

Attention via $\log \sum \exp$ energy

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1 General Framework

Setup. We consider a single set of nodes $\mathbf{v} = \{\mathbf{v}_i : i \in \{1, 2, \dots, N\}\}$, where each node $\mathbf{v}_i \in \mathbb{R}^{d_i}$. The relationships between these nodes are defined by a set of M energy functions $\{E_m : m \in \{1, 2, \dots, M\}\}$. Each energy function E_m defines a subset of nodes acting as *children* $C_m \subseteq \{1, 2, \dots, \text{normalization}\}$ and a subset acting as *parents* $P_m \subseteq \{1, 2, \dots, N\}$, which may overlap.

Energy. Each energy function E_m defines a similarity function:

$$\text{sim}(\mathbf{v}_c, \mathbf{v}_p) \quad : \quad \mathbb{R}^{d_c} \times \mathbb{R}^p \rightarrow \mathbb{R}, \quad (1)$$

which produces a scalar similarity between a child \mathbf{v}_c and a parent \mathbf{v}_p . Let $\{\mathbf{v}_c\} = \{\mathbf{v}_c : c \in C_m\}$ and $\{\mathbf{v}_p\} = \{\mathbf{v}_p : p \in P_m\}$, the energy for E_m is defined as:

$$E_m(\{\mathbf{v}_c\}, \{\mathbf{v}_p\}) = - \sum_{c \in C_m} \ln \left(\sum_{p \in P_m} \exp(\text{sim}(\mathbf{v}_c, \mathbf{v}_p)) \right). \quad (2)$$

The global energy sums over all energy functions:

$$E(\{\mathbf{v}\}) = \sum_{m=1}^M E_m(\{\mathbf{v}_c\}, \{\mathbf{v}_p\}). \quad (3)$$

Gradient Updates. For a single node \mathbf{v}_a , the gradient of the global energy E w.r.t. \mathbf{v}_a decomposes into two terms. Let $\mathcal{M}_c(a) = \{m : a \in C_m\}$ denote the energy functions where \mathbf{v}_a acts as a *child*, and $\mathcal{M}_p(a) = \{m : a \in P_m\}$ the energy functions where \mathbf{v}_a acts as a *parent*. Then:

$$\begin{aligned} -\frac{\partial E}{\partial \mathbf{v}_a} &= \underbrace{\sum_{m \in \mathcal{M}_c(a)} \sum_{p \in P_m} \text{softmax}_p(\text{sim}(\mathbf{v}_a, \mathbf{v}_p)) \frac{\partial}{\partial \mathbf{v}_a} \text{sim}(\mathbf{v}_a, \mathbf{v}_p)}_{\mathbf{v}_a \text{ acting as a child}} \\ &+ \underbrace{\sum_{m \in \mathcal{M}_p(a)} \sum_{c \in C_m} \text{softmax}_a(\text{sim}(\mathbf{v}_c, \mathbf{v}_a)) \frac{\partial}{\partial \mathbf{v}_a} \text{sim}(\mathbf{v}_c, \mathbf{v}_a)}_{\mathbf{v}_a \text{ acting as a parent}}. \end{aligned} \quad (4)$$

The first term captures contributions from \mathbf{v}_a being explained by its parents, while the second term captures contributions from \mathbf{v}_a explaining its children.

2 Gaussian Mixture Models

Setup. We have N data points (children) $\mathbf{x}_i \in \mathbb{R}^d$, $i \in C = \{1, \dots, N\}$, and K mixture components (parents), each with mean $\boldsymbol{\mu}_k \in \mathbb{R}^d$ and covariance $\boldsymbol{\Sigma}_k$, $k \in P = \{1, \dots, K\}$. Let π_k be the mixing proportion.

Similarity function. We define

$$\text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) = \ln \pi_k - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k).$$

Energy.

$$E^{\text{GMM}}(\{\mathbf{x}_i\}, \{\boldsymbol{\mu}_k\}) = - \sum_{i=1}^N \ln \left(\sum_{k=1}^K \exp(\text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k)) \right). \quad (5)$$

Gradients. If we differentiate w.r.t. $\boldsymbol{\mu}_k$, then

$$-\frac{\partial E^{\text{GMM}}}{\partial \boldsymbol{\mu}_k} = \sum_{i=1}^N \text{softmax}_k(\mathbf{A}_{ik}) \boldsymbol{\Sigma}_k^{-1}(\mathbf{x}_i - \boldsymbol{\mu}_k).$$

Setting this gradient to zero yields the usual GMM M-step:

$$\boldsymbol{\mu}_k = \frac{\sum_{i=1}^N \text{softmax}_k(\mathbf{A}_{ik}) \mathbf{x}_i}{\sum_{i=1}^N \text{softmax}_k(\mathbf{A}_{ik})}.$$

3 Hopfield Networks

Setup. We have a set of *children* data vectors $\mathbf{x}_i \in \mathbb{R}^d$, $i \in C = \{1, \dots, N\}$, and a set of *parent* memory vectors $\mathbf{m}_\mu \in \mathbb{R}^d$, $\mu \in P = \{1, \dots, K\}$.

