시계열용 DL 방법론

Pure deep learning - N-BEAT
RNN 계열 - deepAR

인과형 예측기법

Deep Learning 계열

- 시계열 모형은 시계열의 현재값과 과거값 간 안정적인 함수관계를 가정
- Univer approximator property: ANN은 오류역전파 알고리즘을 통해, 임의의 함수를 임의의 정밀도로 근사해낼 수 있는 능력을 가지고 있으므로, 시계열 예측에도 활용할 수 있음
- 기계학습 방법론은 다변량 입력, 복잡한 비선형 관계, 결측치 존재라는 불리한 상황에서도 시계열 예측을 효과적으로 수행할 수 있다고 알려짐
- 시계열을 분석하기 위해 개발된 RNN(Recurrent Neural Networks) 이외도 DNN(Deep Neural Networks), CNN(Convolutional Neural Networks), Attention mechanism 등 다양한 방법들의 결합 활용한 모형들이 있음

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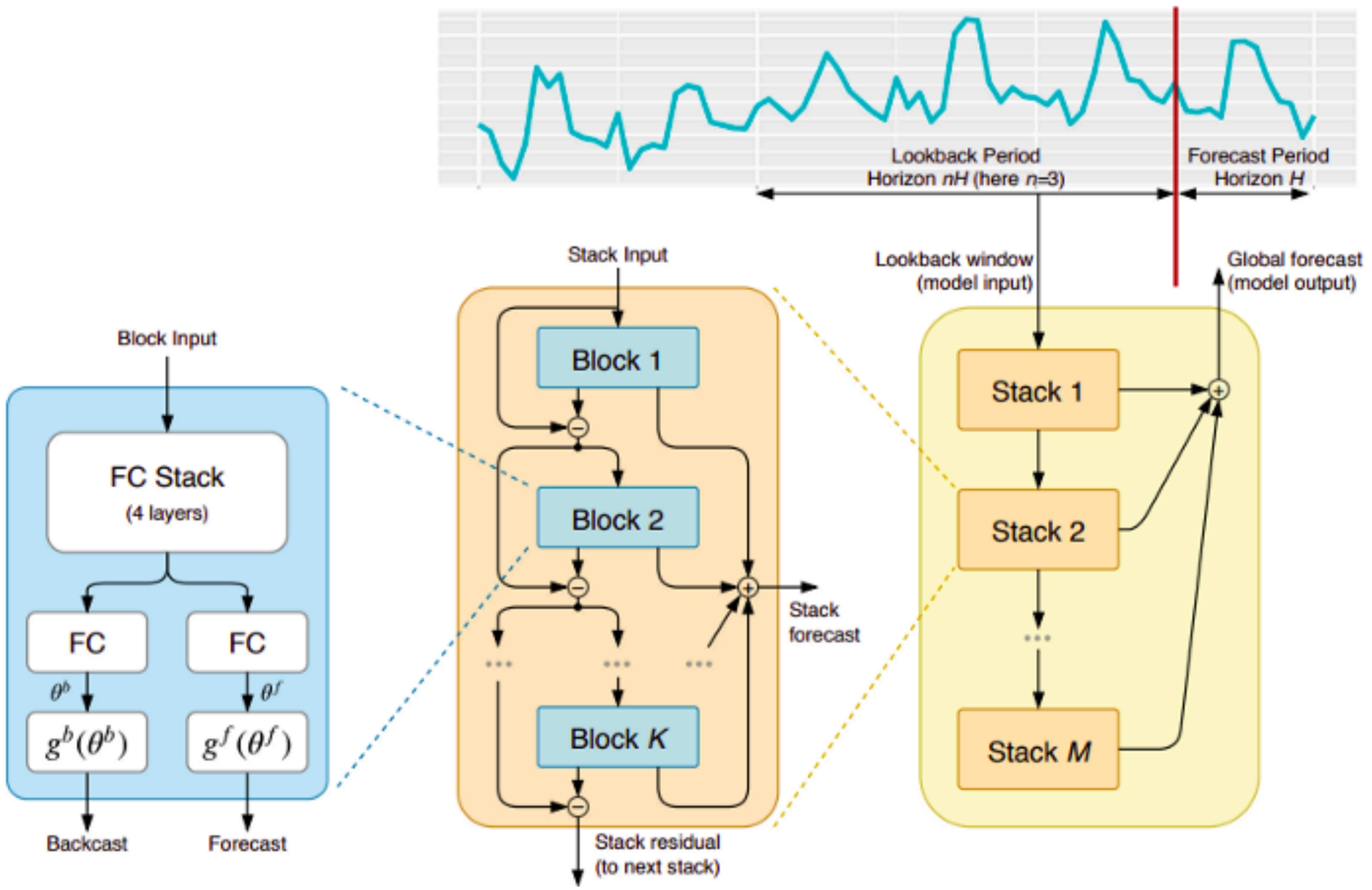
N-BEAT

N-BEAT 개요

- Yoshua Bengio이 창업한 ElementAI에서 제안
- M-competition의 결과와는 달리 순수한 deep learning 구조만으로 시계열을 분석하고자 하는 시도
- 실용적으로 이용할 수 있는 해석 가능한 deep learning 구조를 고안하고자 함



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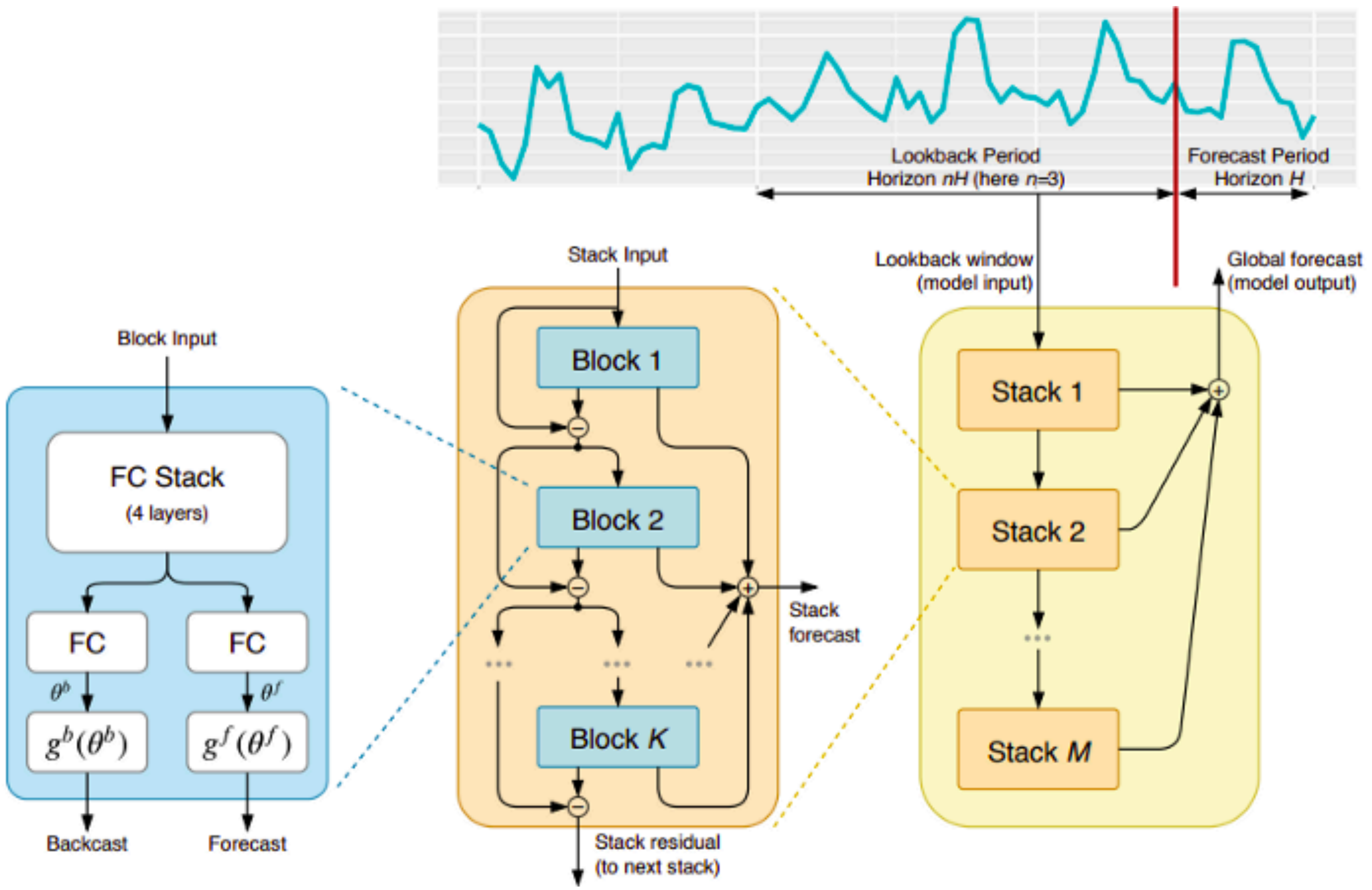
특장점

