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TensorInference: A Julia package for tensor-based probabilistic inference

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Summary

`TensorInference.jl` is a Julia (Bezanson et al., 2017) package designed for performing probabilistic inference in discrete graphical models. It leverages the recent explosion of advances in the field of tensor networks (Orús, 2014, 2019; Robeva & Seigal, 2019) to provide high-performance solutions for common inference problems. Specifically, `TensorInference.jl` offers mechanisms to:

1. calculate the partition function (also known as the probability of evidence).
2. compute the marginal probability distribution over each variable given evidence.
3. find the most likely assignment to all variables given evidence.
4. find the most likely assignment to a set of query variables after marginalizing out the remaining variables.
5. draw samples from the posterior distribution given evidence (Cheng et al., 2019; Han et al., 2018).

The infrastructure based on tensor networks introduces several benefits in handling complex computational tasks. First, it provides a convenient approach to differentiate a tensor network program (Liao et al., 2019), a crucial operation in the computation of the inference tasks listed above. Second, it supports generic element types without sacrificing significant performance. The advantage of this generic element type support is that solutions to diverse problems can be obtained using the same tensor network contraction algorithm but with different element types. This introduces a level of flexibility and adaptability that can handle a broad spectrum of problem domains efficiently (Jin Guo Liu et al., 2022; Jin-Guo Liu et al., 2021). Third, it allows users to define a hyper-optimized contraction order, which is known to have a significant impact on the computational performance of contracting tensor networks (Gao et al., 2021; Markov & Shi, 2008; Pan & Zhang, 2021). `TensorInference.jl` makes a predefined set of state-of-the-art contraction ordering methods available to the users. These methods include a *local search based method* (`TreeSA`) (Kalachev et al., 2022), two *min-cut based methods* (`KaHyParBipartite`) (Gray & Kourtis, 2021) and (`SABipartite`), and a *greedy method* (`GreedyMethod`). Finally, `TensorInference.jl` harnesses the latest developments in computational technology, including a highly optimized set of BLAS (Blackford et al., 2002) routines and GPU technology.

Statement of need

A major challenge in developing intelligent systems is the ability to reason under uncertainty, a challenge that appears in many real-world problems across various domains, including artificial intelligence, medical diagnosis, computer vision, computational biology, and natural language processing. Reasoning under uncertainty involves calculating the probabilities of relevant variables while taking into account any information that is acquired. This process, which can be thought of as drawing global insights from local observations, is known as *probabilistic inference*.

Probabilistic graphical models (PGMs) provide a unified framework to perform probabilistic inference. These models use graphs to represent the joint probability distribution of complex systems concisely by exploiting the conditional independence between variables in the model. Additionally, they form the foundation for various algorithms that enable efficient probabilistic inference.

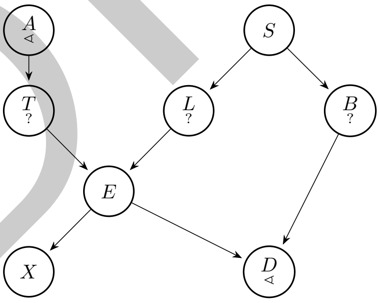
However, even with the representational aid of PGMs, performing probabilistic inference remains an intractable endeavor on many real-world models. The reason is that performing probabilistic inference involves complex combinatorial optimization problems in very high dimensional spaces. To tackle these challenges, more efficient and scalable inference algorithms are needed.

As an attempt to tackle the aforementioned challenges, we present `TensorInference.jl`, a Julia package for probabilistic inference that combines the representational capabilities of PGMs with the computational power of tensor networks. By harnessing the best of both worlds, `TensorInference.jl` aims to enhance the performance of probabilistic inference, thereby expanding the tractability spectrum of exact inference for more complex, real-world models.

`TensorInference.jl` succeeds `JunctionTrees.jl` (Roa-Villescas et al., 2022, 2023), a Julia package implementing the Junction Tree Algorithm (JTA) (Jensen et al., 1990; Lauritzen & Spiegelhalter, 1988). While the latter optimizes computation of individual sum-product messages within the JTA context by employing tensor-based technology at the backend level, `TensorInference.jl` takes a different route. It adopts a holistic tensor network approach, fully integrating the JTA, significantly reducing the algorithm's complexity, and thereby opening new doors for optimization opportunities.

Usage example

The graph below corresponds to the *ASIA network* (Lauritzen & Spiegelhalter, 1988), a simple Bayesian network (Pearl, 1985) used extensively in educational settings. It describes the probabilistic relationships between different random variables which correspond to possible diseases, symptoms, risk factors and test results.



Random variable	Meaning
A	Recent trip to Asia
T	Patient has tuberculosis
S	Patient is a smoker
L	Patient has lung cancer
B	Patient has bronchitis
E	Patient has T and/or L
X	Chest X-Ray is positive
D	Patient has dyspnoea

Figure 1: The ASIA network: a simplified example of a Bayesian network from the context of medical diagnosis (Lauritzen & Spiegelhalter, 1988).

In the example, a patient has recently visited Asia and is now experiencing dyspnea. These conditions serve as the evidence for the observed variables (A and D). The doctor's task is to assess the likelihood of various diseases — tuberculosis, lung cancer, and bronchitis - which constitute the query variables in this scenario (T, L, and B).

We now demonstrate how to use `TensorInference.jl` for conducting a variety of inference tasks on this toy example. Please note that as the API may evolve, we recommend checking the examples directory of the official `TensorInference.jl` repository for the most up-to-date version of this example.

```julia
# Import the TensorInference package, which provides the functionality needed
# for working with tensor networks and probabilistic graphical models.
using TensorInference

# Load the ASIA network model from the `asia.uai` file located in the examples
# directory. Refer to the documentation of this package for a description of the
# format of this file.
instance = read_instance(pkgdir(TensorInference, "examples", "asia", "asia.uai"))

# Create a tensor network representation of the loaded model.
# The variable 7 is the variable of interest, which will be retained in the output.
tn = TensorNetworkModel(instance; openvars=[7])

# Calculate the partition function for each assignment of variable 7.
probability(tn)

# Calculate the marginal probabilities of each random variable in the model.
marginals(tn)

# Retrieve the variables associated with the tensor network model.
get_vars(tn)

# Assume that the "X-ray" result (variable 7) is positive.
# Since setting an evidence may affect the contraction order of the tensor
# network, recompute it.
tn = TensorNetworkModel(instance; evidence=Dict(7 => 0))

# Calculate the maximum log-probability among all configurations.
maximum_logp(tn)

# Generate 10 samples from the probability distribution represented by the
# model.
sample(tn, 10)

# Retrieve both the maximum log-probability and the most probable
# configuration. In this configuration, the most likely outcomes are that the
# patient smokes (variable 3) and has lung cancer (variable 4).
logp, cfg = most_probable_config(tn)

# Compute the most probable values of certain variables (e.g., 4 and 7) while
# marginalizing over others. This is known as Maximum a Posteriori (MAP)
# estimation.
mmap = MMAPModel(instance, queryvars=[4, 7])

# Get the most probable configurations for variables 4 and 7.
most_probable_config(mmap)

# Compute the total log-probability of having lung cancer. The results suggest
# that the probability is roughly half.
log_probability(mmap, [1, 0]), log_probability(mmap, [0, 0])
```

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