LibSPN Keras

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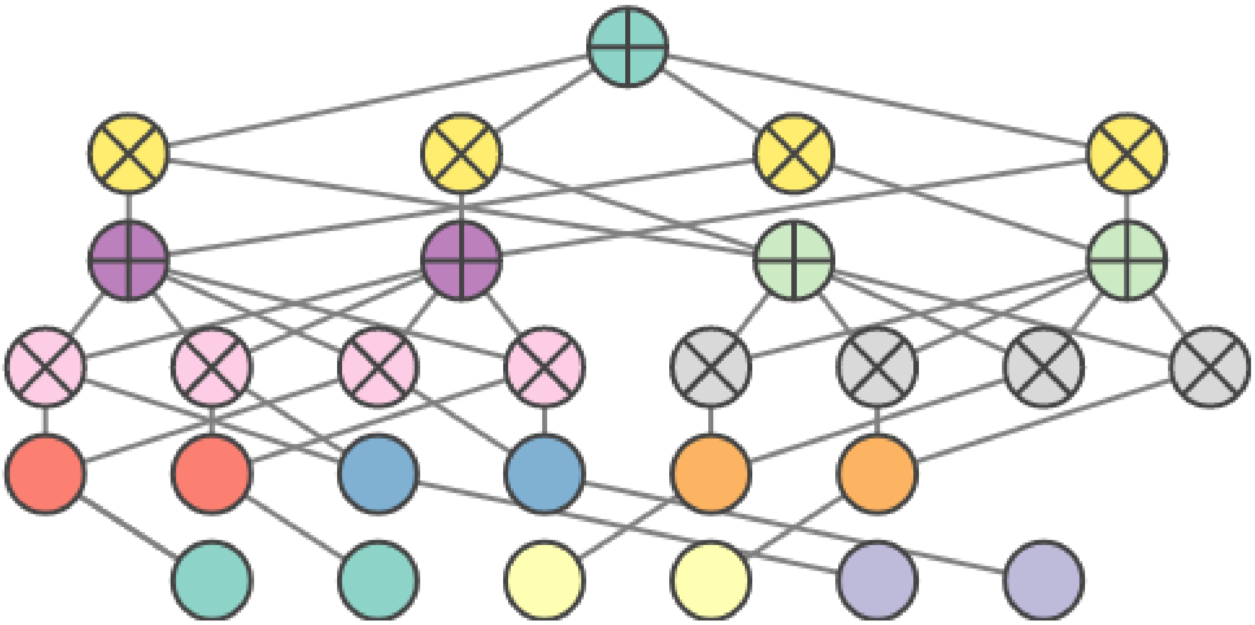
LibSPN Keras is a library for constructing and training Sum-Product Networks. By leveraging the Keras framework with a TensorFlow backend, it offers both ease-of-use and scalability. Whereas the previously available `libspn` focused on scalability, `libspn-keras` offers scalability **and** a straightforward Keras-compatible interface.



CHAPTER

ONE

CONTENTS

1.1 API Reference

1.1.1 Layers

This submodule contains Keras layers for building SPNs. Besides leaf layers and regularization layers, there are two main groups of layers:

- Region layers for arbitrary decompositions of variables. Must be preceded with a `[FlatToRegions, BaseLeaf, PermuteAndPadScopes]` block. Regions are arbitrary sets of variables. A region graph describes how these sets of variables hierarchically define a probability distribution.
- Spatial layers for Deep Generalized Convolutional Sum Product Networks

All layers propagate log probabilities in the forward pass. So in case you want to know about the 'raw' probability, you simply pass the output of a layer through exp.

Leaf layers

Leaf layers transform raw observations to probabilities.

- `NormalLeaf`, `CauchyLeaf` and `LaplaceLeaf` can be used for continuous inputs.
- `IndicatorLeaf` should be used for discrete inputs.

If a variable is not part of the evidence, that means that variable should be marginalized out. This can be done by replacing the output of the corresponding components with 0 since that corresponds with 1 in *log-space*.

Continuous leaf layers

class `libspn_keras.layers.`**`NormalLeaf`**(*num_components*, *location_initializer=None*, *location_trainable=True*, *scale_initializer=None*, *scale_trainable=False*, *accumulator_initializer=None*, *use_accumulators=False*, *scale_constraint=None*, ***kwargs*)

Computes the log probability of multiple components per variable along the final axis.

Each component is modelled as a normal distribution with a diagonal covariance matrix.

Parameters

- **`num_components`** (`int`) – Number of components per variable

- **location_initializer** (Optional[Initializer]) – Initializer for location variable
- **location_trainable** (bool) – Boolean that indicates whether location is trainable
- **scale_initializer** (Optional[Initializer]) – Initializer for scale variable
- **scale_trainable** (bool) – Boolean that indicates whether scale is trainable
- ****kwargs** – kwargs to pass on to the keras.Layer super class

class libspn_keras.layers.**CauchyLeaf**(*num_components*, *location_initializer=None*, *location_trainable=True*, *scale_initializer=None*, *accumulator_initializer=None*, *use_accumulators=False*, *scale_trainable=False*, ***kwargs*)

Computes the log probability of multiple components per variable along the final axis.

Each component is modelled as a Cauchy distribution with a diagonal location matrix.