- **표현하기 쉽고 사용하기 쉬움:**
    - 간단한 module 구조로 쉽게 이해할 수 있음
    - Feature engineering이 최소화 된 구조
- **다중 시계열 모델링 가능:**
    - 다른 스케일의 시계열을 동시에 모델링 할 수 있음
    - 이러한 성질은 inner procedure와 outer proceduer로 구성된 meta-learning을 통해서 이루어짐
    - Inner learning procedure은 block 안에서 이루어지며, local의 일시적인 성격을 모델링
    - Outer learning procedure는 stack 안에서 일어나며, 시계열 전반의 global한 성격을 학습



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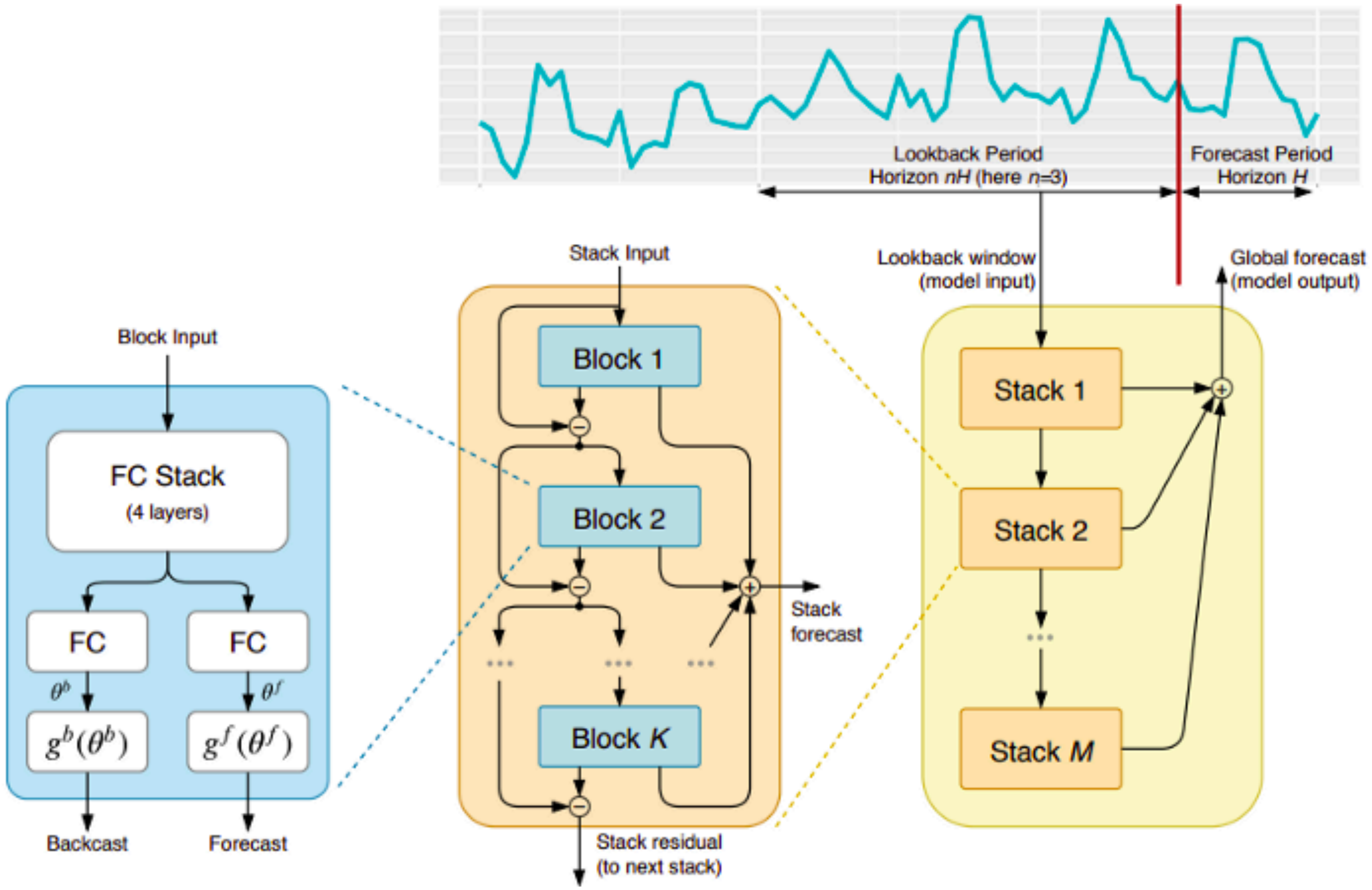
모형 상세

Basic Block (Doubly Residual Stacking)

- *N-BEATS*에서는 *lookback window*를 통해 입력된 데이터를 *backcast*와 *forecast*이라는 두개의 *residual branch* 형태로 활용. 두갈래이므로 *“doubly”*라는 이름이 붙음

- 연속된 block는 이전 block에서의 backcast의 재구성(reconstruction)을 통해 residual error를 모델링 한다는 측면에서 Box-Jenkins 방법을 흉내낸 것으로 볼 수 있음

Note: The original *N-BEATS* implementation only works with univariate time series.



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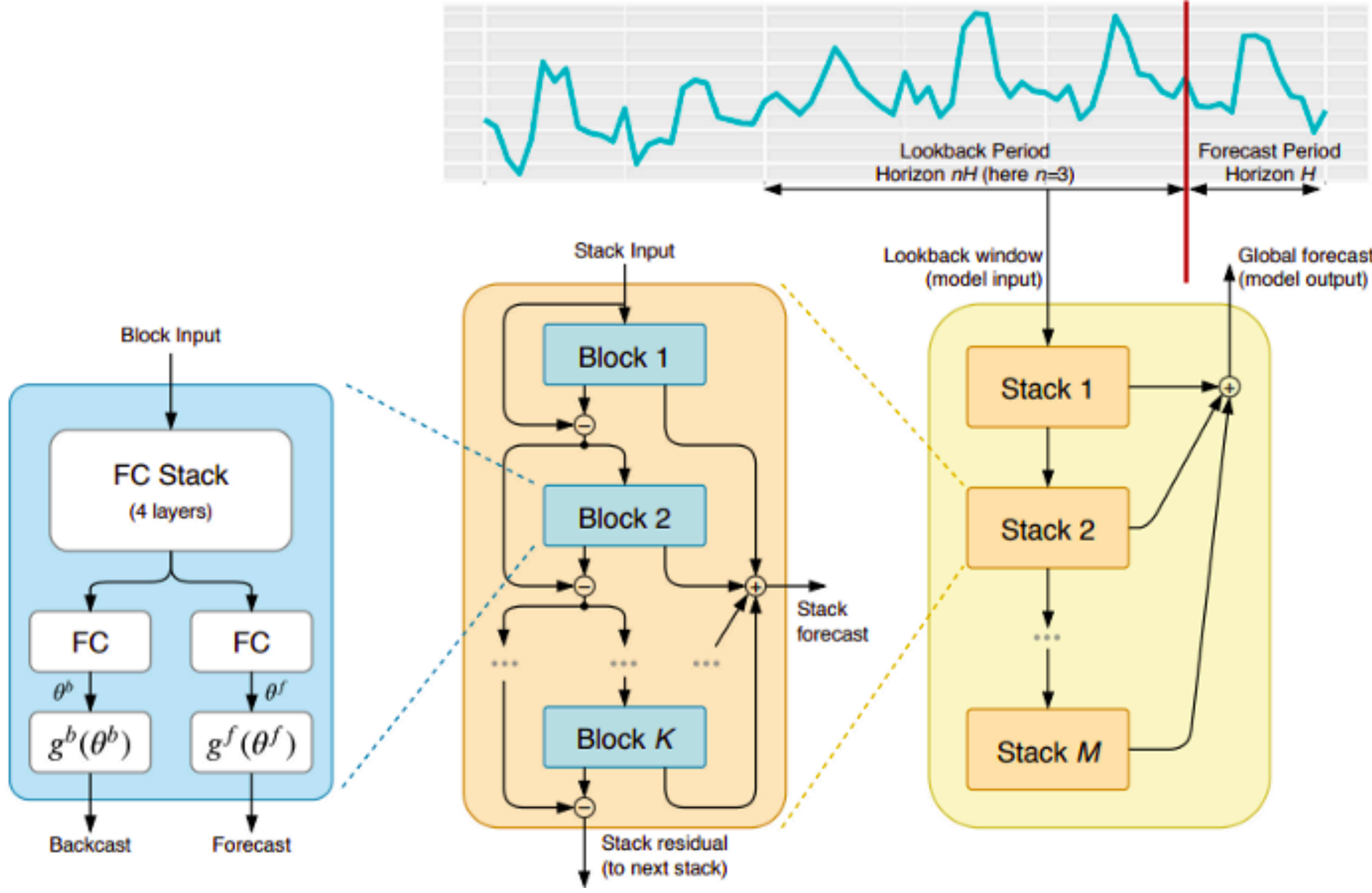
모형 상세