Similarity function.

$$\text{sim}(\mathbf{x}_i, \mathbf{m}_\mu) = \mathbf{x}_i^\top \mathbf{m}_\mu.$$

Energy.

$$E^{\text{Hopfield}}(\{\mathbf{x}_i\}, \{\mathbf{m}_\mu\}) = - \sum_{i=1}^N \ln \left(\sum_{\mu=1}^K \exp(\mathbf{x}_i^\top \mathbf{m}_\mu) \right). \quad (6)$$

Gradients.

$$-\frac{\partial E^{\text{Hopfield}}}{\partial \mathbf{x}_i} = \sum_{\mu=1}^K \text{softmax}_\mu(\mathbf{x}_i^\top \mathbf{m}_\mu) \mathbf{m}_\mu. \quad (7)$$

$$-\frac{\partial E^{\text{Hopfield}}}{\partial \mathbf{m}_\mu} = \sum_{i=1}^N \text{softmax}_\mu(\mathbf{x}_i^\top \mathbf{m}_\mu) \mathbf{x}_i. \quad (8)$$

4 Slot Attention

Setup. Let $\mathbf{x}_j \in \mathbb{R}^d$, $j \in C = \{1, \dots, N\}$ be the children (tokens), and $\boldsymbol{\mu}_i \in \mathbb{R}^d$, $i \in P = \{1, \dots, S\}$ be the parents (slots). We typically apply linear transforms $\mathbf{W}_K, \mathbf{W}_Q \in \mathbb{R}^{d \times d}$ to form

$$\text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i) = (\mathbf{W}_K \mathbf{x}_j)^\top (\mathbf{W}_Q \boldsymbol{\mu}_i).$$

Energy.

$$E^{\text{Slot}}(\{\mathbf{x}_j\}, \{\boldsymbol{\mu}_i\}) = - \sum_{j=1}^N \ln \left(\sum_{i=1}^S \exp(\text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i)) \right). \quad (9)$$

Gradients.

$$-\frac{\partial E^{\text{Slot}}}{\partial \boldsymbol{\mu}_i} = \sum_{j=1}^N \text{softmax}_i(\text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i)) \mathbf{W}_Q^\top \mathbf{W}_K \mathbf{x}_j. \quad (10)$$

$$-\frac{\partial E^{\text{Slot}}}{\partial \mathbf{x}_j} = \sum_{i=1}^S \text{softmax}_i(\text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i)) \mathbf{W}_K^\top \mathbf{W}_Q \boldsymbol{\mu}_i. \quad (11)$$

5 Self-Attention

Setup. In self-attention, every node can act as both a child (query) and a parent (key). Concretely, let us have N tokens $\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$. We form

$$\mathbf{q}_i = \mathbf{W}^Q \mathbf{x}_i, \quad \mathbf{k}_i = \mathbf{W}^K \mathbf{x}_i,$$

for $i = 1, \dots, N$. Thus the set $C = \{1, \dots, N\}$ and $P = \{1, \dots, N\}$ coincide, with

$$\text{sim}(\mathbf{x}_c, \mathbf{x}_p) = (\mathbf{W}^Q \mathbf{x}_c)^\top (\mathbf{W}^K \mathbf{x}_p).$$

Energy.

$$E^{\text{SA}}(\{\mathbf{x}_i\}) = - \sum_{c=1}^N \ln \left(\sum_{p=1}^N \exp \left((\mathbf{W}^Q \mathbf{x}_c)^\top (\mathbf{W}^K \mathbf{x}_p) \right) \right). \quad (12)$$

Gradients. Since each \mathbf{x}_i is *both* a child and a parent, its gradient is a sum of two terms (the child side and the parent side). Writing it out explicitly:

$$\begin{aligned} -\frac{\partial E^{\text{SA}}}{\partial \mathbf{x}_i} &= \underbrace{\sum_{p=1}^N \text{softmax}_p \left((\mathbf{W}^Q \mathbf{x}_i)^\top (\mathbf{W}^K \mathbf{x}_p) \right) \mathbf{W}_Q^\top \mathbf{W}_K \mathbf{x}_p}_{\text{child } i \text{ being explained by parents } p} \\ &\quad + \underbrace{\sum_{c=1}^N \text{softmax}_i \left((\mathbf{W}^Q \mathbf{x}_c)^\top (\mathbf{W}^K \mathbf{x}_i) \right) \mathbf{W}_K^\top \mathbf{W}_Q \mathbf{x}_c}_{\text{parent } i \text{ explaining children } c}. \end{aligned} \quad (13)$$

6 Spatiotemporal Attention

Setup. We consider a hierarchy of L layers, each containing K_l latent variables of dimension D_l . Concretely, let $\mathbf{x}_{k,t}^{(l)} \in \mathbb{R}^{D_l}$ denote the k -th variable (or “slot”) in layer l at time t . The lowest layer ($l = 1$) has $K_1 = N$ observed variables (e.g., pixels) and dimension D_1 (e.g., $[x, y, r, g, b]$), while higher layers have separate dimensions D_l and numbers of slots K_l . Our goal is to define an energy that couples these variables *vertically* (across layers), *concurrently* (within the same layer and time), and *temporally* (across time).

