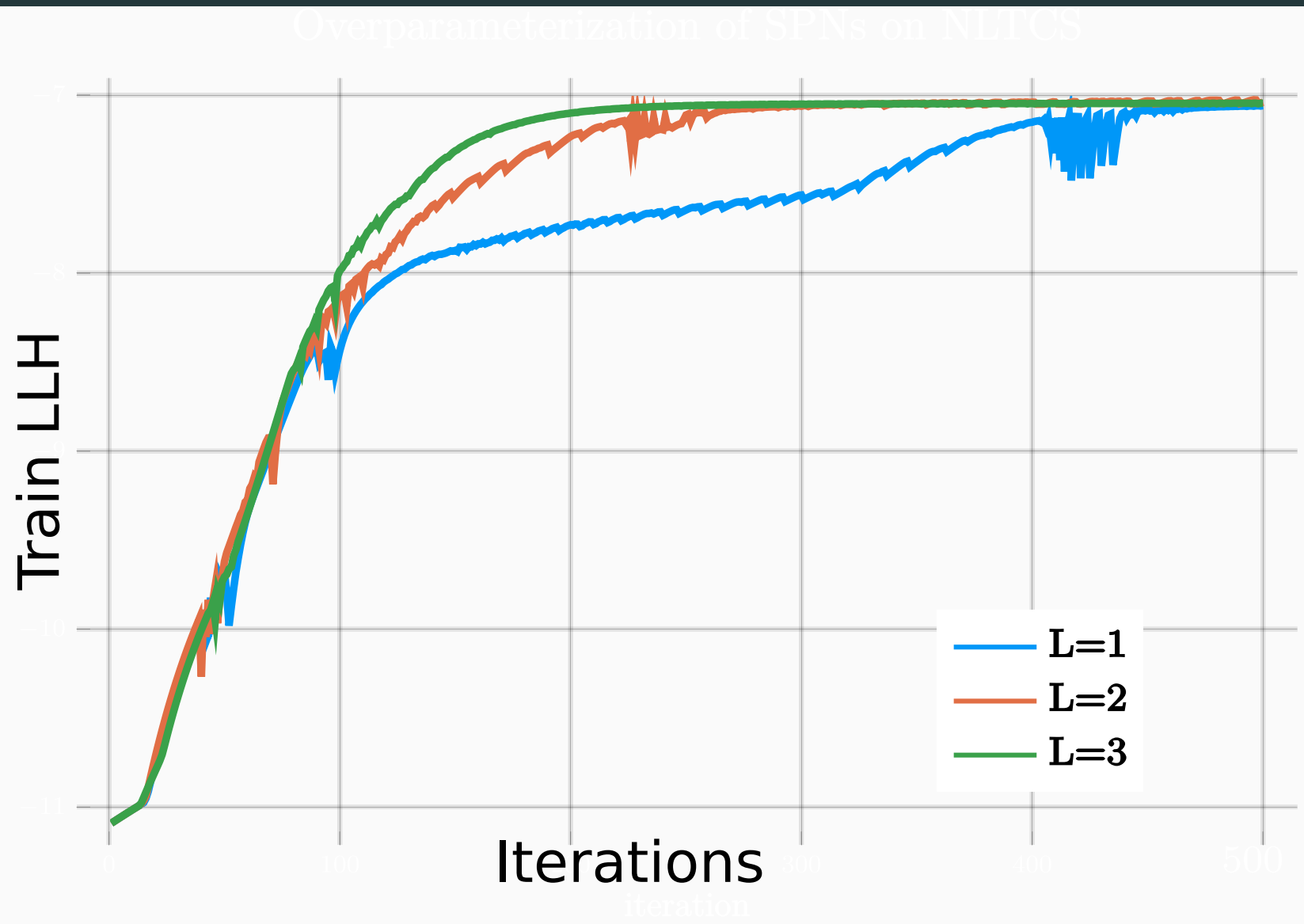
# Over-parametrization in SPNs[5]




$$w_k^{(t)} \approx w_k^{(t)} + \rho^{(t)} \nabla_{w_k^{(t)}} + \sum_{\tau=1}^{t-1} \mu^{(t,\tau)} \nabla_{w_k^{(\tau)}} \tag{1}$$

[5] M. Trapp et al.: Optimisation of Overparametrized Sum-Product Networks. ICML Workshop on Tractable Probabilistic Models, 2019.