Basic Block (Doubly Residual Stacking)



- l번째 block은 입력으로 $\mathbf{x}_l$을 받고, 출력으로는 $\hat{\mathbf{x}}_l$과 $\hat{\mathbf{y}}_l$을 만들어 냄
- Input window의 크기는 forecast horizon H의 정수배 ($2H$~$7H$)로 둠
- 다른 블록들의 입력값 $\mathbf{x}_l$은 이전 블록들의 residual output (input + block을 통과한 출력을 합친 결과)
- $\hat{\mathbf{x}}_l$은 $\mathbf{x}_l$ lookback input에 대한 추정(backcast)이며, $\hat{\mathbf{y}}_l$은 H의 길이를 갖는 forward 예측값 벡터
- 각 *block*의 예측값은 *stack level*에서 한번 합해지고, 전체 *network*에서 합해짐 *(Interpretability*의 근거)

$$\mathbf{x}_l = \mathbf{x}_{l-1} - \hat{\mathbf{x}}_{l-1}, \quad \hat{\mathbf{y}} = \sum_l \hat{\mathbf{y}}_l$$

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모형 상세

Basic Block

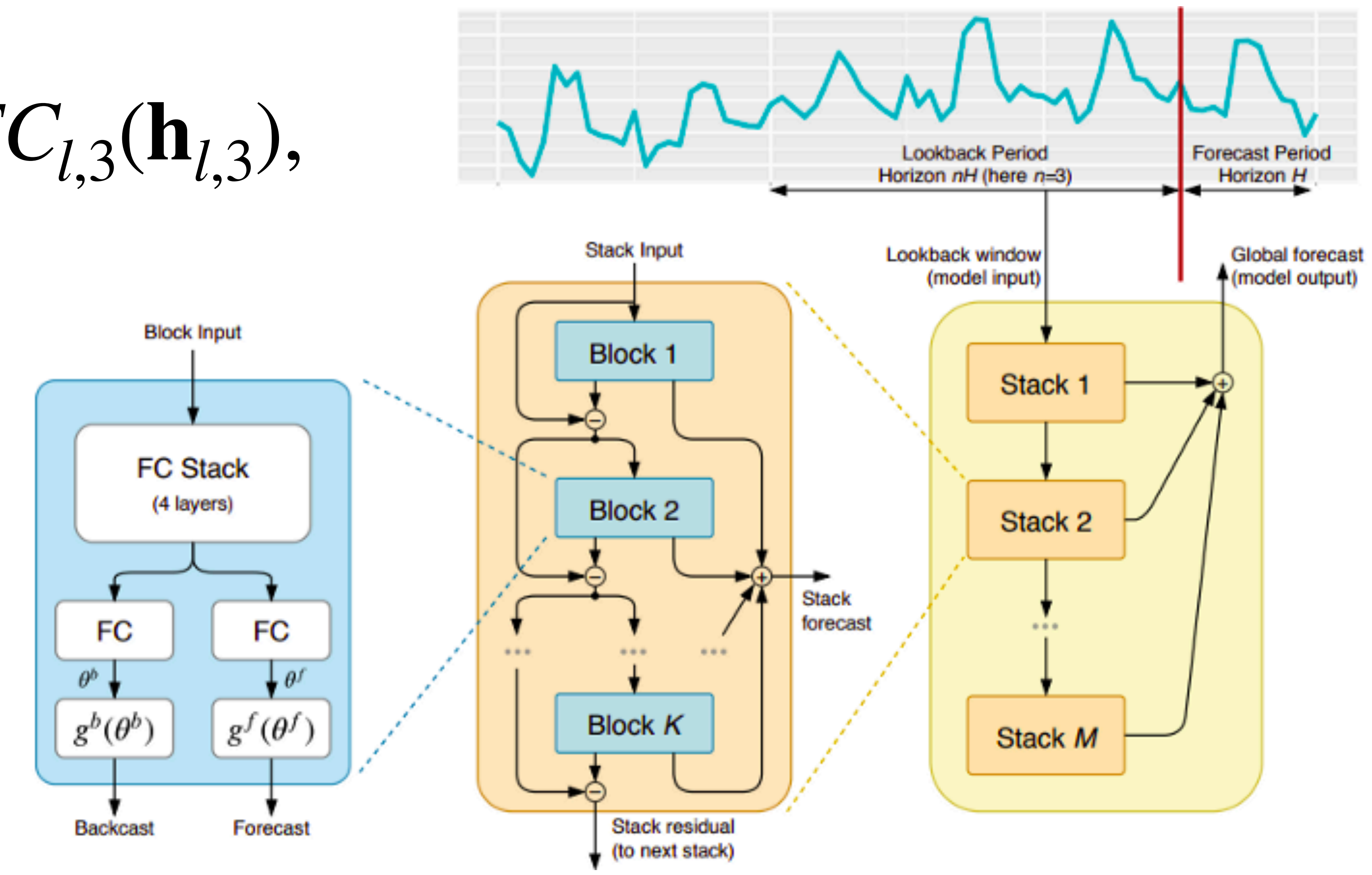
- FC network는 다음과 같이 쓸 수 있음

$$\mathbf{h}_{l,1} = FC_{l,1}(\mathbf{x}_l), \mathbf{h}_{l,2} = FC_{l,2}(\mathbf{h}_{l,1}), \mathbf{h}_{l,3} = FC_{l,3}(\mathbf{h}_{l,2}), \mathbf{h}_{l,4} = FC_{l,3}(\mathbf{h}_{l,3}),$$

FC = Linear

$$\theta_l^b = \text{LINEAR}_l^b(\mathbf{h}_{l,4}), \theta_l^f = \text{LINEAR}_l^f(\mathbf{h}_{l,4})$$

$$\theta_l^f = \mathbf{W}_l^f \mathbf{h}_{l,4}, \mathbf{h}_{l,1} = \text{RELU}(\mathbf{W}_{l,1}\mathbf{x}_l + \mathbf{b}_{l,1})$$



- g함수는 다음과 같이 정의됨

$$\hat{\mathbf{y}}_l = g^f(\theta^f) = \sum_{i=1}^{\dim(\theta_l^f)} \theta_{l,i}^f v_i^f, \quad \hat{\mathbf{x}}_l = g^b(\theta^b) = \sum_{i=1}^{\dim(\theta_l^b)} \theta_{l,i}^b v_i^b$$

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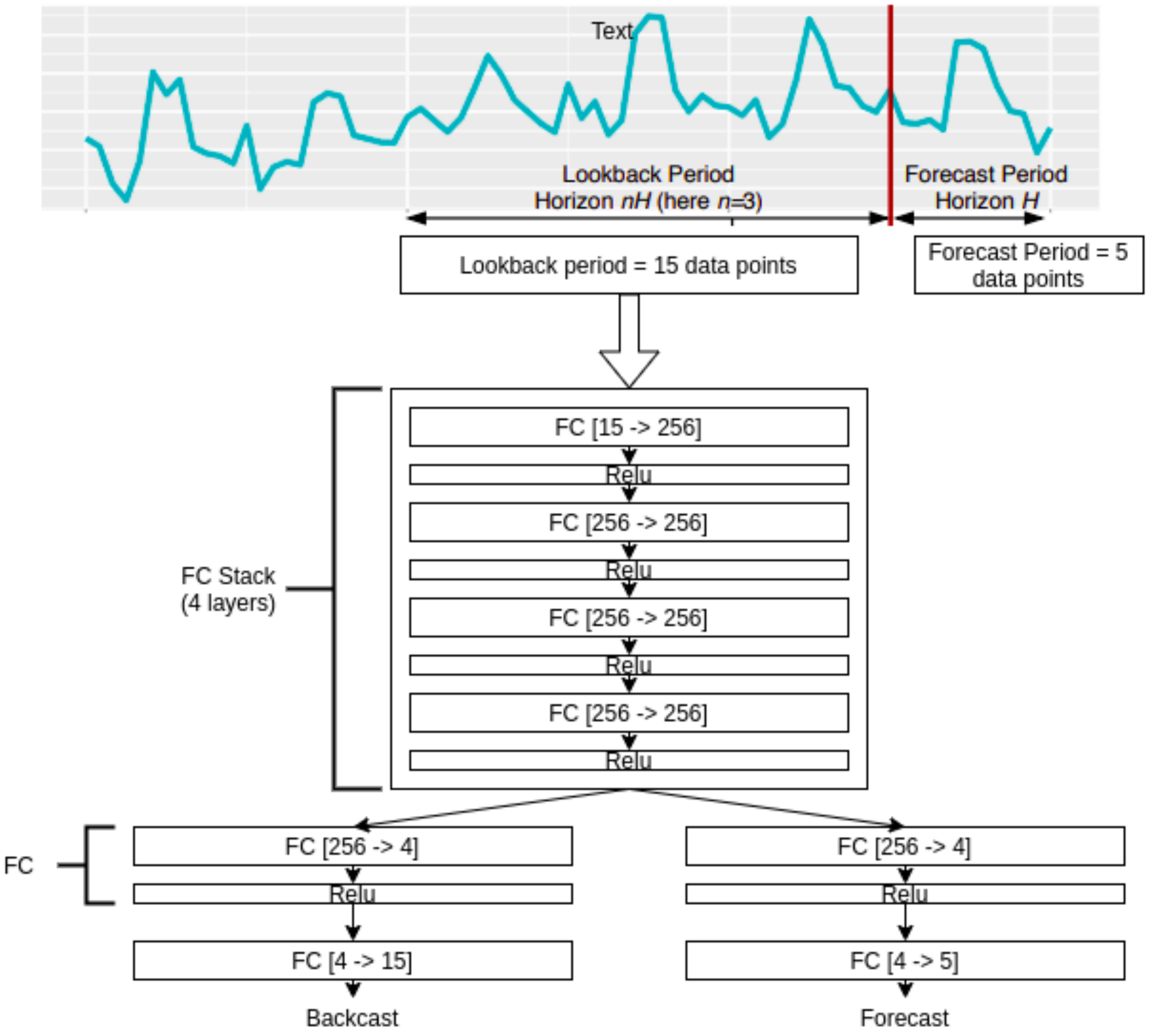
모형 상세