Parameters

- **num_components** (int) – Number of components per variable
- **location_initializer** (Optional[Initializer]) – Initializer for location variable
- **location_trainable** (bool) – Boolean that indicates whether location is trainable
- **scale_initializer** (Optional[Initializer]) – Initializer for scale variable
- ****kwargs** – kwargs to pass on to the keras.Layer super class

class libspn_keras.layers.**LaplaceLeaf**(*num_components*, *location_initializer=None*, *location_trainable=True*, *scale_initializer=None*, *accumulator_initializer=None*, *use_accumulators=False*, ***kwargs*)

Computes the log probability of multiple components per variable along the final axis.

Each component is modelled as a Laplace distribution with a diagonal location matrix.

Parameters

- **num_components** (int) – Number of components per variable
- **location_initializer** (Optional[Initializer]) – Initializer for location variable
- **location_trainable** (bool) – Boolean that indicates whether location is trainable
- **scale_initializer** (Optional[Initializer]) – Initializer for scale variable
- ****kwargs** – kwargs to pass on to the keras.Layer super class

Discrete leaf layers

class libspn_keras.layers.**IndicatorLeaf**(*num_components*, *dtype=tf.int32*, ***kwargs*)

Indicator leaf distribution taking integer inputs and producing a discrete indicator representation.

This effectively comes down to computing a one-hot representation along the final axis.

Parameters

- **num_components** (*int*) – Number of components, or indicators in this context.
- **dtype** (DType) – Dtype of input

- **`**kwargs`** – Kwargs to pass onto the `keras.layers.Layer` superclass.

Region layers

Region layers assume the tensors that are passed between them are of the shape `[num_scopes, num_decomps, num_batch, num_nodes]`. One region is given by the scope index + the decomposition (so it is indexed on the first two axes). This shape is chosen so that `matmul` operations done in `DenseSum` layers don't always require transposing first.

class `libspn_keras.layers.`**`FlatToRegions`**(*num_decomps*, ***kwargs*)

Flat representation to a dense representation.

Reshapes a flat input of shape `[batch, num_vars[, var_dimensionality]]` to `[batch, num_vars == scopes, decomp, var_dimensionality]`

If `var_dimensionality` is 1, the shape can also be `[batch, num_vars]`.

Parameters **`**kwargs`** – Keyword arguments to pass on the keras.Layer super class

class `libspn_keras.layers.`**`PermuteAndPadScopes`**(*permutations=None*, ***kwargs*)

Permutes and pads scopes, usually applied after a `FlatToRegions` and a `BaseLeaf` layer.

Padding can be used to ensure uniform dimension sizes across scopes, decomps and nodes in the layer stack. Padding is achieved by using `-1` for scope indices in `permutations`.

Parameters

- **`num_decomps`** – Number of decompositions
- **`permutations`** (`Union`[`List`[`List`[`int`]], `ndarray`, `None`]) – If None, permutations must be specified later
- **`**kwargs`** – kwargs to pass on to the keras.Layer superclass.

class `libspn_keras.layers.`**`PermuteAndPadScopesRandom`**(*factors=None*, ***kwargs*)

Permutes scopes, usually applied after a `FlatToRegions` and a `BaseLeaf` layer.

Parameters

- **`factors`** (`Optional`[`List`[`int`]]) – Number of factors in preceding product layers. Needed to compute the effective number of scopes, including padded nodes. Can be applied at later stage through `generate_factors`.
- **`**kwargs`** – kwargs to pass on to the `keras.Layer` superclass.

class `libspn_keras.layers.`**`DenseSum`**(*num_sums*, *logspace_accumulators=None*, *accumulator_initializer=None*, *sum_op=None*, *accumulator_regularizer=None*, *logspace_accumulator_constraint=None*, *linear_accumulator_constraint=None*, ***kwargs*)

Computes densely connected sums per scope and decomposition.

Expects incoming `Tensor` to be of shape [num_scopes, num_decomps, num_batch, num_nodes]. If your input is passed through a `FlatToRegions` layer this is already taken care of.

Parameters

- **`num_sums`** (`int`) – Number of sums per scope
- **`logspace_accumulators`** (`Optional`[`bool`]) – If `True`, accumulators will be represented in log-space which is typically used with `BackpropMode.GRADIENT`. If `False`, accumulators will be represented in linear space. Weights are computed by normalizing the accumulators per sum, so that we always end up with a normalized SPN. If

`None` (default) it will be set to `True` for `BackpropMode.GRADIENT` and `False` otherwise.

- **`accumulator_initializer`** (`Optional[Initializer]`) – Initializer for accumulator. Will automatically be converted to log-space values if `logspace_accumulators` is enabled.
- **`accumulator_regularizer`** (`Optional[Regularizer]`) – Regularizer for accumulator (experimental)
- **`linear_accumulator_constraint`** (`Optional[Constraint]`) – Constraint for accumulator defaults to constraint that ensures small positive constant at minimum. Will be ignored if logspace_accumulators is set to True.
- **`sum_op`** (*`SumOpBase`*) – SumOpBase instance which determines how to compute the forward and backward pass of the weighted sums
- **`**kwargs`** – kwargs to pass on to keras.Layer super class

`class` `libspn_keras.layers.`**`DenseProduct`**(*num_factors*, ***kwargs*)

Computes products per decomposition and scope by an 'n-order' outer product.

Assumes the incoming tensor is of shape `[num_scopes, num_decomps, num_batch, num_nodes]` and produces an output of `[num_scopes // num_factors, num_decomps, num_batch, num_nodes ** num_factors]`. It can be considered a *dense* product as it computes all possible products given the scopes it has to merge.