# Over-parametrization Experiment



# Structure Learning

# Challenges in Structure Learning

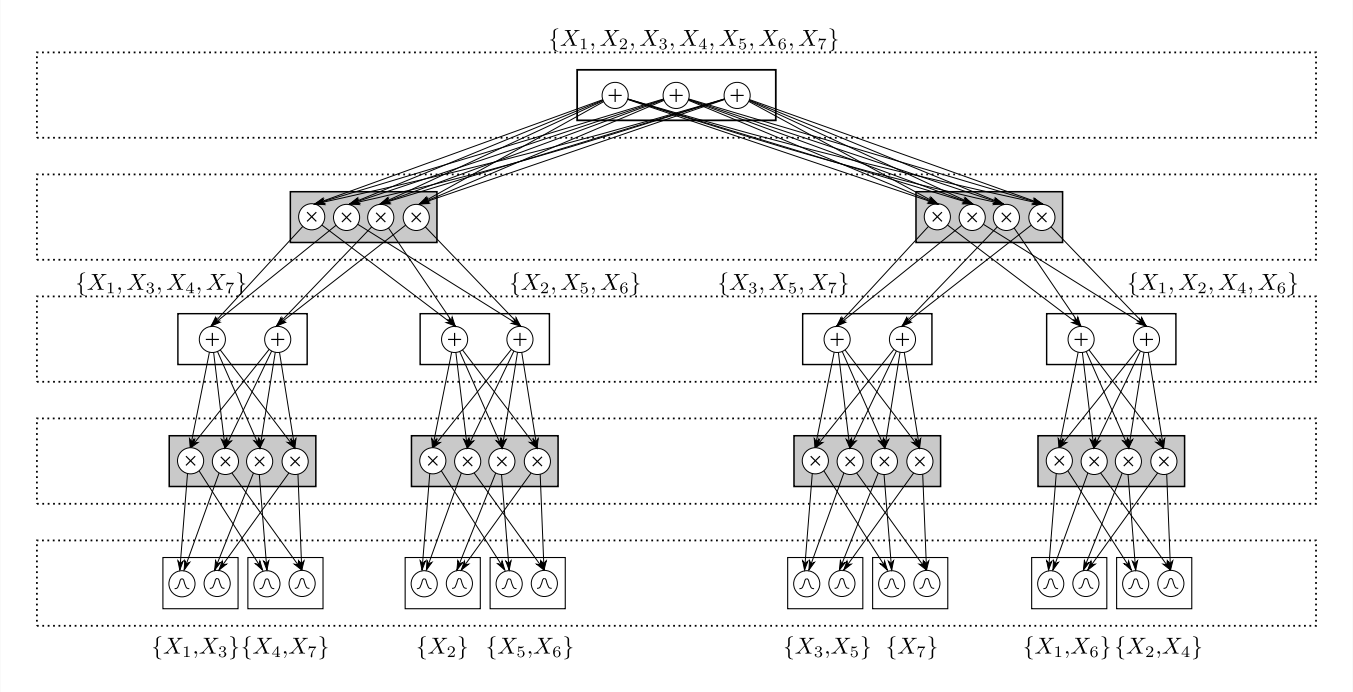
- The structure has to be smooth and decomposable, i.e., a sparsely connected graph.
- Structure learning has to be efficient.
- How to learn structures that generalise well, many approaches learn deep trees that are prune to overfitting.
- What is a good SPN structure? or What is a good principle to derive an SPN structure?

# General-Purpose Learners (Selection)

- LearnSPN [R. Gens & P. Domingos: Learning the structure of sum-product networks. In ICML, 2013.]
- ID-SPN [A. Rooshenas & D. Lowd: Learning Sum-Product Networks with Direct and Indirect Variable Interactions. In ICML, 2014.]
- **RAT-SPN** [R. Peharz et al.: Random sum-product networks: A simple but effective approach to probabilistic deep learning. In UAI, 2019.]
- **Bayesian SPN** [M. Trapp et al.: Bayesian learning of sum-product networks. In NeurIPS, 2019.]