Basic Block



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모형 상세

Interpretability

- 일반 모형에서는 다음의 fully connected layer를 매 block의 마지막에 가짐

$$\hat{\mathbf{y}}_l = \mathbf{V}_l^f \theta_l^f + b_l^f, \quad \hat{\mathbf{x}}_l = \mathbf{V}_l^b \theta_l^b + b_l^b$$

- 설명을 위해서는 각 블록 내 마지막 fully connected layer를 제거하고, 그 대신 설명 가능한 layer를 추가

    -

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모형 상세

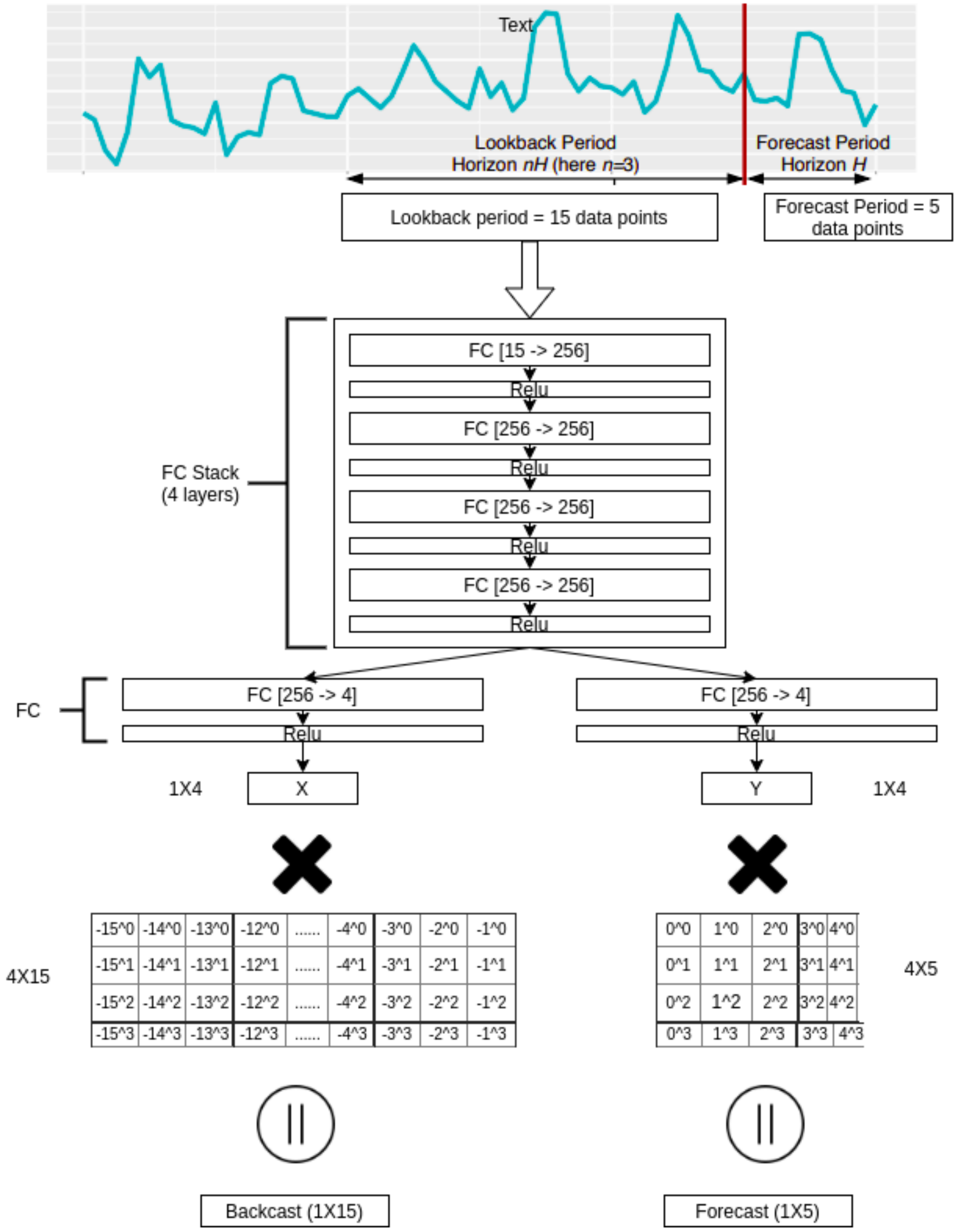
Interpretability

- Trend model
  - Trend model: 단조함수이며 천천히 변하는 함수

$$\hat{\mathbf{y}}_{s,l} = \sum_{i=0}^{p} \theta^{f}_{s,l,i} t^{i} \,,$$

matrix form으로는

$$\hat{\mathbf{y}}^{tr}_{s,l} = \mathbf{T}\theta^{f}_{s,l}, \quad \mathbf{T} = [\mathbf{1}, \mathbf{t}, \ldots, \mathbf{t}^{p}]$$



