

1 Tensor Networks

Our goal now is to focus on a subclass of models over Σ^* . To this end, we analyze *tensor networks*.

We denote a tensor T_v with k axes of sizes $D_v = \{d_1, \dots, d_k\}$ as a function

$$T_v : [d_1] \times \dots \times [d_k] \mapsto \mathbb{R} \quad .$$

As a shorthand, we write

$$[D_v] := [d_1] \times \dots \times [d_k] \quad .$$

Since indexing is usually clear from context, we treat D_v as a multiset of axis sizes.

Given two tensors T_u and T_v that share a common axis of size d_e , their contraction over this axis produces a new tensor T_C with dimension set

$$D_C = (D_u \setminus \{d_e\}) \cup (D_v \setminus \{d_e\}) \quad ,$$

defined as

$$T_C(i) = \sum_{i_e \in [d_e]} T_u(i_{D_u}, i_e) \cdot T_v(i_{D_v}, i_e) \quad ,$$

where $i \in [D_C]$. Note that $d_e \notin D_C$, which is why we explicitly included index i_e in the summation.

Definition 1.1 (Tensor Network over Σ^n). A *tensor network* \mathcal{T} over Σ^n is defined by a graph $G = (V, E)$ with the following structure:

- V is the set of vertices, where each vertex $v = (\text{layer}, \text{index}) \in V$ corresponds to a tensor T_v with axis sizes $D_v = \{d_1, \dots, d_k\}$. Let $V_{\text{layer}} \subseteq V$ denote the set of all vertices at a given layer.
- The input set $I = (T_{0,1}, \dots, T_{0,n}) \subset V$ consists of tensors each having a single axis of size $|\Sigma|$. These serve as the one-hot-encoded inputs corresponding to a string $w \in \Sigma^n$.
- $E \subseteq \{\{u, v\} \mid u \in V_l, v \in V_{l+1}\}$ is the set of edges. Each edge $e = \{u, v\}$ represents a shared index of size d_e between tensors T_u and T_v , which is summed over during contraction.
- The usual tensor network constrains: For each vertex $v \in V$, the degree $\deg(v)$ must match the number of axes $|D_v|$, and shared indices must correspond to same axis sizes.

Once the input tensors are initialized with one-hot encodings derived from a string $w \in \Sigma^n$, the network computes a scalar output $\mathcal{T}(w)$. This induces a probability distribution over Σ^n defined by:

$$S_{n,\mathcal{T}}(w) := \frac{f(\mathcal{T}(w))}{\sum_{w' \in \Sigma^n} f(\mathcal{T}(w'))} \quad ,$$

where $f : \mathbb{R} \mapsto \mathbb{R}_{\geq 0}$ is any arbitrary function like $f \equiv \exp$.

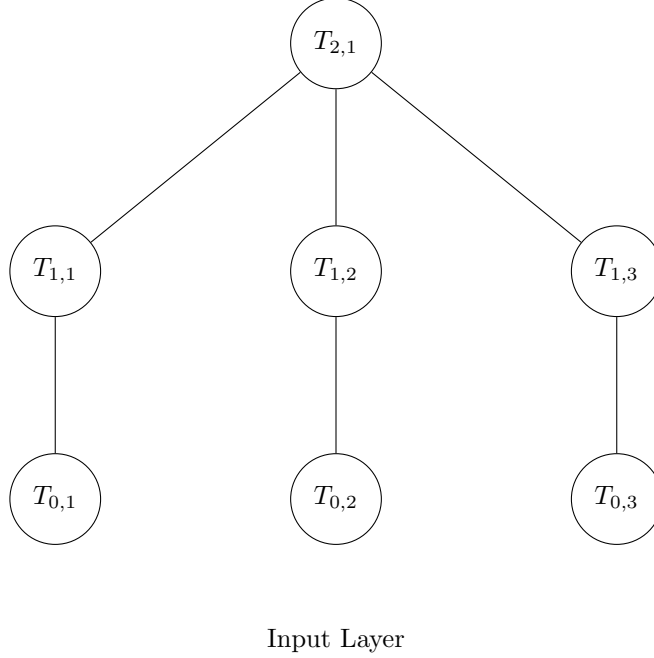


Figure 1: A basic tensor network over Σ^3 .

Definition 1.2 (Normalized and Non-Negative Tensor Networks). Let \mathcal{T} be a tensor network over Σ^n with scalar output $\mathcal{T}(w)$ for each $w \in \Sigma^n$. Define the total mass of the network as

$$|\mathcal{T}| := \sum_{w \in \Sigma^n} \mathcal{T}(w) \quad .$$

We say \mathcal{T} is *normalized* iff $|\mathcal{T}| = 1$.

Furthermore, a tensor network is said to be *non-negative* iff for all $w \in \Sigma^n$ we have $\mathcal{T}(w) \geq 0$.