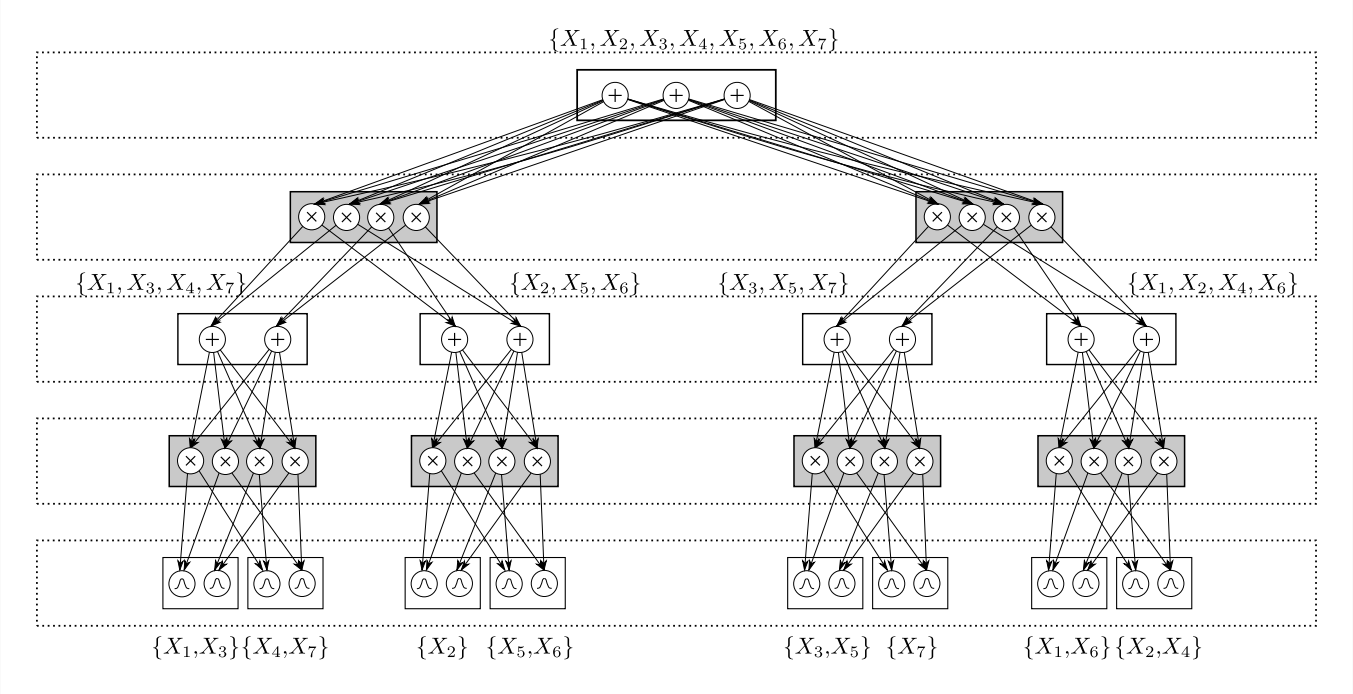
# Random Sum-Product Networks

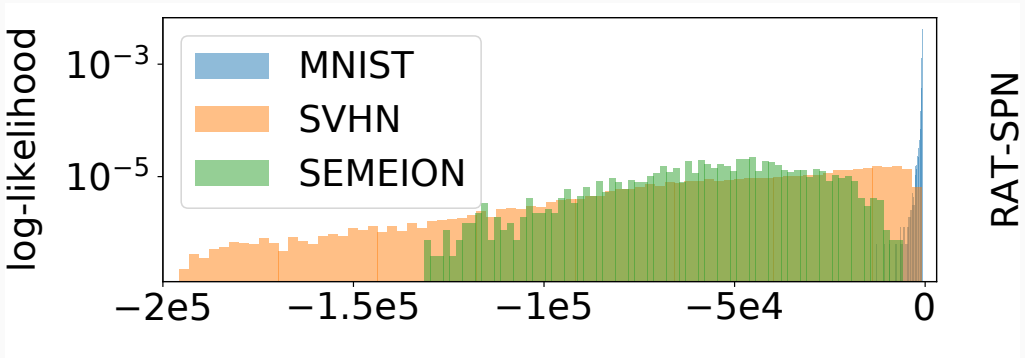
**Idea:** Use a large structure with random decompositions.