Parameters

- **`num_factors`** (*`int`*) – Number of factors per product
- **`**kwargs`** – kwargs to pass on to the keras.Layer super class

`class` `libspn_keras.layers.`**`ReduceProduct`**(*num_factors*, ***kwargs*)

Computes products per decomposition and scope by reduction.

Assumes the incoming tensor is of shape `[num_batch, num_scopes, num_decomps, num_nodes]` and produces an output of `[num_batch, num_scopes // num_factors, num_decomps, num_nodes]`.

Parameters

- **`num_factors`** (`int`) – Number of factors per product
- **`**kwargs`** – kwargs to pass on to the keras.Layer super class.

`class` `libspn_keras.layers.`**`RootSum`**(*return_weighted_child_logits=True*, *logspace_accumulators=None*, *accumulator_initializer=None*, *trainable=True*, *logspace_accumulator_constraint=None*, *accumulator_regularizer=None*, *linear_accumulator_constraint=None*, *sum_op=None*, ***kwargs*)

Final sum of an SPN. Expects input to be in log-space and produces log-space output.

Parameters

- **`return_weighted_child_logits`** (`bool`) – If True, returns a weighted child log probability, which can be used for e.g. (Sparse)CategoricalCrossEntropy losses. If False, computes the weighted sum of the input, which effectively is the log probability of the distribution defined by the SPN.
- **`logspace_accumulators`** (`Optional[bool]`) – If `True`, accumulators will be represented in log-space which is typically used with `BackpropMode.GRADIENT`. If

False, accumulators will be represented in linear space. Weights are computed by normalizing the accumulators per sum, so that we always end up with a normalized SPN. If None (default) it will be set to True for BackpropMode.GRADIENT and False otherwise.

- **accumulator_initializer** (Optional[Initializer]) – Initializer for accumulator. If None, defaults to initializers.Constant(1.0)
- **accumulator_regularizer** (Optional[Regularizer]) – Regularizer for accumulator.
- **linear_accumulator_constraint** (Optional[Constraint]) – Constraint for linear accumulators. Defaults to a constraint that ensures a minimum of a small positive constant. If logspace_accumulators is set to True, this constraint wil be ignored
- **sum_op** (*SumOpBase*) – SumOpBase instance which determines how to compute the forward and backward pass of the weighted sums
- ****kwargs** – kwargs to pass on to the keras.Layer super class

Spatial layers

Spatial layers are layers needed for building DGC-SPNs. The final layer of an SPN should still be a RootSum. Use SpatialToRegions to convert the output from a spatial SPN to a region SPN.

class libspn_keras.layers.**Local2DSum**(*num_sums*, *logspace_accumulators=None*, *accumulator_initializer=None*, *sum_op=None*, *accumulator_regularizer=None*, *logspace_accumulator_constraint=None*, *linear_accumulator_constraint=None*, ***kwargs*)

Computes a spatial local sum, i.e. all cells will have unique weights.

In other words, there is no weight sharing across the spatial axes.

Parameters

- **num_sums** (int) – Number of sums per spatial cell. Corresponds to the number of channels in the output
- **logspace_accumulators** (Optional[bool]) – If True, accumulators will be represented in log-space which is typically used with BackpropMode.GRADIENT. If False, accumulators will be represented in linear space. Weights are computed by normalizing the accumulators per sum, so that we always end up with a normalized SPN. If None (default) it will be set to True for BackpropMode.GRADIENT and False otherwise.
- **accumulator_initializer** (Optional[Initializer]) – Initializer for accumulator
- **accumulator_regularizer** (Optional[Regularizer]) – Regularizer for accumulators
- **linear_accumulator_constraint** (Optional[Constraint]) – Constraint for accumulators (only applied if log_space_accumulators==False)
- **sum_op** (*SumOpBase*) – SumOpBase instance which determines how to compute the forward and backward pass of the weighted sums
- ****kwargs** – kwargs to pass on to the keras.Layer super class

class libspn_keras.layers.**Conv2DSum**(*num_sums*, *logspace_accumulators=None*, *accumulator_initializer=None*, *sum_op=None*, *accumulator_regularizer=None*, *logspace_accumulator_constraint=None*, *linear_accumulator_constraint=None*, ***kwargs*)

Computes a convolutional sum, i.e. weights are shared across the spatial axes.

Parameters

- **num_sums** (`int`) – Number of sums per spatial cell. Corresponds to the number of channels in the output
- **logspace_accumulators** (`Optional[bool]`) – If `True`, accumulators will be represented in log-space which is typically used with `BackpropMode.GRADIENT`. If `False`, accumulators will be represented in linear space. Weights are computed by normalizing the accumulators per sum, so that we always end up with a normalized SPN. If `None` (default) it will be set to `True` for `BackpropMode.GRADIENT` and `False` otherwise.
- **accumulator_initializer** (`Optional[Initializer]`) – Initializer for accumulator
- **sum_op** (*`SumOpBase`*) – SumOpBase instance which determines how to compute the forward and backward pass of the weighted sums
- **accumulator_regularizer** (`Optional[Regularizer]`) – Regularizer for accumulators
- **linear_accumulator_constraint** (`Optional[Constraint]`) – Constraint for accumulators (only applied if log_space_accumulators==False)
- ****kwargs** – kwargs to pass on to the keras.Layer super class

class libspn_keras.layers.**Conv2DProduct**(*strides*, *dilations*, *kernel_size*, *num_channels=None*, *padding='valid'*, *depthwise=False*, ***kwargs*)

Convolutional product as described in (Van de Wolfshaar and Pronobis, 2019).

Expects log-space inputs and produces log-space outputs.