Remark 1.1. We can enforce all tensor networks of our model space to be non-negative by only allowing for non-negative tensors in the networks.

Definition 1.3 (Normalization of Tensor Networks). Let \mathcal{T} be a tensor network over Σ^n , and let $H := V \setminus I$ be the set of non-input tensors, and define $|H|$ as its cardinality. The *induced normalized tensor network* $\frac{\mathcal{T}}{|\mathcal{T}|}$ is the same network as \mathcal{T} , but each entry of each tensor in H is scaled by the factor $\frac{1}{|H|\sqrt{|\mathcal{T}|}}$.

Lemma 1.1. Let $J \subseteq [n]$ and let \mathcal{T} be a tensor network over Σ^n . Define a modified network \mathcal{T}_J where for all $j \in J$, the input tensor $T_{0,j}$ is initialized to the all-ones vector (i.e., $\mathbf{1} \in \mathbb{R}^{|\Sigma|}$). Then for any $w \in \Sigma^{[n] \setminus J}$:

$$\sum_{w_J \in \Sigma^{|J|}} \mathcal{T}(w_J, w) = \mathcal{T}_J(w) \quad .$$

Proof. We proceed by induction on the size of the subset $J \subseteq [n]$.

Base case: $|J| = 0$. Then $J = \emptyset$, so $\mathcal{T}_J = \mathcal{T}$, and the sum over $w_J \in \Sigma^{|J|}$ is a sum over a singleton (the empty word), yielding:

$$\sum_{w_J \in \Sigma^0} \mathcal{T}(w_J, w) = \mathcal{T}(w),$$

and since $\mathcal{T}_J(w) = \mathcal{T}(w)$, the base case holds.

Inductive step: Assume the lemma holds for all subsets of size k , and let $J \subseteq [n]$ with $|J| = k + 1$. Pick any $j_0 \in J$, and define $J' = J \setminus \{j_0\}$, which has size k . By the inductive hypothesis, for any $w \in \Sigma^{[n] \setminus J}$, we have:

$$\sum_{w_{J'} \in \Sigma^k} \mathcal{T}(w_{J'}, w, w_{j_0}) = \mathcal{T}_{J'}(w, w_{j_0}) \quad ,$$

where $w_{j_0} \in \Sigma$ varies over its values.

Now consider the sum over all $w_J \in \Sigma^{k+1}$, which we write as:

$$\sum_{w_{J'} \in \Sigma^k} \sum_{w_{j_0} \in \Sigma} \mathcal{T}(w_{J'}, w_{j_0}, w) \quad .$$

By the inductive hypothesis, this equals:

$$\sum_{w_{j_0} \in \Sigma} \mathcal{T}_{J'}(w_{j_0}, w) \quad .$$

Observe that in $\mathcal{T}_{J'}$, the input tensor at position j_0 is still initialized to a one-hot vector, while the inputs at J' have been replaced with the all-ones vector.

Now, note that the inner sum over w_{j_0} is equivalent to replacing the input at j_0 with the all-ones vector, since the sum represents a sum over vector dot products of vector $\mathbf{v}_{w_{j_0}} := \mathcal{T}_{J'}(w_{j_0}, w)$ with one-hot encoded vectors. It follows from linearity that we can factor out \mathbf{v} , and the sum of the one-hot encoded vector yields the all-ones vector. Thus:

$$\sum_{w_{j_0} \in \Sigma} \mathcal{T}_{J'}(w_{j_0}, w) = \mathcal{T}_J(w) \quad .$$

Hence, by induction, the lemma holds for all subsets $J \subseteq [n]$.

□

Corollary 1.1. *Let \mathcal{T} be a tensor network over Σ^n , and let $\mathcal{T}_{[n]}$ be the network where all input tensors are initialized to the all-ones vector. Then:*

$$\mathcal{T} \text{ is normalized} \iff \mathcal{T}_{[n]} = 1 \quad ,$$

i.e., the total contraction of the network with all-one input tensors equals 1.

Lemma 1.2. *Let \mathcal{T} be a tensor network over Σ^n . The induced normalized tensor network $\frac{\mathcal{T}}{|\mathcal{T}|}$ is indeed normalized, and if additionally \mathcal{T} is non-negative and $f \equiv id$, we have for all $w \in \Sigma^n$:*

$$S_{n, \mathcal{T}}(w) = S_{n, \frac{\mathcal{T}}{|\mathcal{T}|}}(w) \quad .$$

Proof. Let H be the set of non-input tensors in \mathcal{T} , and let $|H| = m$. In the induced normalized network, every tensor in H is scaled by a factor $\alpha = \frac{1}{\sqrt[m]{|\mathcal{T}|}}$. Since the final output $\mathcal{T}(w)$ is a multilinear contraction over the tensors, this means the scalar output for any $w \in \Sigma^n$ becomes:

$$\left(\prod_{v \in H} \alpha \right) \cdot \mathcal{T}(w) = \alpha^m \cdot \mathcal{T}(w) = \frac{1}{|\mathcal{T}|} \cdot \mathcal{T}(w) \quad .$$