# Random Sum-Product Networks

**Idea:** Use a large structure with random decompositions.



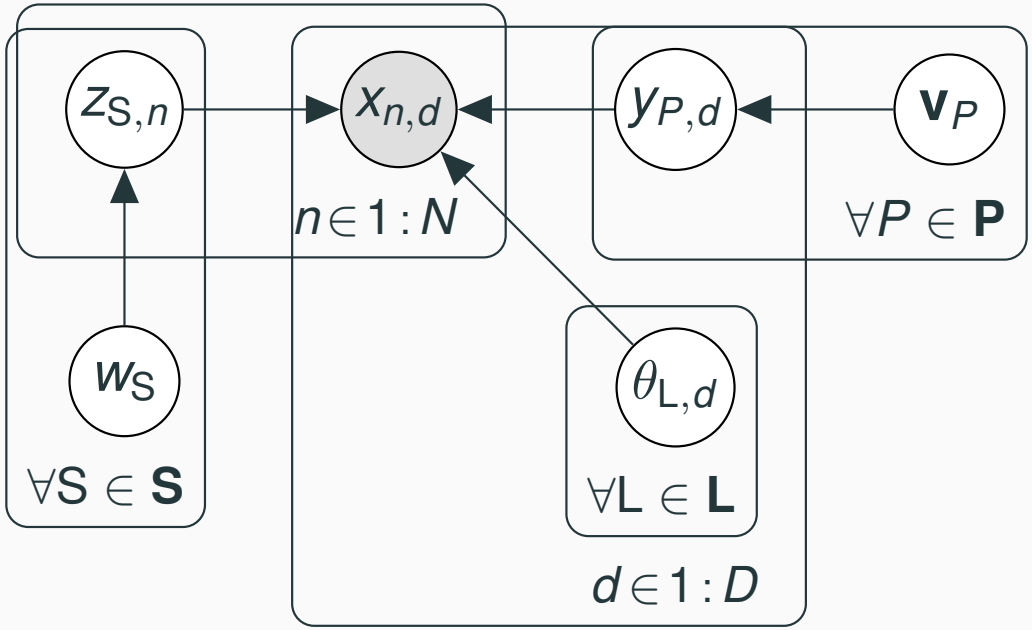
# Bayesian Structure

**Why care about Bayesian structure learning?**

- Occam's razor effect prevents overfitting.
- Works on discrete, continuous and heterogeneous data domains.
- We can use nonparametric formulations, e.g. infinite SPNs, for continual learning.
- Structures can be inferred even in cases of missing values using exact marginalisation.

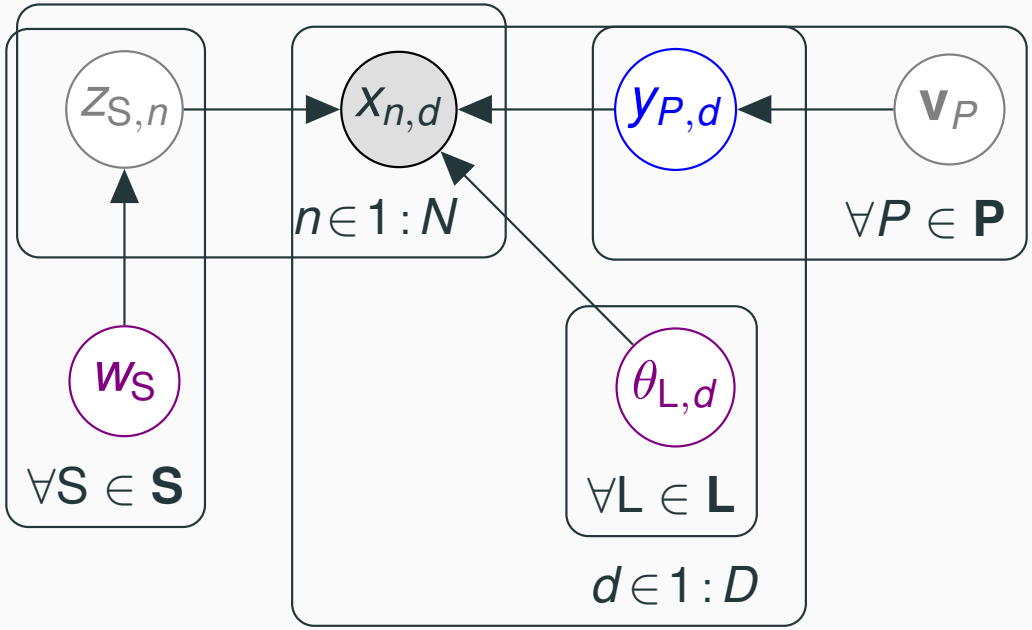
# Bayesian Structure

Generative model for Bayesian learning of SPNs.



# Bayesian Structure

Posterior inference using ancestral sampling within Gibbs.



# Bayesian Structure - Missing Values Experiment

Performance under increasing amount of missing values.