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모형 상세

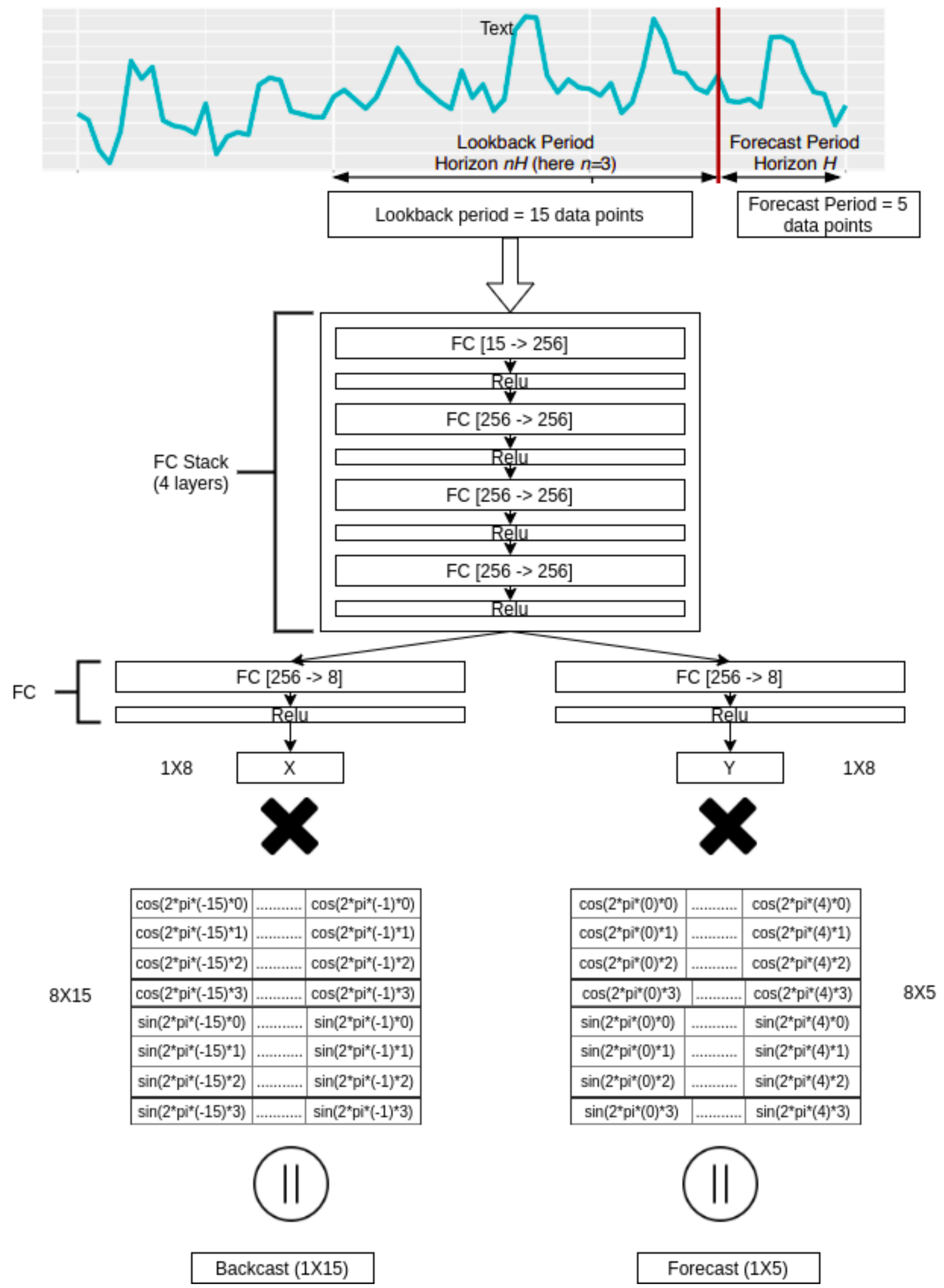
Interpretability

- Seasonality model

$$\hat{\mathbf{y}}_{s,l} = \sum_{i=0}^{\lfloor H/2-1 \rfloor} \theta^{f}_{s,l,i} \cos(2\pi i t) + \theta_{s,l,i+\lfloor H/2 \rfloor} + \sin(2\pi i t)$$

$$\hat{\mathbf{y}}^{season}_{s,l} = \mathbf{S}\theta^{f}_{s,l},$$

$$\mathbf{s} = [\mathbf{1}, \cos(2\pi\mathbf{t}), \ldots, \cos(2\pi\lfloor H/2-1 \rfloor \mathbf{t}), \sin(2\pi\mathbf{t}), \ldots, \sin(2\pi\lfloor H/2-1 \rfloor \mathbf{t}))]$$



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RNN

인과형 예측기법

RNN

- RNN(Recurrent Neural Networks)은 ANN 모형의 입력층에서 출력층으로의 일방향 데이터 전달 구조에 변형을 가하여 은닉층 또는 출력층에서 입력층으로의 피드백 구조를 도입, 네트워크가 기억력을 가지게 만들어 언어 데이터 처리에 우수한 능력을 보임

- 따라서, RNN 모형은 일반적으로 데이터에 존재하는 시간 의존성(Temporal Dependence)을 학습하는 기능을 지니며, 시계열 데이터에 내재되어 있는 temporal structure를 잘 파악해냄

- 특히 LSTM은 데이터에 존재하는 장기간에 걸친 연관관계를 잘 파악해낸다.

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DeepAR

- 개념
- 특장점
- 한계점
- 알고리즘 설명
- Parameter 요약
- 현업 유의점
- Code - 별첨

DeepAR 개요

- **수없이 많은 시계열을 동시에 예측해야 하는 상황이 더욱 빈번해짐**
  - 기존에도 여러 시계열의 정보를 활용하는 multivariate timeseries 기법들이 있었지만, scalable하지 않음
  - 이를 위해 주로 가장 중요한 품목들 위주로 분석을 진행하거나 상위 카테고리로 그룹화 한후 분석 진행

- **기존의 전통적 시계열방법은 판단과 수작업이 많이 들어감**
  - 시계열의 정상성, 단위근 파악 등
  - 특성 파악후 많은 전처리 작업이 필요
    - Ex) 추세 제거, 차분, 지시변수 생성 등
  - 이러한 작업들 역시 scalability에 영향을 줌

Figure 1: Log-log histogram of the number of items versus number of sales for the 500K time series of ec, showing the scale-free nature (approximately straight line) present in the ec dataset (axis labels omitted due to the non-public nature of the data).

https://www.youtube.com/watch?v=okyo61ZZivA

특장점

- **Feature engineering의 수고가 줄어듬**
  - 원래 시계열을 거의 그대로 입력 (내부적으로 autoscaling 적용)
- **확률적인 예측이 가능**
  - 신뢰구간 제공이 가능
  - loss의 종류에 따라서, 기대값이 아니라, 기대 quantile을 구할 수 있음
- **적은 데이터에도 효과가 있음**
  - 수많은 시계열의 정보를 빌려올 수 있음
  - 특히 서로 다른 scale(혹은 분포)의 시계열을 동시 예측 가능
- **다양한 정보를 모델링 할 수 있음**
  - Static한 variable (독립변수)
  - 기타 시계열 혹은 미래의 알려진 값까지 모델링이 가능
- **다양한 likelihood를 고려하여, 다양한 형태의 데이터를 모델링할 수 있음**
  - Binary response, Poison response

Figure 1: Log-log histogram of the number of items versus number of sales for the 500K time series of ec, showing the scale-free nature (approximately straight line) present in the ec dataset (axis labels omitted due to the non-public nature of the data).