Hence,

$$\left(\frac{\mathcal{T}}{|\mathcal{T}|} \right)(w) = \frac{\mathcal{T}(w)}{|\mathcal{T}|} \quad .$$

Summing over all $w \in \Sigma^n$,

$$\left| \frac{\mathcal{T}}{|\mathcal{T}|} \right| = \sum_{w \in \Sigma^n} \frac{\mathcal{T}(w)}{|\mathcal{T}|} = \frac{1}{|\mathcal{T}|} \sum_{w \in \Sigma^n} \mathcal{T}(w) = \frac{|\mathcal{T}|}{|\mathcal{T}|} = 1 \quad .$$

Moreover, since the normalization rescales all outputs by the same constant, the ratio of the terms to the total sum remains unchanged:

$$S_{n, \frac{\mathcal{T}}{|\mathcal{T}|}}(w) = \frac{\left(\frac{\mathcal{T}(w)}{|\mathcal{T}|}\right)}{\sum_{w' \in \Sigma^n} \left(\frac{\mathcal{T}(w')}{|\mathcal{T}|}\right)} = \frac{\mathcal{T}(w)}{|\mathcal{T}|} \cdot \frac{1}{1} = S_{n, \mathcal{T}}(w) \quad .$$

This completes the proof. \square

One might ask whether our definition for tensor networks is bit restrictive, as it only allows for contraction over *pairs* of tensors. But what if we wanted to contract, say, three tensors at once over a common index?

Proposition 1.1. *Let $V' \subseteq V$ be a set of tensors in a tensor network, each containing an axis of dimension d labeled by a shared index i . Contracting all tensors in V' over the shared index i is equivalent to contracting each tensor individually with a single tensor*

$$\delta_{|V'|} : [d]^{|V'|} \mapsto \mathbb{R}_{\geq 0}$$

defined by

$$\delta_{|V'|}(i_1, \dots, i_{|V'|}) = \begin{cases} 1 & \text{if } i_1 = \dots = i_{|V'|} , \\ 0 & \text{otherwise.} \end{cases} \quad .$$

That is, a full contraction over a shared index can be implemented by introducing a single copy tensor connected to each tensor in V' .

Proof. Each tensor T_v for $v \in V'$ has an index $i \in [d]$ corresponding to the shared axis. The contraction over this index is defined by summing over the common value of i across all tensors:

$$\sum_{i=1}^d \prod_{v \in V'} T_v(\dots, i, \dots) \quad .$$

Now consider a new tensor $\delta_{|V'|}$ of order $|V'|$, defined as 1 if all indices are equal and 0 otherwise. Let each tensor T_v maintain its original indices, but connect to $\delta_{|V'|}$ via the position corresponding to v .

The contraction over this shared structure gives:

$$\sum_{i_1, \dots, i_{|V'|}} \left(\prod_{v \in V'} T_v(\dots, i_v, \dots) \right) \delta_{|V'|}(i_1, \dots, i_{|V'|}) \quad .$$

By definition of $\delta_{|V'|}$, this enforces $i_1 = \dots = i_{|V'|}$, reducing the above to:

$$\sum_{i=1}^d \prod_{v \in V'} T_v(\dots, i, \dots) \quad ,$$

which is exactly the original contraction. Hence, the two constructions are equivalent. \square

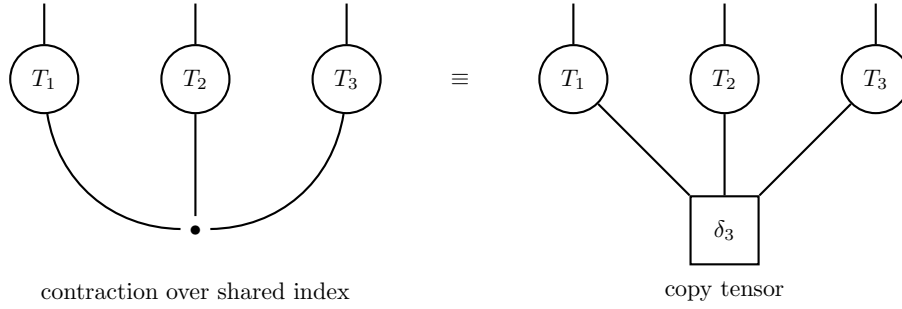


Figure 2: Contracting multiple tensors over one shared index is equivalent to contracting them individually with a single copy tensor.