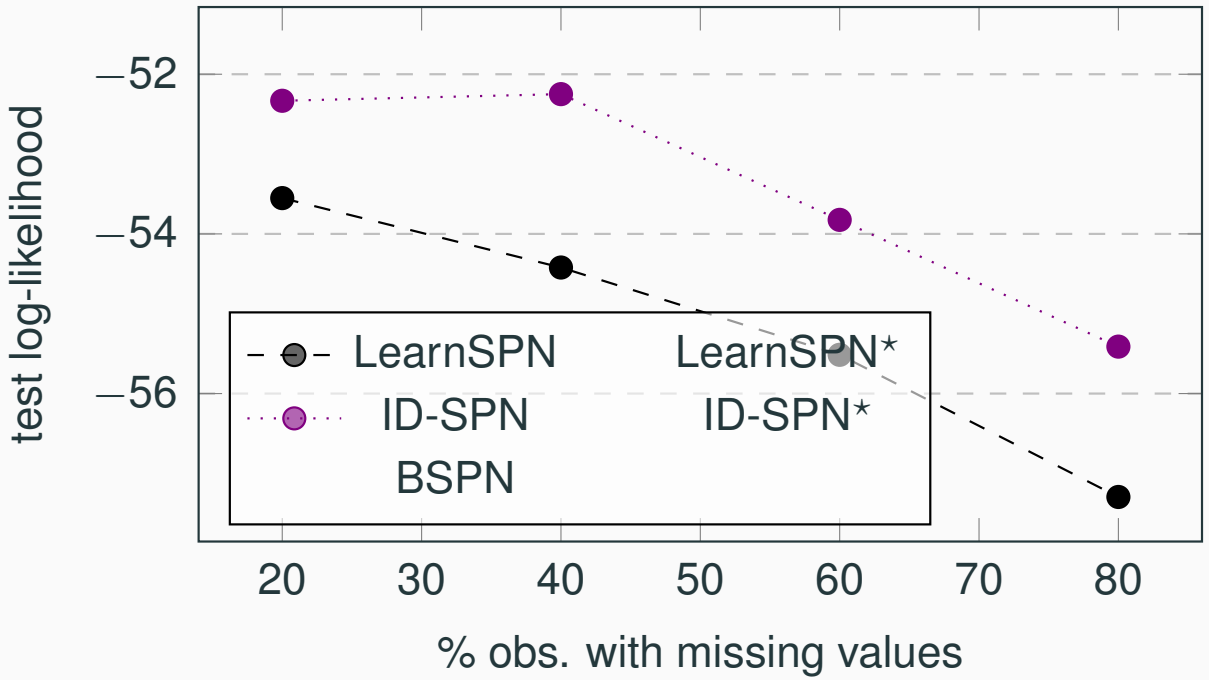



**Figure 3:** Results on EachMovie (D: 500, N: 5526) dataset.

# Bayesian Structure - Missing Values Experiment

Performance under increasing amount of missing values.

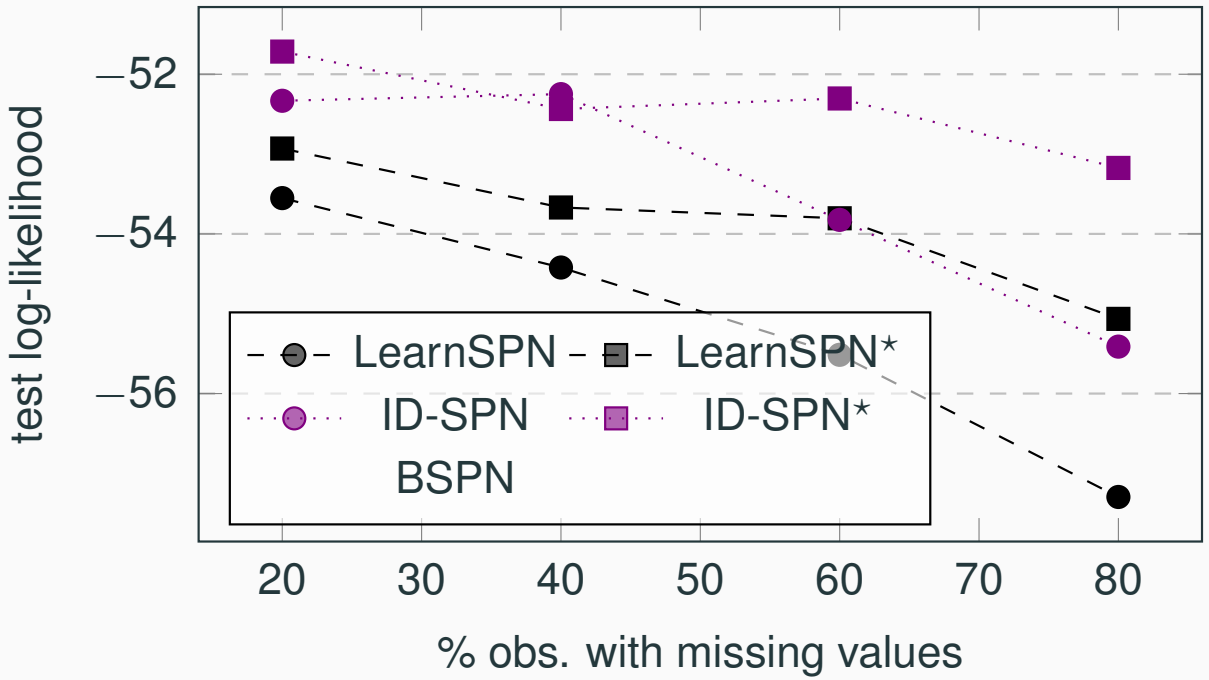



**Figure 3:** Results on EachMovie (D: 500, N: 5526) dataset.

# Bayesian Structure - Missing Values Experiment

Performance under increasing amount of missing values.