Parameters

- **strides** (`List[int]`) – A tuple or list of strides
- **dilations** (`List[int]`) – A tuple or list of dilations
- **kernel_size** (`List[int]`) – A tuple or list of kernel sizes
- **num_channels** (`Optional[int]`) – Number of channels. If None, will be set to num_in_channels ** prod(kernel_sizes). This can be source of OOM problems quickly.
- **padding** (`str`) – Can be either 'full', 'valid' or 'final'. Use 'final' for the top ConvProduct of a DGC-SPN. The other choices have the standard interpretation. Valid padding usually requires non-overlapping patches, whilst full padding is used with overlapping patches and expontentially increasing dilation rates, see also [Van de Wolfshaar, Pronobis (2019)].
- **depthwise** (`bool`) – Whether to use depthwise convolutions. If True, the value of num_channels will be ignored
- ****kwargs** – Keyword arguments to pass on to the keras.Layer superclass.

References

Deep Generalized Convolutional Sum-Product Networks for Probabilistic Image Representations, Van de Wolfshaar, Pronobis (2019)

class `libspn_keras.layers.`**`SpatialToRegions`**(**args*, ***kwargs*)

Reshapes spatial SPN layer to a dense layer.

The dense output has leading dimensions for scopes and decomps (which will be `[1, 1]`).

Dynamic SPN layers

For reusing SPN structures along the temporal dimension one can implement dynamic SPNs. These rely on *template SPNs*, *top SPNs* and an *interface*. The interface of the previous timestep and the template at the current timestep can be combined through `TemporalDenseProduct`.

class `libspn_keras.layers.`**`TemporalDenseProduct`**(**args*, ***kwargs*)

Computes 'temporal' dense products.

This is used to connect an interface stack at $t - 1$ of a dynamic SPN with a template SPN at t. Computes a product of all possible combinations of nodes along the last axis of the two incoming layers.

Parameters **`**kwargs`** – kwargs to pass on to the keras.Layer super class.

Regularization layers

class `libspn_keras.layers.`**`LogDropout`**(*rate*, *noise_shape=None*, *seed=None*, *axis_at_least_one=None*, ***kwargs*)

Log dropout layer.

Applies dropout in log-space. Should not precede product layers in an SPN, since their scope probability then potentially becomes -inf, resulting in NaN-values during training.

Parameters

- **`rate`** (`float`) – Rate at which to randomly dropout inputs.
- **`noise_shape`** (`Optional[Tuple[int, ...]]`) – Shape of dropout noise tensor
- **`seed`** (`Optional[int]`) – Random seed
- **`**kwargs`** – kwargs to pass on to the keras.Layer super class

Normalization layers

class `libspn_keras.layers.`**`NormalizeStandardScore`**(*normalization_epsilon=1e-08*, *sample_wise=True*, ***kwargs*)

Normalizes samples to a standard score.

In other words, the output is the input minus its mean and divided by the standard deviation. This can be used to achieve the same kind of normalization as used in (Poon and Domingos, 2011).

Parameters

- **`normalization_epsilon`** (`float`) – Small positive constant to prevent division by zero, but could also be used a 'smoothing' factor.

- **`sample_wise`** (`bool`) – If `True`, will compute z-scores where statistics are computed sample-wise, otherwise, computes z-scores through computing cross-sample statistics. To use cross-sample statistics, call `NormalizeStandardScore.adapt(train_ds)` where `train_ds` is an instance of `tf.data.Dataset`.
- **`**kwargs`** – kwargs to pass on to the keras.Layer super class

References

Sum-Product Networks, a New Deep Architecture Poon and Domingos, 2011

1.1.2 Models

This submodule provides some out-of-the box model analogues of `tensorflow.keras.Model`. They can be used to train SPNs for e.g. generative scenarios, where there is no label for an input. There's also a `DynamicSumProductNetwork` that can be used for

Feedforward models

class `libspn_keras.models.`**`SumProductNetwork`**(**args*, *unsupervised=True*, ***kwargs*)

An SPN analogue of tensorflow.keras.Model that can be trained generatively.

It does not expect labels y when calling .fit() if `unsupervised` == True.

Parameters **`unsupervised`** (*`bool`*) – If `True` (default) the model does not expect label inputs in .fit() or .evaluate(). Also, losses and metrics should not expect a target output, just a y_hat.

class `libspn_keras.models.`**`SequentialSumProductNetwork`**(*layers*, *infer_no_evidence=False*, *unsupervised=None*, ***kwargs*)

An analogue of `tensorflow.keras.Sequential` that can be trained in an unsupervised way.

It does not expect labels y when calling .fit() if `unsupervised` == True. Inherits from `keras.Sequential`, so layers are passed to it as a list.

Parameters

- **`unsupervised`** (*`bool`*) – If `True` the model does not expect label inputs in .fit() or .evaluate(). Also, losses and metrics should not expect a target output, just a y_hat. By default, it will be inferred from `infer_no_evidence` and otherwise defaults to `True`.
- **`infer_no_evidence`** (*`bool`*) – If `True`, the model expects an evidence mask defined as a boolean tensor which is used to mask out variables that are not part of the evidence.

Temporal models

class `libspn_keras.models.`**`DynamicSumProductNetwork`**(*template_network*, *interface_network_t0*, *interface_network_t_minus_1*, *top_network*, *return_last_step=True*, *unsupervised=True*, ***kwargs*)

SPN that re-uses its nodes at each time step.

The input is expected to be pre-padded sequences with a full tensor shape of [num_batch, max_sequence_len, num_variables].

