Lecture 11: Attention Layer

Deep Learning for Actuarial Modeling
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Ronald Richman, Salvatore Scognamiglio, Mario V. Wüthrich

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1. Attention layer

Overview

- *Attention layers* are the key building blocks of Transformers. They are designed to identify the most relevant information in the input data.
- The central idea is to learn a weighting scheme that prioritizes the most important parts and their interactions of the input information.
- Different attention mechanisms are available in the literature. Our focus is on the most commonly used variant called *scaled dot-product attention*.

Attention layers were introduced in the seminal paper of Vaswani *et al.* (2017).

Attention layers were first designed for sequential data (e.g., time-series).

The starting point is an input sequence of elements:

$$\boldsymbol{X}_{1:t} = \left[\boldsymbol{X}_1, \ \ldots, \ \boldsymbol{X}_t\right]^\top \in \mathbb{R}^{t \times q},$$

where:

- t is length of the sequence,
- q is dimension of the series,
- $\boldsymbol{X}_u \in \mathbb{R}^q$ is the u-th element of the sequence, with $1 \leq u \leq t$.

2. Query, Key and Value

In order to be applied, an attention layer requires the following elements:

- Queries $\boldsymbol{q}_u \in \mathbb{R}^q$, $1 \leq u \leq t$
  - The query $\boldsymbol{q}_u$ represents what the u-th element is trying to find in the overall input
  - Act like a *question* asking: "What information is relevant to me?"
- Keys $\boldsymbol{k}_u \in \mathbb{R}^q$, $1 \leq u \leq t$.
  - The key $\boldsymbol{k}_u$ describes what the u-th element can provide to others.
  - Function like a *label* indicating: "This is the kind of information I carry".
- Values $\boldsymbol{v}_u \in \mathbb{R}^q$, $1 \leq u \leq t$
  - The value $\boldsymbol{v}_u$ contains the actual content that can be shared
  - When a query matches a key, the corresponding value is passed along as useful context.

The query $\boldsymbol{q}_u$ tries to find a key $\boldsymbol{k}_s$ that gives a match. E.g., in a sentence the query of the subject 'car' tries to find a verb 'accelerate' in the sentence, which then gives a match for a dangerous driving maneuver. In that case, a high attention is paid to the corresponding *value* $\boldsymbol{v}_s$.

Queries, keys and values are represented by the three matrices

$$\begin{aligned} Q &= [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_t]^\top \in \mathbb{R}^{t \times q}, \\ K &= [\boldsymbol{k}_1, \ldots, \boldsymbol{k}_t]^\top \in \mathbb{R}^{t \times q}, \\ V &= [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_t]^\top \in \mathbb{R}^{t \times q}. \end{aligned}$$

In self-attention models, Q, K, and V are derived from the input sequence $\boldsymbol{X}_{1:t}$ by applying some **time -distributed layers**.

2.1 Time-distributed layer

Overview

A *time-distributed layer* applies the same operation (with the same parameters) to every component (time step) of sequential input data.

- Consider a time-distributed FNN layer with q_1 units applied to the input tensor $\boldsymbol{X}_{1:t} \in \mathbb{R}^{t \times q}$.
- This performs the mapping

$$\begin{aligned} \boldsymbol{z}^{\text{t-FNN}} \quad : \quad & \mathbb{R}^{t \times q} \to \mathbb{R}^{t \times q_1}, \\ & \boldsymbol{X}_{1:t} \mapsto \boldsymbol{z}^{\text{t-FNN}}(\boldsymbol{X}_{1:t}) = \left(\boldsymbol{z}^{\text{FNN}}(\boldsymbol{X}_1), \ldots, \boldsymbol{z}^{\text{FNN}}(\boldsymbol{X}_t)\right)^\top, \end{aligned}$$

  where $\boldsymbol{z}^{\text{FNN}} : \mathbb{R}^q \to \mathbb{R}^{q_1}$ is a FNN layer.
- This transformation leaves the time dimension t unchanged.
- Important, the same parameters (network weights and biases) are shared across all time steps $1 \leq u \leq t$. This makes the FNN layer a so-called *time-distributed* one.

To derive $\boldsymbol{q}_u$, $\boldsymbol{k}_u$, and $\boldsymbol{v}_u$, three time-distributed q-dimensional FNNs

$$\boldsymbol{z}_{\kappa}^{\text{t-FNN}} : \mathbb{R}^{t \times q} \to \mathbb{R}^{t \times q}, \qquad \boldsymbol{X}_{1:t} \mapsto \boldsymbol{z}_{\kappa}^{\text{t-FNN}}(\boldsymbol{X}_{1:t}),$$

for $\kappa = Q, K, V$, where applied.