Similarity Functions. We introduce three types of similarity, each with its own projection matrices. For inter-layer connections (linking layers $l - 1$ and l), we define:

$$\text{sim}_v^{(l)}(\mathbf{x}, \mathbf{x}') = (\mathbf{W}_v^{K,(l)} \mathbf{x})^\top (\mathbf{W}_v^{Q,(l)} \mathbf{x}'), \quad (14)$$

For intra-layer (slots within the same layer and time):

$$\text{sim}_c^{(l)}(\mathbf{x}, \mathbf{x}') = (\mathbf{W}_c^{Q,(l)} \mathbf{x})^\top (\mathbf{W}_c^{K,(l)} \mathbf{x}'), \quad (15)$$

For temporal connections (the same slot across different times):

$$\text{sim}_t^{(l)}(\mathbf{x}, \mathbf{x}') = (\mathbf{W}_t^{Q,(l)} \mathbf{x})^\top (\mathbf{W}_t^{K,(l)} \mathbf{x}'). \quad (16)$$

Here, $\mathbf{W}_\bullet^{Q,(l)}$ and $\mathbf{W}_\bullet^{K,(l)}$ are learnable projection matrices for layer l . The intra-layer and temporal parameters parallel the key-query mechanism in self-attention, while the inter-layer parameters are analogous to the inverted attention mechanism used in slot attention.

Energy At each layer l , the total energy is split into three terms:

$$\begin{aligned}
E_v^{(l)} &= - \sum_{t=1}^T \sum_{c=1}^{K_{l-1}} \underbrace{\ln \left(\sum_{k=1}^{K_l} \exp(\text{sim}_v^{(l)}(\mathbf{x}_{c,t}^{(l-1)}, \mathbf{x}_{k,t}^{(l)})) \right)}_{\text{Inter-layer energy}}, \\
E_c^{(l)} &= - \sum_{t=1}^T \sum_{k=1}^{K_l} \underbrace{\ln \left(\sum_{\substack{k'=1 \\ k' \neq k}}^{K_l} \exp(\text{sim}_c^{(l)}(\mathbf{x}_{k,t}^{(l)}, \mathbf{x}_{k',t}^{(l)})) \right)}_{\text{Intra-layer energy}}, \\
E_t^{(l)} &= - \sum_{k=1}^{K_l} \sum_{t=2}^T \underbrace{\ln \left(\sum_{t' < t} \exp(\text{sim}_t^{(l)}(\mathbf{x}_{k,t}^{(l)}, \mathbf{x}_{k,t'}^{(l)})) \right)}_{\text{Temporal energy}}.
\end{aligned} \tag{17}$$

Summing these over all layers $l \in \{1, \dots, L\}$ defines the total energy E . These terms correspond to inter-layer connections ($E_v^{(l)}$) and match the energy function for slot attention, intra-layer connections ($E_c^{(l)}$) which match the energy function for self attention, and temporal connections ($E_t^{(l)}$), which match the energy function for *causal* self attention (as each variable is only explained by past variables).

Gradients Consider a single variable $\mathbf{x}_{k,t}^{(l)}$. Its gradient with respect to the energy decomposes into four parts:

$$-\frac{\partial E}{\partial \mathbf{x}_{k,t}^{(l)}} = \underbrace{-\frac{\partial E_v^{(l)}}{\partial \mathbf{x}_{k,t}^{(l)}}}_{\text{bottom-up}} + \underbrace{-\frac{\partial E_v^{(l+1)}}{\partial \mathbf{x}_{k,t}^{(l)}}}_{\text{top-down}} + \underbrace{-\frac{\partial E_c^{(l)}}{\partial \mathbf{x}_{k,t}^{(l)}}}_{\text{intra-layer}} + \underbrace{-\frac{\partial E_t^{(l)}}{\partial \mathbf{x}_{k,t}^{(l)}}}_{\text{temporal}}. \tag{18}$$

Bottom-up: We define a similarity matrix $\mathbf{A}_{c,k}$, representing the interactions between $\mathbf{x}_{k,t}^{(l)}$ in layer l and $\mathbf{x}_{c,t}^{(l-1)}$ in the layer below.

$$\mathbf{A}_{c,k} = \text{sim}_v^{(l)}(\mathbf{x}_{c,t}^{(l-1)}, \mathbf{x}_{k,t}^{(l)}), \tag{19}$$

The gradient with respect to $\mathbf{x}_{k,t}^{(l)}$ is:

$$-\frac{\partial E_v^{(l)}}{\partial \mathbf{x}_{k,t}^{(l)}} = \sum_{c=1}^{K_{l-1}} \text{softmax}_k(\mathbf{A}_{c,k}) \mathbf{W}_v^{Q,(l)\top} \mathbf{W}_v^{K,(l)} \mathbf{x}_{c,t}^{(l-1)}. \tag{20}$$

This term aggregates contributions from the children in layer $l-1$, weighted by the attention $\text{softmax}_c(\mathbf{A}_{c,k})$, and is analogous to Slot Attention or Gaussian mixture models.