Parameters

- **`template_network`** (`Model`) – Template network that is applied to the leaves and ends with nodes that cover all variables for each timestep.
- **`interface_network_t0`** (`Model`) – Interface network for t = t0, applied on top of the template network's output at the current timestep.
- **`interface_network_t_minus_1`** (`Model`) – Interface network for t = t0 - 1, applied to the output of the interfaced output of the previous timestep
- **`top_network`** (`Model`) – Network on top of the interfaced network at the current timestep (covers all variables of the current timestep, including those of previous timesteps). This network must end with a root sum layer.
- **`return_last_step`** (*`bool`*) – Whether to return only the roots at the last step with shape [num_batch, root_num_out] or whether to [num_batch, max_sequence_len, root_num_out]
- **`unsupervised`** (*`bool`*) –

1.1.3 Sum Operations

LibSPN-Keras offers a convenient way to control the backward pass for sum operations used in the SPNs you build. Internally, LibSPN-Keras defines a couple of sum operations with different backward passes, for gradient as well as EM learning. All of these operations inherit from the `SumOpBase` class in `libspn_keras/sum_ops.py`.

NOTE

By default, LibSPN-Keras uses `SumOpGradBackprop`.

Getting And Setting a Sum Op

These methods allow for setting and getting the current default `SumOpBase`. By setting a default all sum layers (`DenseSum`, `Conv2DSum`, `Local2DSum` and `RootSum`) will use that sum op, unless you explicitly provide a `SumOpBase` instance to any of those classes when initializing them.

`libspn_keras.config.sum_op.`**`set_default_sum_op`**`(`*op*`)`

Set default sum op to conveniently use it throughout an SPN architecture.

Parameters **`op`** (*`SumOpBase`*) – Implementation of sum op with corresponding backward pass definitions

Return type `None`

`libspn_keras.config.sum_op.`**`get_default_sum_op`**`()`

Get default sum op.

Return type `SumOpBase`

Returns A `SumOpBase` instance that was set with `set_default_sum_op`

Sum Operation With Gradients In Backward Pass

class `libspn_keras.sum_ops.`**`SumOpGradBackprop`**(*logspace_accumulators=None*)

Sum op primitive with gradient in backpropagation when computed through TensorFlow's autograd engine.

Internally, weighted sums are computed with default gradients for all ops being used.

Parameters **`logspace_accumulators`** (`Optional[bool]`) – If provided overrides default log-space choice. For a `SumOpGradBackprop` the default is `True`

Sum Operations With EM Signals In Backward Pass

class `libspn_keras.sum_ops.`**`SumOpEMBackprop`**

Sum op primitive with EM signals in backpropagation.

These are dense EM signals as opposed to the other EM based instances of `SumOpBase`.

class `libspn_keras.sum_ops.`**`SumOpHardEMBackprop`**(*sample_prob=None*)

Sum op with hard EM signals in backpropagation when computed through TensorFlow's autograd engine.

Parameters **`sample_prob`** (`Union[float, Tensor, None]`) – Sampling probability in the range of [0, 1]. Sampling logits are taken from the normalized log probability of the children of each sum.

class `libspn_keras.sum_ops.`**`SumOpUnweightedHardEMBackprop`**(*sample_prob=None*)

Sum op with hard EM signals in backpropagation when computed through TensorFlow's autograd engine.

Instead of using weighted sum inputs to select the maximum child, it relies on unweighted child inputs, which has the advantage of alleviating a self-amplifying chain of hard EM signals in deep SPNs.

Parameters **`sample_prob`** (`Union[float, Tensor, None]`) – Sampling probability in the range of [0, 1]. Sampling logits are taken from the normalized log probability of the children of each sum.

1.1.4 Initializers

In addition to initializers in `tensorflow.keras.initializers`, `libspn-keras` implements a few more useful initialization schemes for both leaf layers as well as sum weights.

Setting Defaults

Since accumulator initializers are often the same for all layers in an SPN, `libspn-keras` provides the following functions to get and set default accumulator initializers. These can still be overridden by providing the initializers explicitly at initialization of a layer.

`libspn_keras.config.accumulator_initializer.`**`set_default_accumulator_initializer`**(*initializer*)

Configure the default accumulator that will be used for sum accumulators.

Parameters **`initializer`** (`Initializer`) – The initializer which will be used by default for sum accumulators.

Return type `None`

`libspn_keras.config.accumulator_initializer.`**`get_default_accumulator_initializer`**()

Obtain default accumulator initializer.

Return type `Initializer`

Returns The default accumulator initializer that will be use in sum accumulators, unless specified explicitly at initialization.

Location initializers

For a leaf distribution of the location scale family, the following initializers are useful

class `libspn_keras.initializers.`**`PoonDomingosMeanOfQuantileSplit`**(*data=None*, *samplewise_normalization=True*, *normalization_epsilon=0.01*)

Initializes the data according to the algorithm described in (Poon and Domingos, 2011).

The data is divided over K quantiles where K is the number of nodes along the last axis of the tensor to be initialized. The quantiles are computed over all samples in the provided `data`. Then, the mean per quantile is taken as the value for initialization.

Parameters

- **`data`** (*`numpy.ndarray`*) – Data to compute quantiles over
- **`samplewise_normalization`** (`bool`) – Whether to 'Z-score normalize' the data sample-wise before computing the quantiles and means.
- **`normalization_epsilon`** (`float`) – Non-zero constant to account for near-zero standard deviations in normalizations.