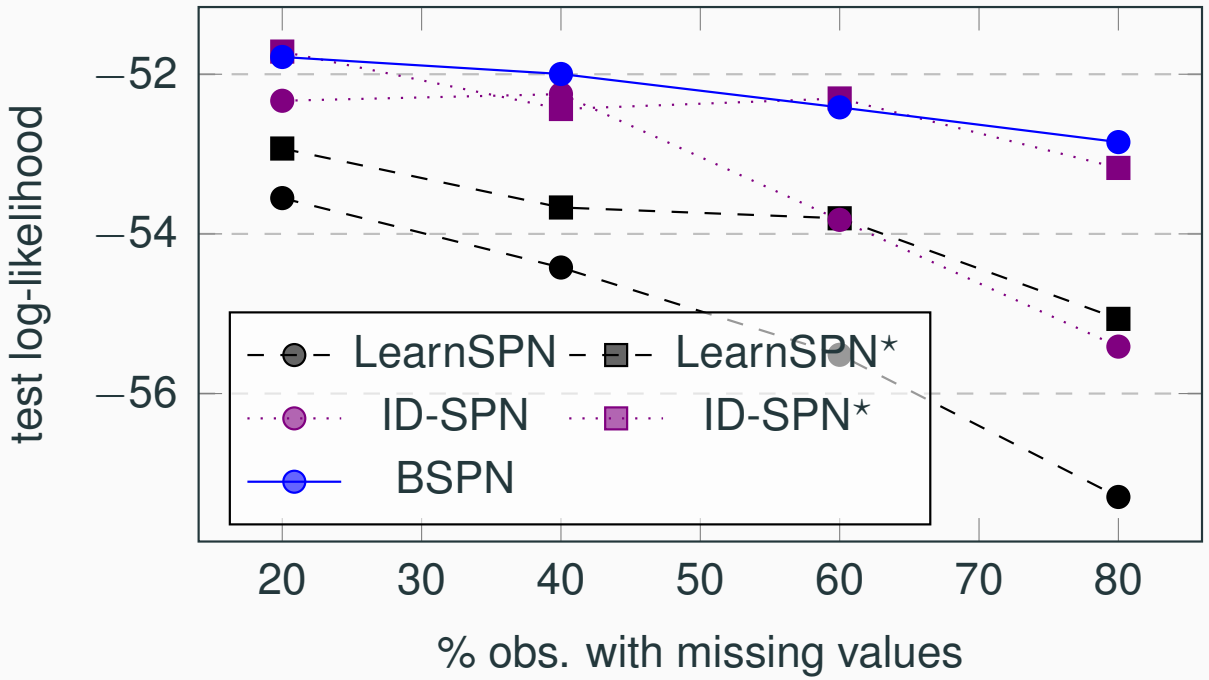



**Figure 3:** Results on EachMovie (D: 500, N: 5526) dataset.

# Applications

# Existing Applications

Some existing applications of SPNs:

- Computer vision, e.g. image classification, medical image processing, attend-infer-repeat.
- Language processing, e.g. language modelling, bandwidth extension.
- Robotics, e.g. semantic mapping.
- **Non-linear regression**, and many more[6]

[6] https://github.com/arranger1044/awesome-spn#applications

# Gaussian Processes

A Gaussian Process (GP) is a collection of random variables indexed by an arbitrary covariate space $\mathcal{T}$, where any finite subset is Gaussian distributed.

A GP can be understood as a prior over functions.