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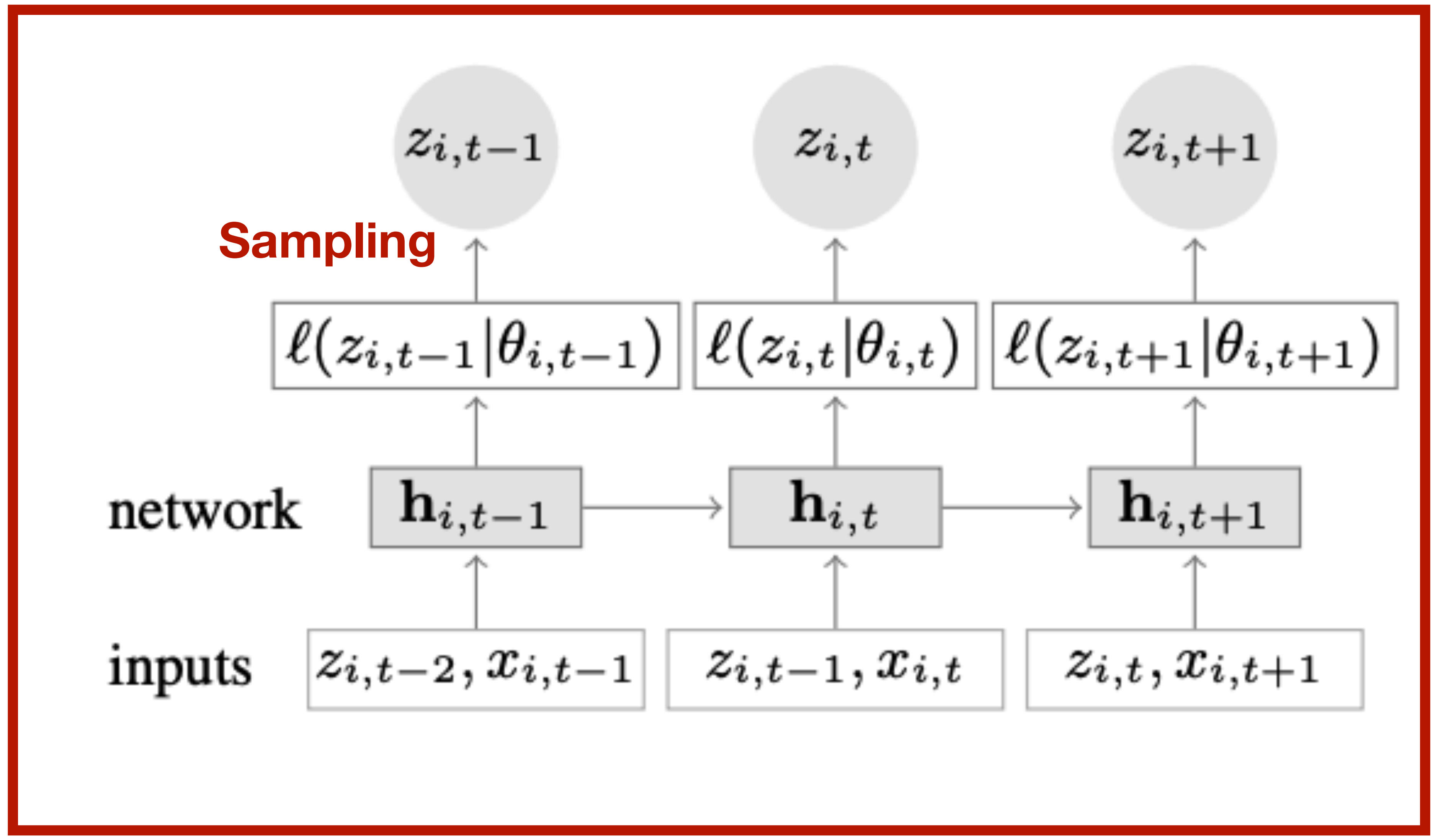
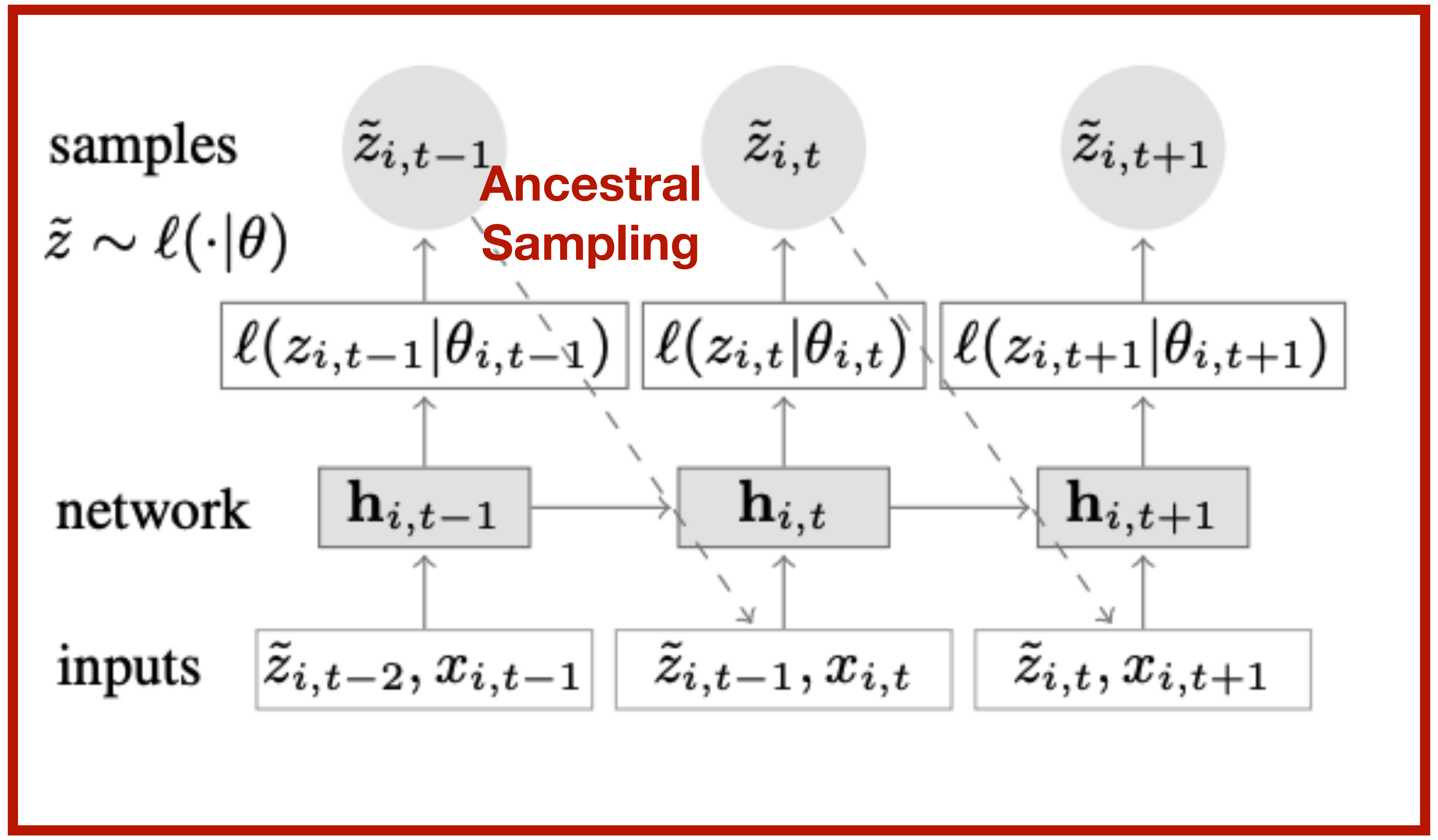
모형 상세

Sequence to sequence 구조



Encoder

Training Phase



Decoder

Prediction Phase

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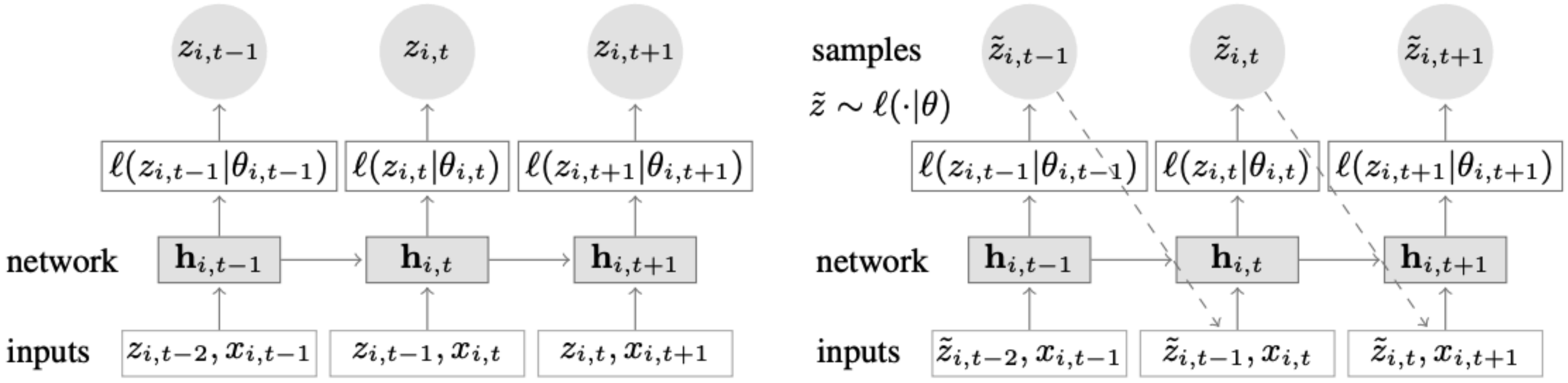
모형 상세

Likelihood



- 신경망은 시계열 정보, z,의 likelihood, $l(z|\theta)$,의 paramter를 예측하는 데 활용
- 논문에서는 두개의 likelihood를 사용
  - Gaussian likelihood

Softplus activation

$$l_G(z\,|\,\mu,\sigma) = (s\pi\sigma^2)^{-1/2}\exp\left(-(z-\mu)^2/(2\sigma^2)\right), \quad \mu(\mathbf{h}_{i,t}) = \mathbf{w}_\mu^T\mathbf{h}_{i,t}, \quad \sigma(\mathbf{h}_{i,t}) = \log(1+\exp(\mathbf{w}_\sigma^T\mathbf{h}_{i,t}+b\sigma))$$

  - Negative binomial likelihood: positive count

$$l_{NB}(z\,|\,\mu,\alpha) = \frac{\Gamma\left(z+\frac{1}{\alpha}\right)}{\Gamma(z+1)\Gamma\left(\frac{1}{\alpha}\right)}\left(\frac{1}{1+\alpha\mu}\right)^{1/\alpha}\left(\frac{\alpha\mu}{1+\alpha\mu}\right)^{z}, \quad \mu(\mathbf{h}_{i,t}) = \log(1+\exp(\mathbf{w}_\mu^T\mathbf{h}_{i,t}+b\mu)), \quad \alpha(\mathbf{h}_{i,t}) = \log(1+\exp(\mathbf{w}_\alpha^T\mathbf{h}_{i,t}+b\alpha))$$