Top-down: We define a similarity matrix $\mathbf{A}_{k,p}$, representing the interactions between $\mathbf{x}_{k,t}^{(l)}$ in layer l and $\mathbf{x}_{p,t}^{(l+1)}$ in the layer above.

$$\mathbf{A}_{k,p} = \text{sim}_v^{(l+1)}(\mathbf{x}_{k,t}^{(l)}, \mathbf{x}_{p,t}^{(l+1)}), \tag{21}$$

The gradient with respect to $\mathbf{x}_{k,t}^{(l)}$ is:

$$-\frac{\partial E_v^{(l+1)}}{\partial \mathbf{x}_{k,t}^{(l)}} = \sum_{p=1}^{K_{l+1}} \text{softmax}_p(\mathbf{A}_{k,p}) \mathbf{W}_v^{K,(l+1)\top} \mathbf{W}_v^{Q,(l+1)} \mathbf{x}_{p,t}^{(l+1)}. \tag{22}$$

This term captures the influence of $\mathbf{x}_{k,t}^{(l)}$ being treated as a child, weighted by the attention $\text{softmax}_p(\mathbf{A}_{k,p})$, and reflects the top-down influence from layer $l+1$, and is analogous to Hopfield attention or the parent term in self-attention.

Intra-layer: We define two similarity matrices, $\mathbf{A}_{k,k'}$ and $\mathbf{A}_{k',k}$, representing the bidirectional interactions between $\mathbf{x}_{k,t}^{(l)}$ and other slots $\mathbf{x}_{k',t}^{(l)}$:

$$\begin{aligned}\mathbf{A}_{k,k'} &= \text{sim}_c^{(l)}(\mathbf{x}_{k,t}^{(l)}, \mathbf{x}_{k',t}^{(l)}), \\ \mathbf{A}_{k',k} &= \text{sim}_c^{(l)}(\mathbf{x}_{k',t}^{(l)}, \mathbf{x}_{k,t}^{(l)}),\end{aligned}\tag{23}$$

where

$$\text{sim}_c^{(l)}(\mathbf{x}_{k,t}^{(l)}, \mathbf{x}_{k',t}^{(l)}) = (\mathbf{W}_c^{Q,(l)} \mathbf{x}_{k,t}^{(l)})^\top (\mathbf{W}_c^{K,(l)} \mathbf{x}_{k',t}^{(l)}).$$

The gradient with respect to $\mathbf{x}_{k,t}^{(l)}$ is:

$$\begin{aligned}-\frac{\partial E_c^{(l)}}{\partial \mathbf{x}_{k,t}^{(l)}} &= \underbrace{\sum_{k' \neq k} \text{softmax}_k(\mathbf{A}_{k',k}) \mathbf{W}_c^{K,(l)\top} \mathbf{W}_c^{Q,(l)} \mathbf{x}_{k',t}^{(l)}}_{\mathbf{x}_{k,t}^{(l)} \text{ acting as parent (explaining others)}} \\ &\quad + \underbrace{\sum_{k' \neq k} \text{softmax}_{k'}(\mathbf{A}_{k,k'}) \mathbf{W}_c^{Q,(l)\top} \mathbf{W}_c^{K,(l)} \mathbf{x}_{k',t}^{(l)}}_{\mathbf{x}_{k,t}^{(l)} \text{ acting as child (being explained by others)}}.\end{aligned}\tag{24}$$

The first term captures the influence of $\mathbf{x}_{k,t}^{(l)}$ as a parent, aggregating the contributions from other slots $\mathbf{x}_{k',t}^{(l)}$ it explains, weighted by $\text{softmax}_{k'}(\mathbf{A}_{k',k})$. The second term reflects $\mathbf{x}_{k,t}^{(l)}$'s role as a child, being explained by other slots $\mathbf{x}_{k',t}^{(l)}$, weighted by $\text{softmax}_k(\mathbf{A}_{k,k'})$.