These give us the time-slices for fixed time points $1 \leq u \leq t$

$$\boldsymbol{q}_u = \boldsymbol{z}_Q^{\text{FNN}}(\boldsymbol{X}_u) = \phi_Q\left(\boldsymbol{w}_0^{(Q)} + W^{(Q)}\boldsymbol{X}_u\right) \in \mathbb{R}^q,$$

$$\boldsymbol{k}_u = \boldsymbol{z}_K^{\text{FNN}}(\boldsymbol{X}_u) = \phi_K\left(\boldsymbol{w}_0^{(K)} + W^{(K)}\boldsymbol{X}_u\right) \in \mathbb{R}^q,$$

$$\boldsymbol{v}_u = \boldsymbol{z}_V^{\text{FNN}}(\boldsymbol{X}_u) = \phi_V\left(\boldsymbol{w}_0^{(V)} + W^{(V)}\boldsymbol{X}_u\right) \in \mathbb{R}^q,$$

with corresponding network weights, biases, and activation functions.

Equivalently, this reads in matrix notation as

$$Q = \boldsymbol{z}_Q^{\text{t-FNN}}(\boldsymbol{X}_{1:t}) = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_t]^\top \in \mathbb{R}^{t \times q},$$

$$K = \boldsymbol{z}_K^{\text{t-FNN}}(\boldsymbol{X}_{1:t}) = [\boldsymbol{k}_1, \ldots, \boldsymbol{k}_t]^\top \in \mathbb{R}^{t \times q},$$

$$V = \boldsymbol{z}_V^{\text{t-FNN}}(\boldsymbol{X}_{1:t}) = [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_t]^\top \in \mathbb{R}^{t \times q}.$$

3. Attention head

- The *attention head* is defined by the mapping

$$H : \mathbb{R}^{t\times q} \times \mathbb{R}^{t\times q} \times \mathbb{R}^{t\times q} \to \mathbb{R}^{t\times q}, \qquad (Q, K, V) \mapsto H = H(Q, K, V),$$

with scaled *dot-product attention*

$$H = A\,V = \text{softmax}\left(\frac{QK^\top}{\sqrt{q}}\right) V \in \mathbb{R}^{t\times q}.$$

- The *attention matrix* $A \in \mathbb{R}^{t\times t}$ is obtained by applying the softmax function *row-wise* to matrix $A' = QK^\top/\sqrt{q}$, that is,

$$A = \text{softmax}(A'), \qquad \text{where} \quad a_{u,s} = \frac{\exp(a'_{u,s})}{\sum_{k=1}^{t} \exp(a'_{u,k})} \in (0,1).$$

- This ensures that the rows sums of A are equal to one.

- Recalling the notation

$$Q = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_t]^\top \in \mathbb{R}^{t \times q} \quad \text{and} \quad K = [\boldsymbol{k}_1, \ldots, \boldsymbol{k}_t]^\top \in \mathbb{R}^{t \times q},$$

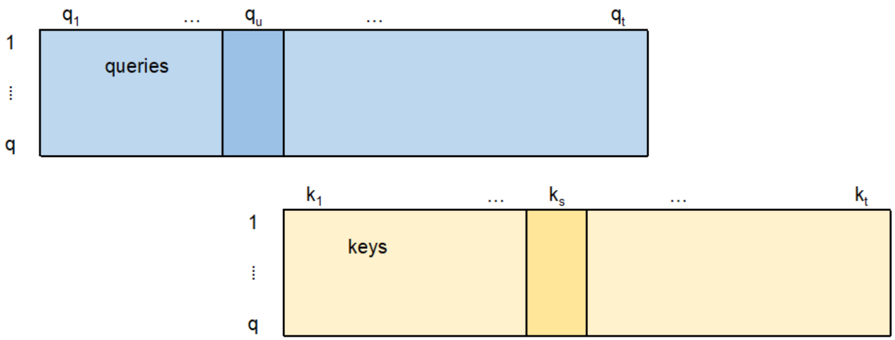
the elements $a'_{u,s}$ of matrix A' are given by the dot-product

$$a'_{u,s} = \frac{1}{\sqrt{q}}\, \boldsymbol{q}_u^\top \boldsymbol{k}_s = \frac{1}{\sqrt{q}} \, \langle \boldsymbol{q}_u, \boldsymbol{k}_s \rangle = \boldsymbol{q}_u \cdot \boldsymbol{k}_s / \sqrt{q}.$$

These are three different ways to express the scalar product between the query $\boldsymbol{q}_u$ and the key $\boldsymbol{k}_s$; see also next graph.

- The scaling factor $\sqrt{q}$ removes the input dimension dependence. I.e., it prevents the dot-product operation from being too flat or too spiky.

- Each entry of the attention head $H = A\,V$ is a weighted average of the columns of the value matrix V. The weights $a_{u,s}$ determine the *importance* of each row vector $\boldsymbol{v}_s$ of V; see next illustration.