References

Sum-Product Networks, a New Deep Architecture Poon and Domingos, 2011

class `libspn_keras.initializers.`**`KMeans`**(*data=None*, *samplewise_normalization=True*, *data_fraction=0.2*, *normalization_epsilon=0.01*, *stop_epsilon=0.0001*, *num_iters=100*, *group_centroids=True*, *max_num_clusters=8*, *jitter_factor=0.05*, *centroid_initialization='kmeans++'*, *downsample=None*, *use_groups=False*)

Initializer learned through K-means from data.

The centroids learned from K-means are used to initialize the location parameters of a location-scale leaf, such as a `NormalLeaf`. This is particularly useful for variables with dimensionality of greater than 1.

Notes

Currently only works for spatial SPNs.

Parameters

- **`data`** (*`numpy.ndarray`*) – Data on which to perform K-means.
- **`samplewise_normalization`** (*`bool`*) – Whether to normalize data before learning centroids.
- **`data_fraction`** (*`float`*) – Fraction of the data to use for K-means (chosen randomly)
- **`normalization_epsilon`** (*`float`*) – Normalization constant (only used when `sample_normalization` is `True`.

- **stop_epsilon** (float) – Non-zero constant for difference in MSE on which to stop K-means fitting.
- **num_iters** (*int*) – Maximum number of iterations.
- **group_centroids** (*bool*) – If True, performs another round of K-means to group the centroids along the scope axes.
- **max_num_clusters** (*int*) – Maximum number of clusters (use this to limit the memory needed)
- **jitter_factor** (*float*) – If the number of clusters is larger than allowed according to max_num_clusters, the learned max_num_clusters centroids are repeated and then jittered with noise generated from a truncated normal distribution with a standard deviation of jitter_factor
- **centroid_initialization** (*str*) – Centroid initialization algorithm. If "kmeans++", will iteratively initialize clusters far apart from each other. Otherwise, the centroids will be initialized from the data randomly.

class libspn_keras.initializers.**Equidistant**(*minval=0.0*, *maxval=1.0*)

Initializer that generates tensors where the last axis is initialized with 'equidistant' values.

Parameters

- **minval** (float) – A python scalar or a scalar tensor. Lower bound of the range of random values to generate.
- **maxval** (float) – A python scalar or a scalar tensor. Upper bound of the range of random values to generate. Defaults to 1 for float types.

Weight initializers

When training with either HARD_EM or HARD_EM_UNWEIGHTED, you can use the EpsilonInverseFanIn initializer.

class libspn_keras.initializers.**EpsilonInverseFanIn**(*axis=- 2*, *epsilon=0.0001*)

Initializes all values in a tensor with ϵK^{-1}.

Where K is the dimension at axis.

This is particularly useful for (unweighted) hard EM learning and should generally be avoided otherwise.

Parameters

- **axis** (int) – The axis for input nodes so that K^{-1} is the inverse fan in. Usually, this is -2.
- **epsilon** (float) – A small non-zero constant

class libspn_keras.initializers.**Dirichlet**(*axis=- 2*, *alpha=0.1*)

Initializes all values in a tensor with $Dir(\alpha)$.

Parameters

- **axis** (int) – The axis over which to sample from a $Dir(\alpha)$.
- **alpha** (float) – The α parameter of the Dirichlet distribution. If a scalar, this is broadcast along the given axis.

1.1.5 Losses

Supervised generative learning

The following loss can be used when trying to maximize $p(X, Y)$.

class `libspn_keras.losses.`**`NegativeLogJoint`**(*reduction='auto'*, *name=None*)

Compute $-\log(p(X, Y))$.

Assumes that its input is $\log(p(X|Y))$ where Y is indexed on the second axis. This can be used for supervised generative learning with gradient-based optimizers or (hard) expectation maximization.

Unsupervised generative learning

The following loss can be used when trying to maximize $p(X)$.

class `libspn_keras.losses.`**`NegativeLogLikelihood`**(*reduction='auto'*, *name=None*)

Marginalize logits over last dimension so that it computes $-\log(p(X))$.

This can be used for unsupervised generative learning.

1.1.6 Optimizers

Apart from the one(s) below, any optimizer in `tensorflow.keras.optimizers` can be used.

class `libspn_keras.optimizers.`**`OnlineExpectationMaximization`**(*learning_rate=0.05*, *gliding_average=True*, ***kwargs*)

Online expectation maximization which requires sum layers to use any of the EM-based SumOpBase instances.

Internally, this is just an SGD optimizer with unit learning rate.

1.1.7 Metrics

class `libspn_keras.metrics.`**`LogLikelihood`**(*name='llh'*, ***kwargs*)

Compute log marginal $1/N \sum \log(p(X))$.

Assumes that the last layer of the SPN is a `RootSum`. It ignores the `y_true` argument, since a target for Y is absent in unsupervised learning.

1.1.8 Constraints

Linear Weight Constraints

These should be used for linear accumulators.

class `libspn_keras.constraints.`**`GreaterEqualEpsilonNormalized`**(*epsilon=1e-10*, *axis=- 2*)

Constraints the weight to be greater than or equal to epsilon and then normalizes.

Parameters **`epsilon`** (`float`) – Constant, usually small non-zero

class `libspn_keras.constraints.`**`GreaterEqualEpsilon`**(*epsilon=1e-10*)

Constraints the weight to be greater than or equal to epsilon.

Parameters **`epsilon`** (`float`) – Constant, usually small non-zero

Log Weight Constraints

These should be used for log accumulators.

class `libspn_keras.constraints.`**`LogNormalized`**(*axis=- 2*)

Normalizes log-space weights.