7 Temporal:

Setup. We define a similarity matrix $\mathbf{A}_{t,t'}$ representing the interaction between a slot $\mathbf{x}_{k,t}^{(l)}$ at time t and its past representation $\mathbf{x}_{k,t'}^{(l)}$ at time t' , for $t' < t$:

$$\mathbf{A}_{t,t'} = \text{sim}_t^{(l)}(\mathbf{x}_{k,t}^{(l)}, \mathbf{x}_{k,t'}^{(l)}) = (\mathbf{W}_t^{Q,(l)} \mathbf{x}_{k,t}^{(l)})^\top (\mathbf{W}_t^{K,(l)} \mathbf{x}_{k,t'}^{(l)}).\tag{25}$$

Gradient. Assuming causal attention (i.e. no future times), the gradient w.r.t. $\mathbf{x}_{k,t}^{(l)}$ is:

$$-\frac{\partial E_t^{(l)}}{\partial \mathbf{x}_{k,t}^{(l)}} = \sum_{t' < t} \text{softmax}_{t'}(\mathbf{A}_{t,t'}) \mathbf{W}_t^{Q,(l)\top} \mathbf{W}_t^{K,(l)} \mathbf{x}_{k,t'}^{(l)}.\tag{26}$$

Thus $\mathbf{x}_{k,t}^{(l)}$ is influenced only by its own past $\mathbf{x}_{k,t'}^{(l)}$ ($t' < t$), as in causal self-attention.

Remark (Full Version). We can generalize to let each latent $\mathbf{s}_{k,t}$ attend *all* data features and *all* slot latents at *any* time. This merges the three energies into a single large log-sum-exp, imposing direct competition among data, concurrency, and temporal parents, but increases complexity to $\mathcal{O}((N+K)T)^2$.

8 Cross Attention

Setup. We have a set of child vectors (queries) $\mathbf{Q} \in \mathbb{R}^{d \times N_Q}$ and a set of parent vectors (keys) $\mathbf{K} \in \mathbb{R}^{d \times N_K}$. Let

$$C = \{1, \dots, N_Q\}, \quad P = \{1, \dots, N_K\},$$

so $\mathbf{v}_c = \mathbf{q}_c$ is the c -th query, and $\mathbf{v}_p = \mathbf{k}_p$ is the p -th key. Suppose we have learnable weight matrices $\mathbf{W}^Q, \mathbf{W}^K \in \mathbb{R}^{d \times d}$. Then

$$\mathbf{q}_c = \mathbf{W}^Q \mathbf{x}_c^Q, \quad \mathbf{k}_p = \mathbf{W}^K \mathbf{x}_p^K,$$

where \mathbf{x}_c^Q is the raw c -th query token and \mathbf{x}_p^K the raw p -th key token.

Similarity function.

$$\text{sim}(\mathbf{q}_c, \mathbf{k}_p) = \mathbf{q}_c^\top \mathbf{k}_p.$$

Energy.

$$E^{\text{Cross}}(\{\mathbf{q}_c\}, \{\mathbf{k}_p\}) = - \sum_{c=1}^{N_Q} \ln \left(\sum_{p=1}^{N_K} \exp(\mathbf{q}_c^\top \mathbf{k}_p) \right). \quad (27)$$

Gradients.

$$-\frac{\partial E^{\text{Cross}}}{\partial \mathbf{q}_c} = \sum_{p=1}^{N_K} \text{softmax}_p(\mathbf{q}_c^\top \mathbf{k}_p) \mathbf{k}_p. \quad (28)$$

$$-\frac{\partial E^{\text{Cross}}}{\partial \mathbf{k}_p} = \sum_{c=1}^{N_Q} \text{softmax}_p(\mathbf{q}_c^\top \mathbf{k}_p) \mathbf{q}_c. \quad (29)$$

When mapping back to the raw tokens \mathbf{x}_c^Q or \mathbf{x}_p^K , chain-rule multiplies by \mathbf{W}^Q or \mathbf{W}^K , respectively.

9 Predictive coding

Setup. We again have child vectors $\{\mathbf{x}_i\}_{i=1}^N$ and a set of parent $\boldsymbol{\mu}_k \in \mathbb{R}^d, k = 1, \dots, K$. However, rather than a direct difference $\mathbf{x}_i - \boldsymbol{\mu}_k$, let us assume the *model* maps $\boldsymbol{\mu}_k$ through some non-linear function $f_\phi(\cdot)$ before comparing to \mathbf{x}_i . For instance, f_ϕ could be a neural network.

Similarity function. Define

$$\text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) = -\frac{1}{2} \|\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)\|^2.$$

Energy.

$$E^{\text{PC}}(\{\mathbf{x}_i\}, \{\boldsymbol{\mu}_k\}) = - \sum_{i=1}^N \ln \left(\sum_{k=1}^K \exp \left(-\frac{1}{2} \|\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)\|^2 \right) \right). \quad (30)$$

Gradients.

$$\alpha_{i,k} = \text{softmax}_k \left(-\frac{1}{2} \|\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)\|^2 \right).$$

$$-\frac{\partial E^{\text{PC}}}{\partial \mathbf{x}_i} = \sum_{k=1}^K \alpha_{i,k} (\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)).$$

$$-\frac{\partial E^{\text{PC}}}{\partial \boldsymbol{\mu}_k} = \sum_{i=1}^N \alpha_{i,k} \underbrace{\frac{\partial f_\phi(\boldsymbol{\mu}_k)}{\partial \boldsymbol{\mu}_k}}_{\text{Jacobian of } f_\phi} (\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)).$$

Here, $\frac{\partial f_\phi(\boldsymbol{\mu}_k)}{\partial \boldsymbol{\mu}_k}$ is the $d \times d$ Jacobian (or more general shape if $\boldsymbol{\mu}_k$ and $f_\phi(\boldsymbol{\mu}_k)$ differ in dimension).