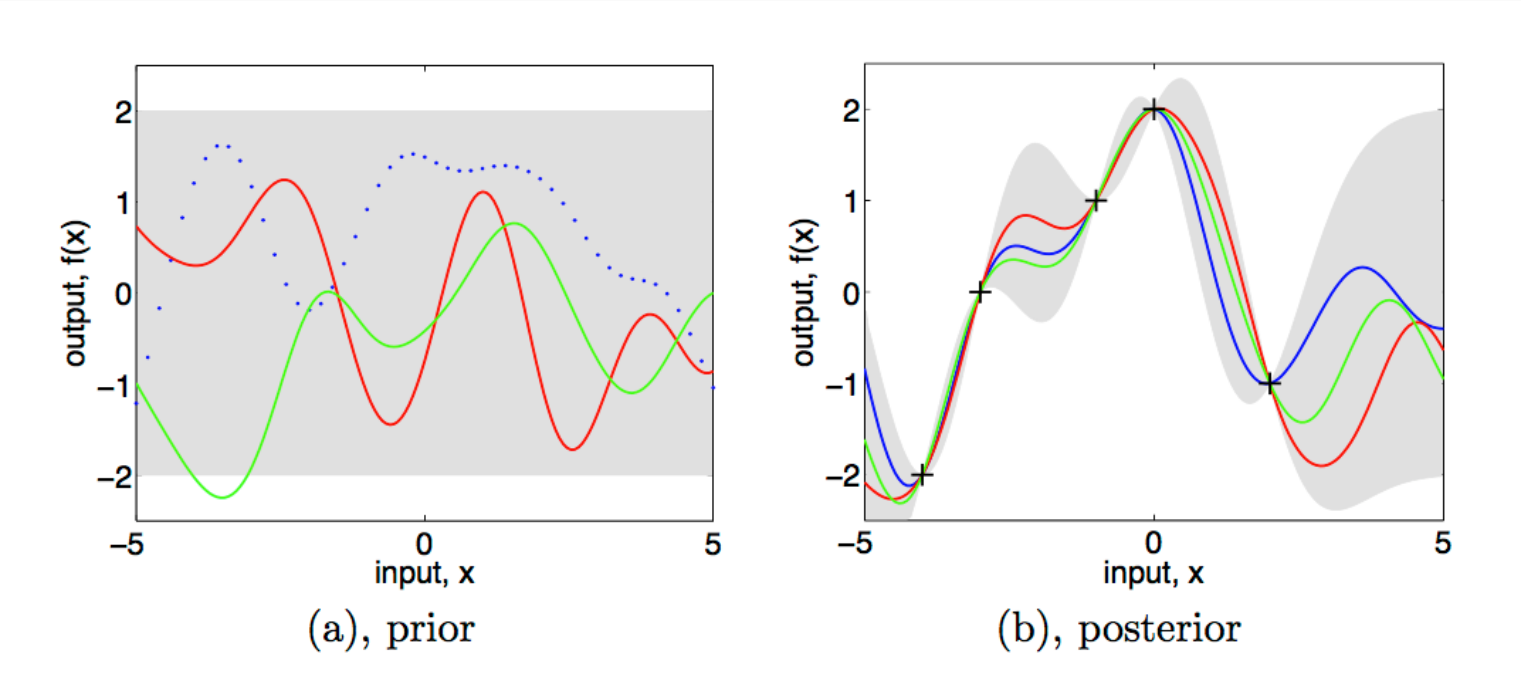



**Figure 4:** C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, 2006.

# Gaussian Processes

A GP is uniquely specified by a *mean-function* $m : \mathcal{T} \to \mathbb{R}$ and a *covariance function* $k : \mathcal{T} \times \mathcal{T} \to \mathbb{R}$.

The posterior predictive distribution (used for predictions) of a GP is Gaussian, i.e.,

$$p(f^* \mid \boldsymbol{f}) = \mathcal{N}\left(k_{\mathbf{x}^*,\mathbf{X}}^T k_{\mathbf{X},\mathbf{X}}^{-1} \boldsymbol{f}, k_{\mathbf{x}^*,\mathbf{x}^*} - k_{\mathbf{x}^*,\mathbf{X}} k_{\mathbf{X},\mathbf{X}}^{-1} k_{\mathbf{x}^*,\mathbf{X}}^T\right) \tag{2}$$

**Problem:** How to compute the inversion of $k_{\mathbf{X},\mathbf{X}}$?

# Gaussian Processes

We can use the Cholesky decomposition.

**Problem:** The Cholesky decomposition scales $\mathcal{O}(N^3)$.

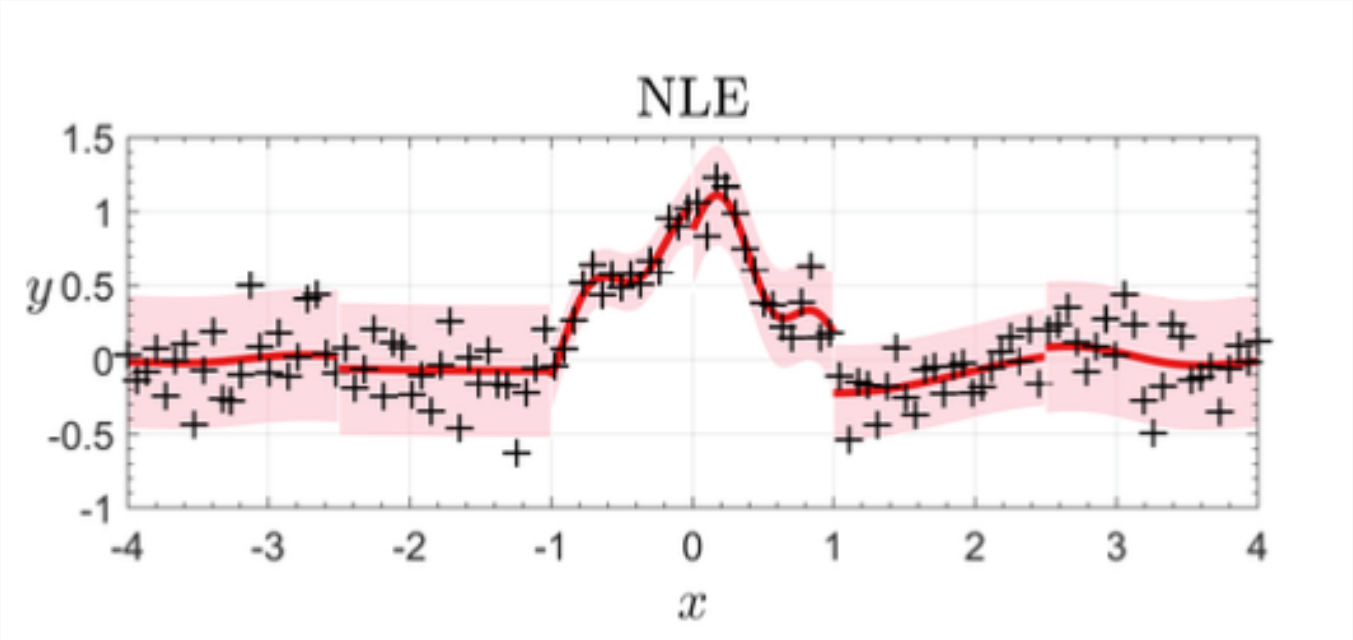
Solutions:

1. Approximate the posterior using a variational approximation, or
2. Use local experts to approximate the GP or approximate the computation of predictions.

# Local Experts

*Local experts to approximate the GP or approximate the computation of predictions.*

A natural way is to partition $\mathcal{T}$ into sub-sets $\mathcal{T}^{(k)}$ , $k = 1, \ldots, K$. This is called the naive-local-experts model.



# Local Experts

Existing solutions to discontinuities.

1. Product-of-Experts (PoE) / Bayesian Committee Machine (BCM)
   - Instead of partition $T$, partition $\mathcal{X}$ into sub-sets $\mathcal{X}^{(k)}$.
   - Use an algorithm that works only on the sub-sets.
   - **Problem:** Not a stochastic process, results in over-conservative or over-confident estimates.
2. Mixture-of-Experts (MoE)
   - Use a gating network to assign observations to experts instead of hard boundaries.
   - Often intractable (due to the gating network).
3. Impose Continuity Constraints
   - Suffers from inconsistent variances and does not scale.

# Deep Structured Mixtures of Gaussian Processes

Why not use a large finite mixture of NLEs?

[7] M. Trapp et al.: Deep structure mixtures of Gaussian Processes. To appear in AISTATS, 2020.

# Deep Structured Mixtures of Gaussian Processes

Why not use a large finite mixture of NLEs?

Deep Structured Mixture of GPs (DSMGP):[7]

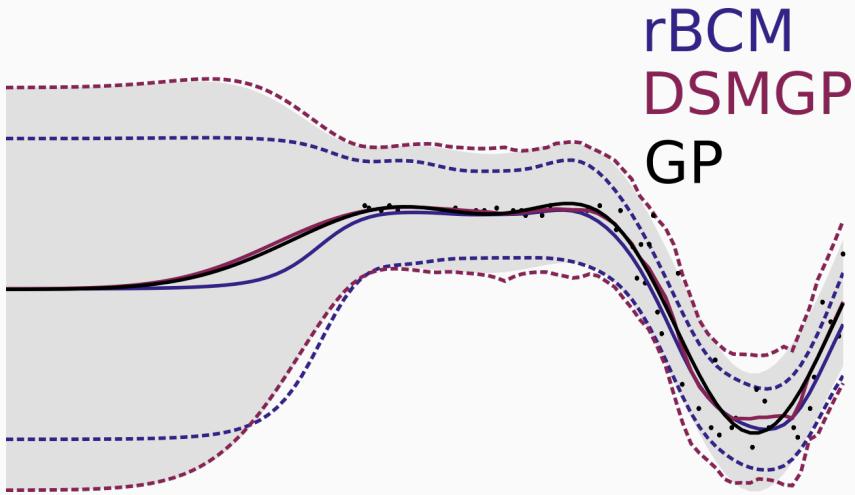
1. A DSMGP is an SPN (large structured mixture) over Gaussian measures.
2. DSMGPs perform exact Bayesian model averaging over a large set of NLEs.

[7] M. Trapp et al.: Deep structure mixtures of Gaussian Processes. To appear in AISTATS, 2020.

# Deep Structured Mixtures of Gaussian Processes

Benefits of DSMGPs:

- DSMGPs are a sound stochastic process.
- We can perform exact posterior inference in DSMGPs.
- DSMGPs have similar computational costs compared to other expert-based approaches and capture predictive uncertainties consistently better.



Thank you for your attention!