- If the query $\boldsymbol{q}_u$ points into the same direction as the key $\boldsymbol{k}_s$, we receive a large attention weight $a_{u,s}$. This implies that the corresponding entry $\boldsymbol{v}_s$ on the s-th row of the value matrix V receives a big attention.
- I.e., the information $\boldsymbol{v}_s$ at time s is important for period u (the query $\boldsymbol{q}_u$ at time u).

4. Multi-head Attention

Overview

- A Transformer layer can also have multiple attention heads, allowing the model to focus more effectively on different parts of the input sequence simultaneously.
- Rather than computing a single attention output, *multi-head attention* applies the attention mechanism multiple times in *parallel*, with each attention head using different weights and parameters.

- The *multi-head attention* mechanism applies $n_h \geq 2$ parallel attention heads to $\boldsymbol{X}_{1:t}$.
- Assume the j-th attention head is given by the query, key and value Q_j, K_j, and V_j, respectively, defining the j-th attention head

$$H_j = H_j(\boldsymbol{X}_{1:t}) = \text{softmax}\left(\frac{Q_j K_j^\top}{\sqrt{q}}\right) V_j \in \mathbb{R}^{t \times q}.$$

- These heads are concatenated and linearly transformed

$$H_{\text{MH}}(\boldsymbol{X}_{1:t}) = \text{Concat}\left(H_1, H_2, \ldots, H_{n_h}\right) W \in \mathbb{R}^{t \times q},$$

  for an output weight matrix $W \in \mathbb{R}^{n_h q \times q}$.
- This multi-head attention is further processed as described above.

5. Other Layers in Transformers

In addition to attention and feed-forward components, transformer architectures also commonly include:

- Layer Normalization
  - Helps stabilize and speed up training by reducing internal covariate shift.
- Drop-out Layer
  - Used as a regularization technique to prevent overfitting.

5.1 Layer normalization

Overview

- *Layer normalization*, introduced by Ba, Kiros and Hinton (2016), is a technique used to improve the learning process, to accelerate convergence, and to enhance the model's predictive performance.
- A layer normalization is applied to individual instances across all covariate (feature) components; this is not affected by the batch size.
- In contrast, *batch normalization* of Ioffe and Szegedy (2015) is applied for a fixed covariate (feature) component across all instances in the batch; additionally, batch normalization often involves a moving average mechanism for having stability across multiple batches.

- Layer normalization is a mapping

$$\boldsymbol{z}^{\text{norm}} : \mathbb{R}^q \to \mathbb{R}^q, \qquad \boldsymbol{X} \mapsto \boldsymbol{z}^{\text{norm}}(\boldsymbol{X}) = \left(\gamma_j \left(\frac{X_j - \bar{X}}{\sqrt{s^2 + \epsilon}} \right) + \delta_j \right)_{1 \le j \le q},$$

where $\epsilon > 0$ is a small constant added for numerical stability.

- The empirical mean $\bar{X} \in \mathbb{R}$ and variance $s^2 \in \mathbb{R}^+$ are computed as

$$\bar{X} = \frac{1}{q} \sum_{j=1}^{q} X_j \qquad \text{and} \qquad s^2 = \frac{1}{q} \sum_{j=1}^{q} (X_j - \bar{X})^2.$$

- $\boldsymbol{\gamma} = (\gamma_1, \ldots, \gamma_q)^\top \in \mathbb{R}^q$ and $\boldsymbol{\delta} = (\delta_1, \ldots, \delta_q)^\top \in \mathbb{R}^q$ are vectors of trainable parameters.

5.2 Drop-out layer

Overview

- *Drop-out* is a widely used regularization technique in networks.
- We have already briefly discussed it in the FNN chapter.
- It randomly removes neurons (units) during the model training to enhance the model's generalization capabilities.

Drop-out has been introduced by Srivastava *et al.* (2014) and Wager, Wang and Liang (2013).

- Drop-out is typically implemented by multiplying the output of a specific layer by i.i.d. realizations of Bernoulli random variables with a fixed drop-out rate $\alpha \in (0,1)$ in each step of SGD training.

- Drop-out is formalized by

$$\boldsymbol{z}^{\text{drop}} : \mathbb{R}^q \to \mathbb{R}^q, \qquad \boldsymbol{X} \mapsto \boldsymbol{z}^{\text{drop}}(\boldsymbol{X}) = \boldsymbol{Z} \odot \boldsymbol{X},$$

  where $\boldsymbol{Z} = (Z_1, Z_2, \ldots, Z_q)^\top \in \{0,1\}^q$ is a vector of i.i.d. Bernoulli random variables that are re-sampled in each SGD step, and $\odot$ denotes the element-wise Hadamard product.

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References II

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