10 Switching Linear Dynamical System

Setup. Consider a time series of observations $\{\mathbf{x}_t\}_{t=1}^T$, where each $\mathbf{x}_t \in \mathbb{R}^d$. We assume there are K distinct (linear) dynamical modes, each with parameters $\{\mathbf{A}_k, \mathbf{b}_k, \boldsymbol{\Sigma}_k\}$. Let π_k be the mixing weight of mode k . A typical *switching linear dynamical system* (SLDS) posits:

$$\mathbf{x}_{t+1} \approx \mathbf{A}_k \mathbf{x}_t + \mathbf{b}_k, \quad k \in \{1, \dots, K\},$$

with Gaussian noise $\boldsymbol{\Sigma}_k$. We treat \mathbf{x}_{t+1} as a *child* and the $\{\mathbf{A}_k, \mathbf{b}_k\}$ (together with \mathbf{x}_t) as *parents* in a mixture-of-linear-dynamics fashion.

Similarity function. Define, for each mode k ,

$$\text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k) = \ln \pi_k - \frac{1}{2} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k)^\top \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k).$$

Energy. Summing over all time steps $t = 1, \dots, T-1$, we write

$$E^{\text{SLDS}}(\{\mathbf{x}_t\}, \{\mathbf{A}_k, \mathbf{b}_k\}) = - \sum_{t=1}^{T-1} \ln \left(\sum_{k=1}^K \exp(\text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k)) \right). \quad (31)$$

Gradients. Let

$$\alpha_{t,k} = \text{softmax}_k(\text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k)),$$

i.e. the normalized exponent for mode k .

$$\begin{aligned} -\frac{\partial E^{\text{SLDS}}}{\partial \mathbf{x}_{t+1}} &= \sum_{k=1}^K \alpha_{t,k} \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k). \\ -\frac{\partial E^{\text{SLDS}}}{\partial \mathbf{x}_t} &= \sum_{k=1}^K \alpha_{t,k} (-\mathbf{A}_k^\top \Sigma_k^{-1}) (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k) \quad (t = 1, \dots, T-1). \\ -\frac{\partial E^{\text{SLDS}}}{\partial \mathbf{A}_k} &= \sum_{t=1}^{T-1} \alpha_{t,k} \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k) \mathbf{x}_t^\top. \\ -\frac{\partial E^{\text{SLDS}}}{\partial \mathbf{b}_k} &= \sum_{t=1}^{T-1} \alpha_{t,k} \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k). \end{aligned}$$

11 Layer Normalization

Setup. We consider a batch of input vectors $\{\mathbf{x}_i\}_{i=1}^B$, where each vector $\mathbf{x}_i \in \mathbb{R}^D$. Each vector is normalized by subtracting the mean and dividing by the standard deviation, with learnable scaling and bias parameters $\gamma, \delta \in \mathbb{R}^D$. For numerical stability, a small constant $\epsilon > 0$ is added to the variance.

Energy. The energy for layer normalization is given by:

$$E^{\text{LN}}(\{\mathbf{x}_i\}) = \sum_{i=1}^B \left[\gamma \sqrt{\frac{1}{D} \sum_{j=1}^D (x_{ij} - \bar{\mathbf{x}}_i)^2 + \epsilon} + \sum_{j=1}^D \delta_j x_{ij} \right],$$

where:

$$\bar{\mathbf{x}}_i = \frac{1}{D} \sum_{j=1}^D x_{ij}.$$

Derivative. The normalized outputs are obtained as the derivative of the energy with respect to the inputs:

$$\begin{aligned} \frac{\partial E^{\text{LN}}}{\partial x_{ij}} &= \gamma_j \frac{x_{ij} - \bar{\mathbf{x}}_i}{\sqrt{\frac{1}{D} \sum_{k=1}^D (x_{ik} - \bar{\mathbf{x}}_i)^2 + \epsilon}} + \delta_j. \\ \bar{\mathbf{x}}_i &= \frac{1}{D} \sum_{k=1}^D x_{ik}. \end{aligned}$$

12 Coordinate ascent

Consider an energy of the form

$$E(\{\mathbf{x}_j\}, \{\boldsymbol{\mu}_i\}; \theta) = - \sum_{j=1}^N \ln \left(\sum_{i=1}^S \exp(\text{sim}_\theta(\mathbf{x}_j, \boldsymbol{\mu}_i)) \right),$$

with θ denoting the parameters of the similarity function. In an EM procedure, we alternate:

- **E-step:** Update latent variables using fixed θ .
- **M-step:** Update parameters θ in closed form given fixed latent assignments.