α: Shape parameter

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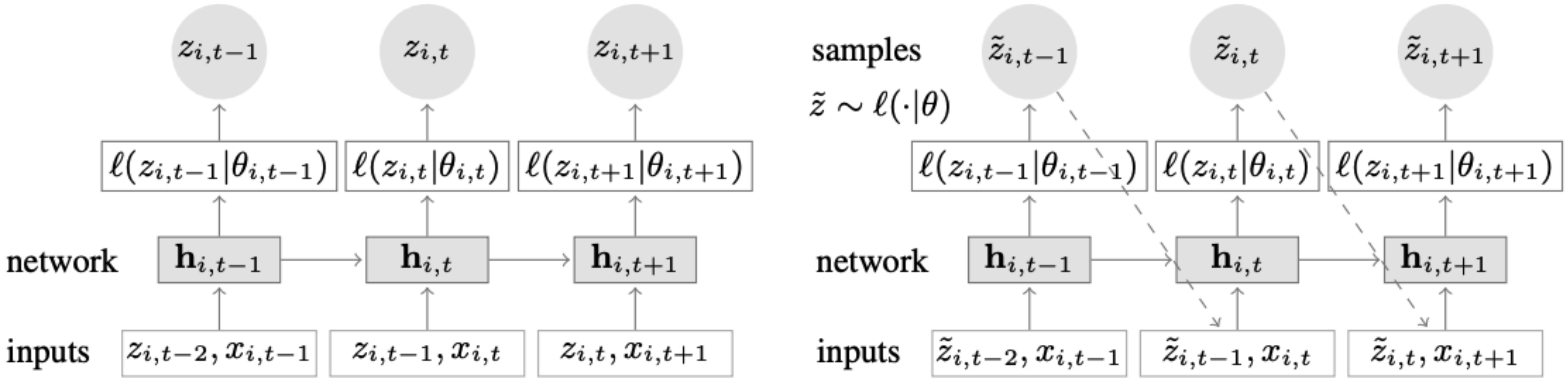
모형 상세

Likelihood



- Input:
  - 과거의 관측치 값: $z_1, \ldots, z_{t_0-1}$
  - 독립변수들: $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_T$
- Output: 추정된 결합확률 분포: $P(Z_{t_0}, Z_{t_0+1}, \ldots, Z_T)$
- 정해진 크기의 임의의 window 내의 값들을 이용하여, MLE를 구하는 방식으로 학습
- 결국 likelihood는 다음과 같음

$$\sum_{i=1}^{N} \sum_{t=1}^{T} \log l(z_{i,t} \mid y_t(\mathbf{h}_{i,t}))$$

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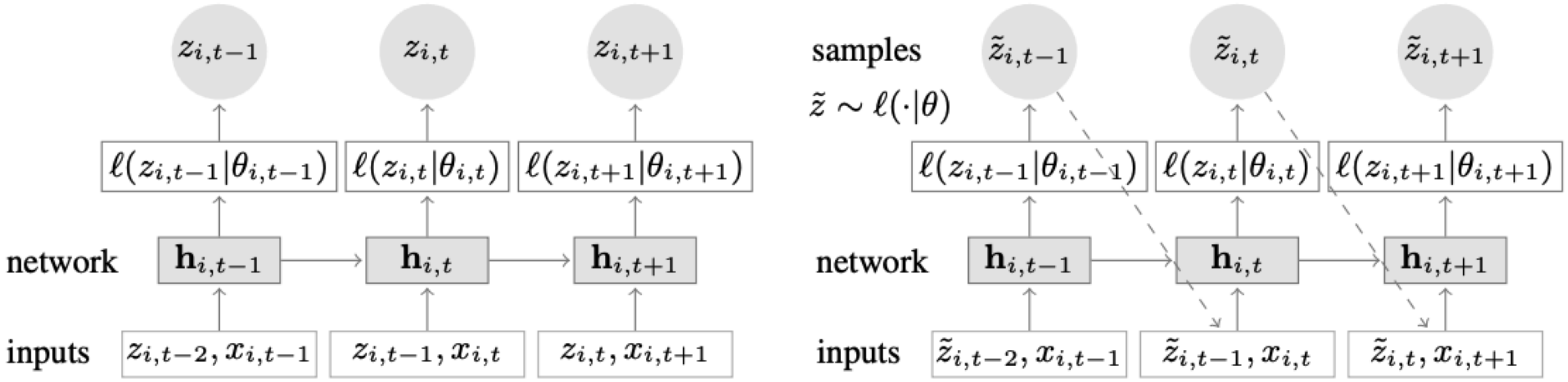
모형 상세

Scale problem, long-tail problem



- 두가지 문제가 존재함
  - 시계열의 scale이 크게 다르다. (대다수의 품목이 아주 적게 팔린다)
  - 주로 관심을 가져야 할 시계열의 개수가 크게 적다. (소수의 품목만이 아주 많이 팔린다.)

- 두가지 해결책을 제시
  - Automatic Scaling
  - Weighted sampling to counter-balance power-law behavior

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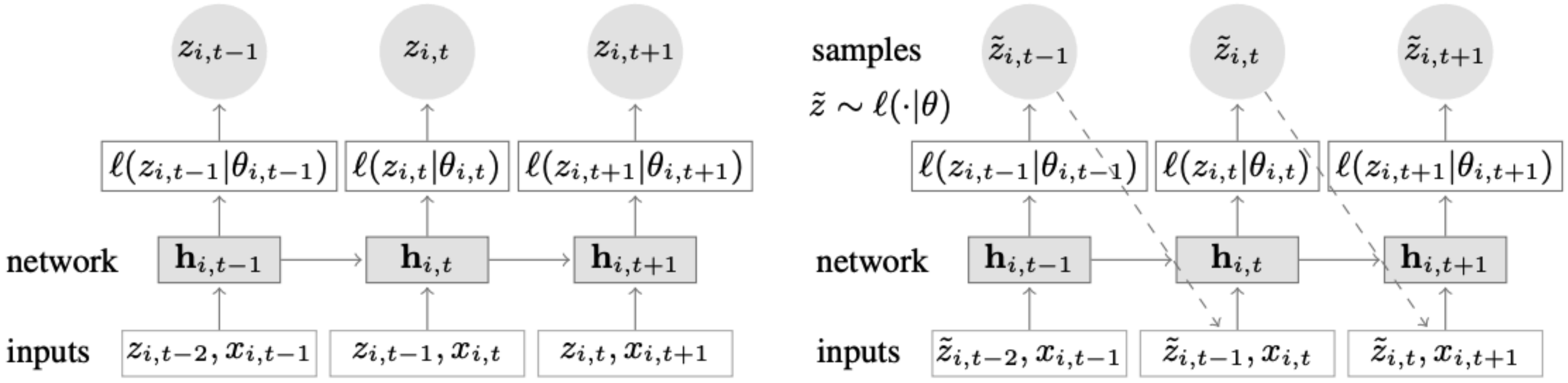
모형 상세

Automatic scaling



Automatic scaling:

- ***i*번째 시계열의 자기상관 입력인** z 를 v_i라는 scaling factor를 이용해서 scaling함
- v_i는 단순히 시계열의 평균값으로, 논문에서는 다음의 식을 활용 (Heuristic method)

$$v_i = 1 + \frac{1}{t_0} \sum_{t=1}^{t_0} z_{i,t}$$

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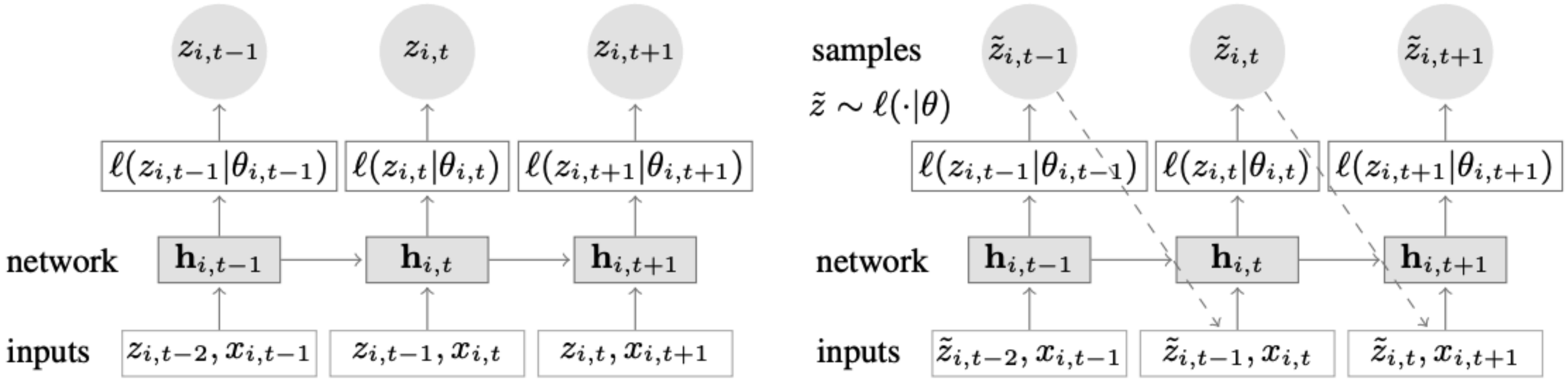
모형 상세

Long tail



Handling heavy tail distribution (Weighted sampling):