Parameters **`axis`** (*`int`*) – Axis along whichto normalize

Scale Constraints

The following constraint is useful for ensuring stable scale parameters in location-scale leaf layers.

class `libspn_keras.constraints.`**`Clip`**(*min*, *max=None*)

Constraints the weights to be between `min` and `max`.

Parameters

- **`min`** (`float`) – Minimum clip value
- **`max`** (`Optional[float]`) – Maximum clip value

1.1.9 Region graphs

The region graph utilities can be made to create SPNs by explicitly defining the region structure. This can be used to e.g. conveniently express some learned structure.

For some examples on how to use region graphs check out this tutorial.

class `libspn_keras.`**`RegionVariable`**(*index*)

Represents a region in the SPN.

Regions graphs are DAGs just like SPNs, but they do not represent sums and products. They are merely used for defining the scope structure of the SPN.

A RegionVariable is a leaf node without children, as opposed to a RegionNode which is a node with children.

Parameters **`index`** (`int`) – Index of the variable

class `libspn_keras.`**`RegionNode`**(*children*)

Represents a region in the SPN.

Regions graphs are DAGs just like SPNs, but they do not represent sums and products. They are merely used for defining the scope structure of the SPN.

A RegionNode is a node with children, as opposed to a RegionVariable, which is a leaf node.

Parameters **`children`** (*`list of RegionNode or`* `RegionVariable`) – children of this node. Scope of the resulting node is the union of the scopes of its children. The scopes of these children must not overlap (pairwise disjoint)

`libspn_keras.`**`region_graph_to_dense_spn`**(*region_graph_root*, *leaf_node*, *num_sums_iterable*, *return_weighted_child_logits*, *logspace_accumulators=False*, *accumulator_initializer=None*, *linear_accumulator_constraint=None*, *product_first=True*, *num_classes=None*, *with_root=True*)

Convert a region graph (built from `RegionNode` and `RegionVar`) to a dense SPN.

Parameters

- **`region_graph_root`** (`RegionNode`) – Root of the region graph
- **`leaf_node`** (`BaseLeaf`) – Node to insert at the leaf of the SPN
- **`num_sums_iterable`** (`Iterator[int]`) – Number of sums for all but the last root sum layer from bottom to top
- **`logspace_accumulators`** (`bool`) – Whether to represent accumulators of weights in logspace or not
- **`accumulator_initializer`** (`Optional[Initializer]`) – Initializer for accumulators
- **`linear_accumulator_constraint`** (`Optional[Constraint]`) – Constraint for linear accumulator, default: GreaterThanEpsilon
- **`product_first`** (`bool`) – Whether to start with a product layer
- **`num_classes`** (`Optional[int]`) – Number of classes at output. If `None`, will not use 'latent' sums at the end but will instead directly connect the root to the final layer of the dense stack. This means if set to `None` the SPN cannot be used for classification.
- **`with_root`** (`bool`) – If `True`, sets a `RootSum` as the final layer.
- **`return_weighted_child_logits`** (`bool`) – Whether to return weighted child logits. If ``

Return type `Sequential`

Returns A Sum-Product Network as a tf.keras.Sequential model.

1.1.10 Visualization

For educational purposes, the following module can be used to visualize dense SPNs.

`libspn_keras.visualize.`**`visualize_dense_spn`**(*dense_spn*, *show_legend=False*, *show_padding=True*, *transparent=False*, *node_size=30*)

Visualize dense SPN, consisting of `DenseSum`, `DenseProduct`, `RootSum` and leaf layers.

Parameters

- **`dense_spn`** (`Model`) – An SPN of type `tensorflow.keras.Sequential`
- **`show_legend`** (`bool`) – Whether to show legend of scopes and layers on the right
- **`show_padding`** (`bool`) – Whether to show padded nodes
- **`transparent`** (`bool`) – If `True`, the background is transparent.
- **`node_size`** (`int`) – Size of the nodes drawn in the graph. Adjust to avoid clutter.

Return type `Figure`

Returns A `plotly.graph_objects.Figure` instance. Use `.show()` to render the visualization.

CHAPTER TWO

DOCUMENTATION

The documentation of the library is hosted on ReadTheDocs.

CHAPTER THREE

WHAT ARE SPNS?

Sum-Product Networks (SPNs) are a probabilistic deep architecture with solid theoretical foundations, which demonstrated state-of-the-art performance in several domains. Yet, surprisingly, there are no mature, general-purpose SPN implementations that would serve as a platform for the community of machine learning researchers centered around SPNs. LibSPN Keras is a new general-purpose Python library, which aims to become such a platform. The library is designed to make it straightforward and effortless to apply various SPN architectures to large-scale datasets and problems. The library achieves scalability and efficiency, thanks to a tight coupling with TensorFlow and Keras, two frameworks already in use by a large community of researchers and developers in multiple domains.

CHAPTER FOUR

DEPENDENCIES

Currently, LibSPN Keras is tested with `tensorflow>=2.0` and `tensorflow-probability>=0.8.0`.

CHAPTER FIVE

INSTALLATION

```
pip install libspn-keras
```

CHAPTER

SIX

NOTE ON STABILITY OF THE REPO

Currently, the repo is in an alpha state. Hence, one can expect some sporadic breaking changes.