For *slot attention*, we have:

$$\begin{aligned} \theta &= \{\mathbf{W}_K, \mathbf{W}_Q\}, \\ \text{sim}_\theta(\mathbf{x}_j, \boldsymbol{\mu}_i) &= (\mathbf{W}_K \mathbf{x}_j)^\top (\mathbf{W}_Q \boldsymbol{\mu}_i). \\ \mathbf{A} \text{ with entries } A_{ji} &= \text{softmax}_i \left((\mathbf{W}_K \mathbf{x}_j)^\top (\mathbf{W}_Q \boldsymbol{\mu}_i) \right). \end{aligned}$$

E-step: Update Slots

Fix $\mathbf{W}_K, \mathbf{W}_Q$. The gradient for each slot $\boldsymbol{\mu}_i$ is

$$-\frac{\partial E^{\text{Slot}}}{\partial \boldsymbol{\mu}_i} = \sum_{j=1}^N A_{ji} \mathbf{W}_Q^\top \mathbf{W}_K \mathbf{x}_j.$$

Use this gradient to iteratively update $\{\boldsymbol{\mu}_i\}$ until convergence.

M-step: Update Parameters

Given fixed slots $\{\boldsymbol{\mu}_i\}$ and attention matrix \mathbf{A} , we aim to update the parameters $\mathbf{W}_K, \mathbf{W}_Q$. This is motivated by setting the gradient of the energy with respect to these parameters to zero:

$$-\frac{\partial E^{\text{Slot}}}{\partial \mathbf{W}_K} = 0, \quad -\frac{\partial E^{\text{Slot}}}{\partial \mathbf{W}_Q} = 0.$$

Under the fixed assignments provided by \mathbf{A} and slots $\{\boldsymbol{\mu}_i\}$, these conditions are equivalent to solving a weighted least-squares problem. Specifically, we consider minimizing the objective

$$\min_{\mathbf{W}_K, \mathbf{W}_Q} \sum_{j=1}^N \sum_{i=1}^S A_{ji} \left\| \mathbf{W}_K \mathbf{x}_j - \mathbf{W}_Q \boldsymbol{\mu}_i \right\|^2,$$

since the stationary point of this quadratic form corresponds to zero gradients with respect to $\mathbf{W}_K, \mathbf{W}_Q$.

Update \mathbf{W}_Q : Differentiate w.r.t. \mathbf{W}_Q , set to zero:

$$\sum_{j,i} A_{ji} \left(\mathbf{W}_K \mathbf{x}_j - \mathbf{W}_Q \boldsymbol{\mu}_i \right) \boldsymbol{\mu}_i^\top = 0,$$

yielding

$$\mathbf{W}_Q = \left(\sum_{j,i} A_{ji} \mathbf{W}_K \mathbf{x}_j \boldsymbol{\mu}_i^\top \right) \left(\sum_{j,i} A_{ji} \boldsymbol{\mu}_i \boldsymbol{\mu}_i^\top \right)^{-1}.$$

Update \mathbf{W}_K : Similarly, differentiate w.r.t. \mathbf{W}_K , set to zero:

$$\sum_{j,i} A_{ji} \left(\mathbf{W}_K \mathbf{x}_j - \mathbf{W}_Q \boldsymbol{\mu}_i \right) \mathbf{x}_j^\top = 0,$$

yielding

$$\mathbf{W}_K = \left(\sum_{j,i} A_{ji} \mathbf{W}_Q \boldsymbol{\mu}_i \mathbf{x}_j^\top \right) \left(\sum_{j,i} A_{ji} \mathbf{x}_j \mathbf{x}_j^\top \right)^{-1}.$$

Iterate: Alternate between the E-step (updating $\{\boldsymbol{\mu}_i\}$) and the M-step (updating $\mathbf{W}_K, \mathbf{W}_Q$) until convergence.

A Appendix: Derivation of Gradient Updates

Let us consider a generic term:

$$-\ln\left(\sum_{m=1}^M \exp(f_m(\mathbf{x}))\right),$$

where $\mathbf{x} \in \mathbb{R}^d$ is some variable, and each f_m is a scalar function. We compute its gradient:

$$\begin{aligned} \frac{\partial}{\partial \mathbf{x}} \left[-\ln\left(\sum_{m=1}^M \exp(f_m(\mathbf{x}))\right) \right] &= -\frac{1}{\sum_{m'} \exp(f_{m'}(\mathbf{x}))} \sum_{m=1}^M \exp(f_m(\mathbf{x})) \frac{\partial f_m(\mathbf{x})}{\partial \mathbf{x}} \\ &= -\sum_{m=1}^M \left[\frac{\exp(f_m(\mathbf{x}))}{\sum_{m'} \exp(f_{m'}(\mathbf{x}))} \right] \frac{\partial f_m(\mathbf{x})}{\partial \mathbf{x}}. \end{aligned}$$

Defining $\text{softmax}_m(f(\mathbf{x})) = \frac{\exp(f_m(\mathbf{x}))}{\sum_{m'} \exp(f_{m'}(\mathbf{x}))}$, this is

$$-\sum_{m=1}^M \text{softmax}_m(f(\mathbf{x})) \frac{\partial f_m(\mathbf{x})}{\partial \mathbf{x}},$$

which matches the softmax-weighted gradient structure.

B Appendix

Here, we collect the explicit partial derivatives of sim for each model discussed.

Gaussian Mixture Models

$$\begin{aligned} \text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) &= \ln \pi_k - \frac{1}{2} (\mathbf{x}_i - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k). \\ \frac{\partial}{\partial \boldsymbol{\mu}_k} \text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) &= \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_i - \boldsymbol{\mu}_k). \end{aligned}$$

Cross Attention

$$\begin{aligned} \text{sim}(\mathbf{q}_c, \mathbf{k}_p) &= \mathbf{q}_c^\top \mathbf{k}_p. \\ \frac{\partial}{\partial \mathbf{q}_c} \text{sim}(\mathbf{q}_c, \mathbf{k}_p) &= \mathbf{k}_p, \quad \frac{\partial}{\partial \mathbf{k}_p} \text{sim}(\mathbf{q}_c, \mathbf{k}_p) = \mathbf{q}_c. \end{aligned}$$

Hopfield Networks

$$\begin{aligned} \text{sim}(\mathbf{x}_i, \mathbf{m}_\mu) &= \mathbf{x}_i^\top \mathbf{m}_\mu. \\ \frac{\partial}{\partial \mathbf{x}_i} \text{sim}(\mathbf{x}_i, \mathbf{m}_\mu) &= \mathbf{m}_\mu, \quad \frac{\partial}{\partial \mathbf{m}_\mu} \text{sim}(\mathbf{x}_i, \mathbf{m}_\mu) = \mathbf{x}_i. \end{aligned}$$

Slot Attention

$$\begin{aligned} \text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i) &= (\mathbf{W}_K \mathbf{x}_j)^\top (\mathbf{W}_Q \boldsymbol{\mu}_i). \\ \frac{\partial}{\partial \mathbf{x}_j} \text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i) &= \mathbf{W}_K^\top \mathbf{W}_Q \boldsymbol{\mu}_i, \quad \frac{\partial}{\partial \boldsymbol{\mu}_i} \text{sim}(\mathbf{x}_j, \boldsymbol{\mu}_i) = \mathbf{W}_Q^\top \mathbf{W}_K \mathbf{x}_j. \end{aligned}$$

Self-Attention

$$\begin{aligned} \text{sim}(\mathbf{x}_c, \mathbf{x}_p) &= (\mathbf{W}^Q \mathbf{x}_c)^\top (\mathbf{W}^K \mathbf{x}_p). \\ \frac{\partial}{\partial \mathbf{x}_c} \text{sim}(\mathbf{x}_c, \mathbf{x}_p) &= \mathbf{W}^{Q\top} \mathbf{W}^K \mathbf{x}_p, \quad \frac{\partial}{\partial \mathbf{x}_p} \text{sim}(\mathbf{x}_c, \mathbf{x}_p) = \mathbf{W}^{K\top} \mathbf{W}^Q \mathbf{x}_c. \end{aligned}$$

Switching Linear Dynamical System

$$\begin{aligned}
\text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k) &= \ln \pi_k - \frac{1}{2} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k)^\top \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k). \\
\frac{\partial}{\partial \mathbf{x}_{t+1}} \text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k) &= \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k), \\
\frac{\partial}{\partial \mathbf{x}_t} \text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k) &= -\mathbf{A}_k^\top \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k), \\
\frac{\partial}{\partial \mathbf{A}_k} \text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k) &= \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k) \mathbf{x}_t^\top, \\
\frac{\partial}{\partial \mathbf{b}_k} \text{sim}(\mathbf{x}_{t+1}, \mathbf{x}_t; \mathbf{A}_k, \mathbf{b}_k) &= \Sigma_k^{-1} (\mathbf{x}_{t+1} - \mathbf{A}_k \mathbf{x}_t - \mathbf{b}_k).
\end{aligned}$$

Predictive Coding

$$\begin{aligned}
\text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) &= -\frac{1}{2} \|\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)\|^2. \\
\frac{\partial}{\partial \mathbf{x}_i} \text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) &= \mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k), \\
\frac{\partial}{\partial \boldsymbol{\mu}_k} \text{sim}(\mathbf{x}_i, \boldsymbol{\mu}_k) &= \frac{\partial f_\phi(\boldsymbol{\mu}_k)}{\partial \boldsymbol{\mu}_k} (\mathbf{x}_i - f_\phi(\boldsymbol{\mu}_k)).
\end{aligned}$$