CHAPTER

SEVEN

FEATURE OVERVIEW

- Gradient based training for generative and discriminative problems
- Hard EM training for generative problems
- Hard EM training with unweighted weights for generative problems
- Soft EM training for generative problems
- Deep Generalized Convolutional Sum-Product Networks
- SPNs with arbitrary decompositions
- Fully compatible with Keras and TensorFlow 2.0
- Input dropout
- Sum child dropout
- Image completion
- Model saving
- Discrete inputs through an `IndicatorLeaf` node
- Continuous inputs through `NormalLeaf`, `CauchyLeaf` or `LaplaceLeaf`. Each of these distributions support both univariate as well as *multivariate* inputs.

CHAPTER

EIGHT

EXAMPLES / TUTORIALS

1. **Benchmark**: `libspn-keras` and Einsum Networks.
2. **Image Classification**: A Deep Generalized Convolutional Sum-Product Network (DGC-SPN).
3. **Image Completion**: A Deep Generalized Convolutional Sum-Product Network (DGC-SPN).
4. **Understanding region SPNs**
5. More to come, and if you would like to see a tutorial on anything in particular please raise an issue!

Check out the way we can build complex DGC-SPNs in a layer-wise fashion:

```
import libspn_keras as spnk
from tensorflow import keras

spnk.set_default_sum_op(spnk.SumOpGradBackprop())
spnk.set_default_accumulator_initializer(
    keras.initializers.TruncatedNormal(stddev=0.5, mean=1.0)
)

sum_product_network = keras.Sequential([
  spnk.layers.NormalizeStandardScore(input_shape=(28, 28, 1)),
  spnk.layers.NormalLeaf(
      num_components=16,
      location_trainable=True,
      location_initializer=keras.initializers.TruncatedNormal(
          stddev=1.0, mean=0.0)
  ),
  # Non-overlapping products
  spnk.layers.Conv2DProduct(
      depthwise=True,
      strides=[2, 2],
      dilations=[1, 1],
      kernel_size=[2, 2],
      padding='valid'
  ),
  spnk.layers.Local2DSum(num_sums=16),
  # Non-overlapping products
  spnk.layers.Conv2DProduct(
      depthwise=True,
      strides=[2, 2],
      dilations=[1, 1],
      kernel_size=[2, 2],
      padding='valid'
  ),
  spnk.layers.Local2DSum(num_sums=32),
```

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```
    # Overlapping products, starting at dilations [1, 1]
    spnk.layers.Conv2DProduct(
        depthwise=True,
        strides=[1, 1],
        dilations=[1, 1],
        kernel_size=[2, 2],
        padding='full'
    ),
    spnk.layers.Local2DSum(num_sums=32),
    # Overlapping products, with dilations [2, 2] and full padding
    spnk.layers.Conv2DProduct(
        depthwise=True,
        strides=[1, 1],
        dilations=[2, 2],
        kernel_size=[2, 2],
        padding='full'
    ),
    spnk.layers.Local2DSum(num_sums=64),
    # Overlapping products, with dilations [2, 2] and full padding
    spnk.layers.Conv2DProduct(
        depthwise=True,
        strides=[1, 1],
        dilations=[4, 4],
        kernel_size=[2, 2],
        padding='full'
    ),
    spnk.layers.Local2DSum(num_sums=64),
    # Overlapping products, with dilations [2, 2] and 'final' padding to combine
    # all scopes
    spnk.layers.Conv2DProduct(
        depthwise=True,
        strides=[1, 1],
        dilations=[8, 8],
        kernel_size=[2, 2],
        padding='final'
    ),
    spnk.layers.SpatialToRegions(),
    # Class roots
    spnk.layers.DenseSum(num_sums=10),
    spnk.layers.RootSum(return_weighted_child_logits=True)
])

sum_product_network.summary(line_length=100)
```

Which produces:

```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
normal_leaf (NormalLeaf)     (None, 28, 28, 16)        25088
_________________________________________________________________
conv2d_product (Conv2DProduc (None, 14, 14, 16)        4
_________________________________________________________________
local2d_sum (Local2DSum)     (None, 14, 14, 16)        50176
_________________________________________________________________
conv2d_product_1 (Conv2DProd (None, 7, 7, 16)          4
```

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```
_________________________________________________________________
local2d_sum_1 (Local2DSum)    (None, 7, 7, 32)          25088
_________________________________________________________________
conv2d_product_2 (Conv2DProd (None, 8, 8, 32)          4
_________________________________________________________________
local2d_sum_2 (Local2DSum)    (None, 8, 8, 32)          65536
_________________________________________________________________
conv2d_product_3 (Conv2DProd (None, 10, 10, 32)        4
_________________________________________________________________
local2d_sum_3 (Local2DSum)    (None, 10, 10, 64)        204800
_________________________________________________________________
conv2d_product_4 (Conv2DProd (None, 14, 14, 64)        4
_________________________________________________________________
local2d_sum_4 (Local2DSum)    (None, 14, 14, 64)        802816
_________________________________________________________________
conv2d_product_5 (Conv2DProd (None, 8, 8, 64)          4
_________________________________________________________________
spatial_to_regions (SpatialT (None, 1, 1, 4096)        0
_________________________________________________________________
dense_sum (DenseSum)          (None, 1, 1, 10)          40960
_________________________________________________________________
root_sum (RootSum)            (None, 10)                10
=================================================================
Total params: 1,214,498
Trainable params: 1,201,930
Non-trainable params: 12,568
_________________________________________________________________
```

CHAPTER NINE

TODOS

- Structure learning
- Advanced regularization e.g. pruning or auxiliary losses on weight accumulators

PYTHON MODULE INDEX

INDEX