- Scale에 비례해서 학습셋에 포함될 확률을 높여줌

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Attention Mechanism

Seq2seq & its limit

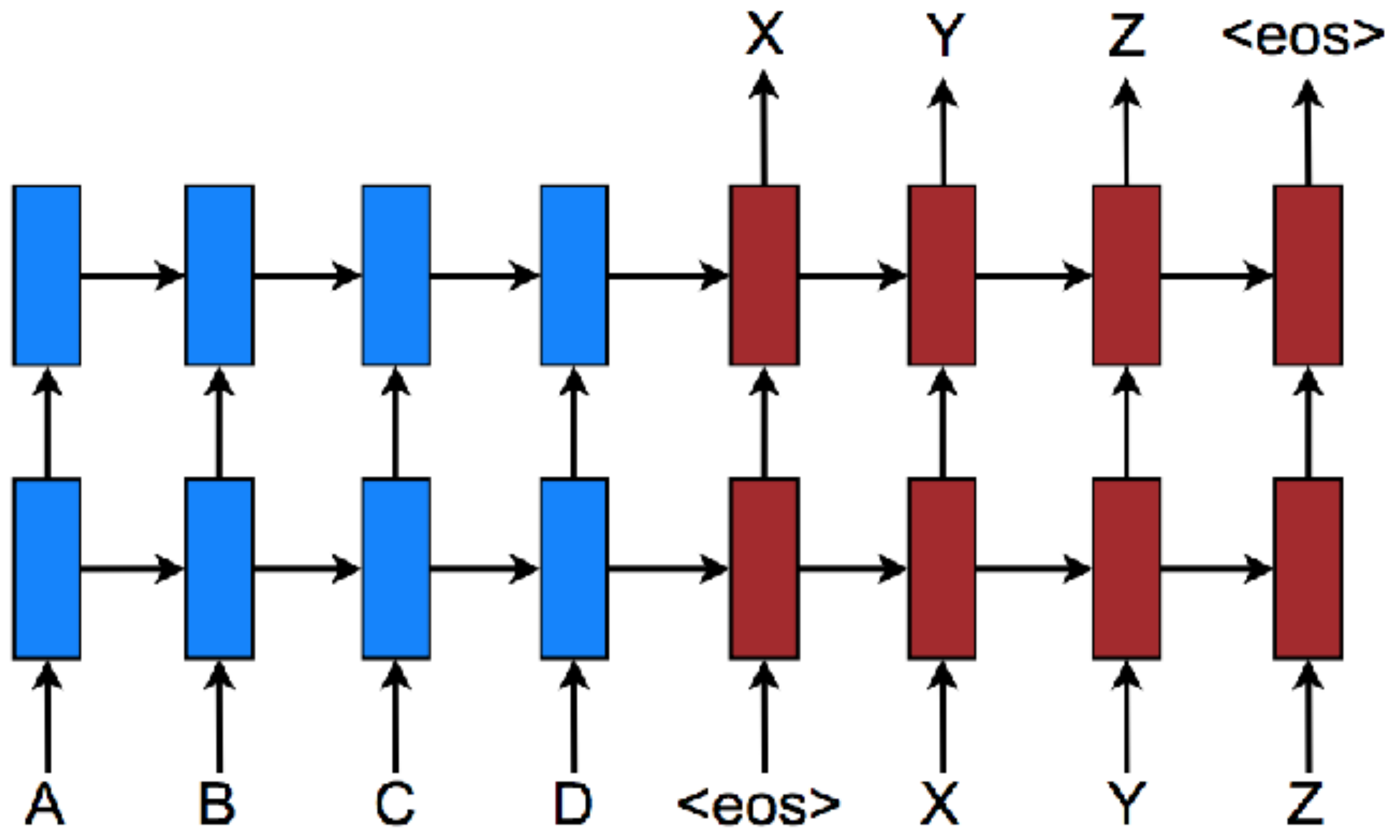

Figure 1: **Neural machine translation** – a stacking recurrent architecture for translating a source sequence `A B C D` into a target sequence `X Y Z`. Here, `<eos>` marks the end of a sentence.

When the source sequence is too long and contains multiple information-rich phrases apart from each other

What if we had a mechanism to allow the decoder to selectively (dynamically) focus on the information-rich phrases in the source sequence?

Attention mechanism

NEURAL MACHINE TRANSLATION
BY JOINTLY LEARNING TO ALIGN AND TRANSLATE

Dzmitry Bahdanau
Jacobs University Bremen, Germany

KyungHyun Cho **Yoshua Bengio***
Université de Montréal

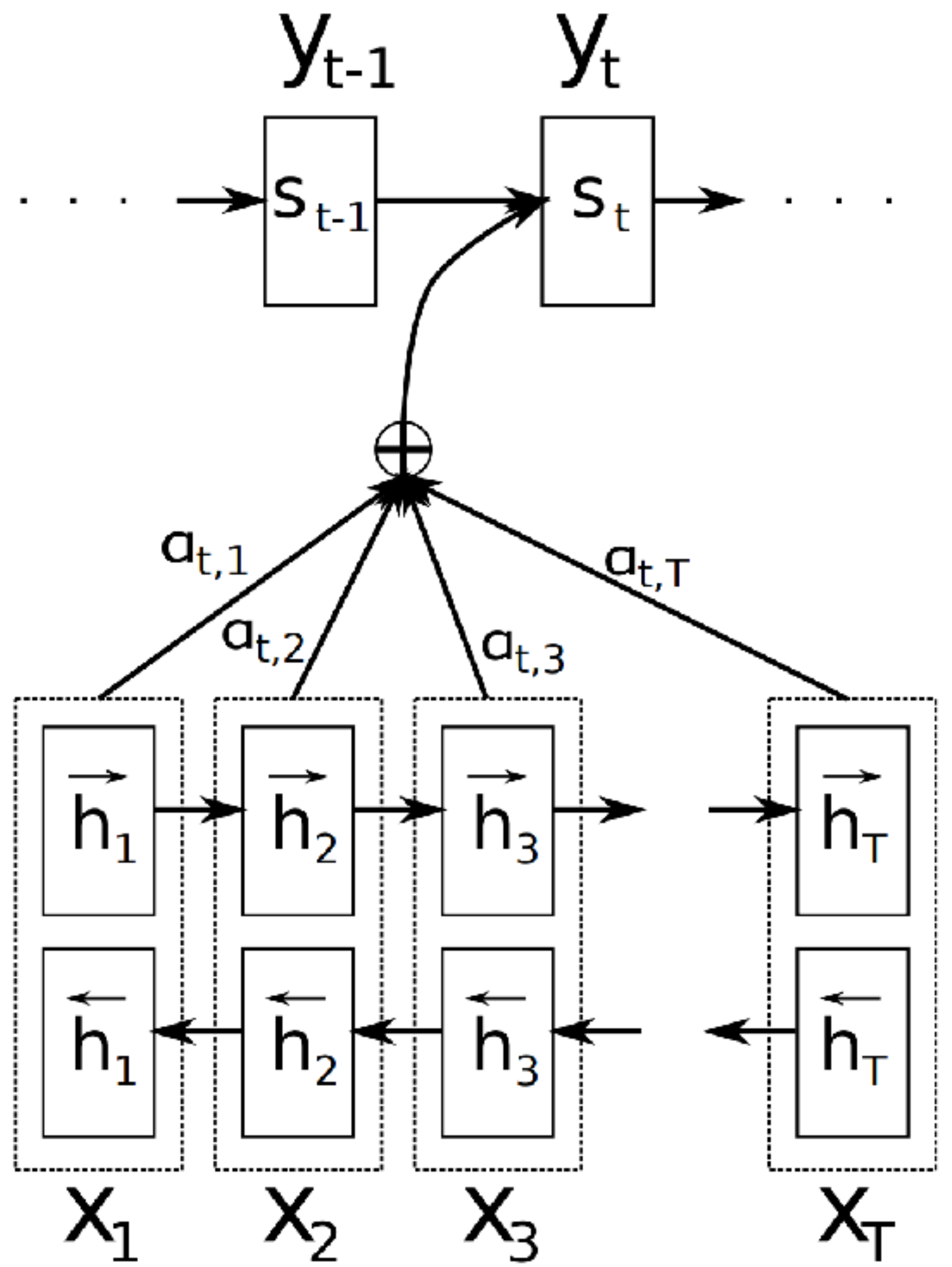

Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

Attention mechanism can do

Long term memories - attending to memories

- Dealing with gradient vanishing problem

Exceeding limitations of a global representation

- Attending/focusing to smaller parts of data
- patches in images - words or phrases in sentences

http://download.mpi-inf.mpg.de/d2/mmalinow-slides/attention_networks.pdf

Attention mechanism can do

Decoupling representation from a problem

- Different problems required different sizes of representations
- LSTM with longer sentences requires larger vectors

Overcoming computational limits for visual data

- Focusing only on the parts of images
- Scalability independent of the size of images

Adds some interpretability to the models (error inspection)

How to implement Attention

Attention mechanism

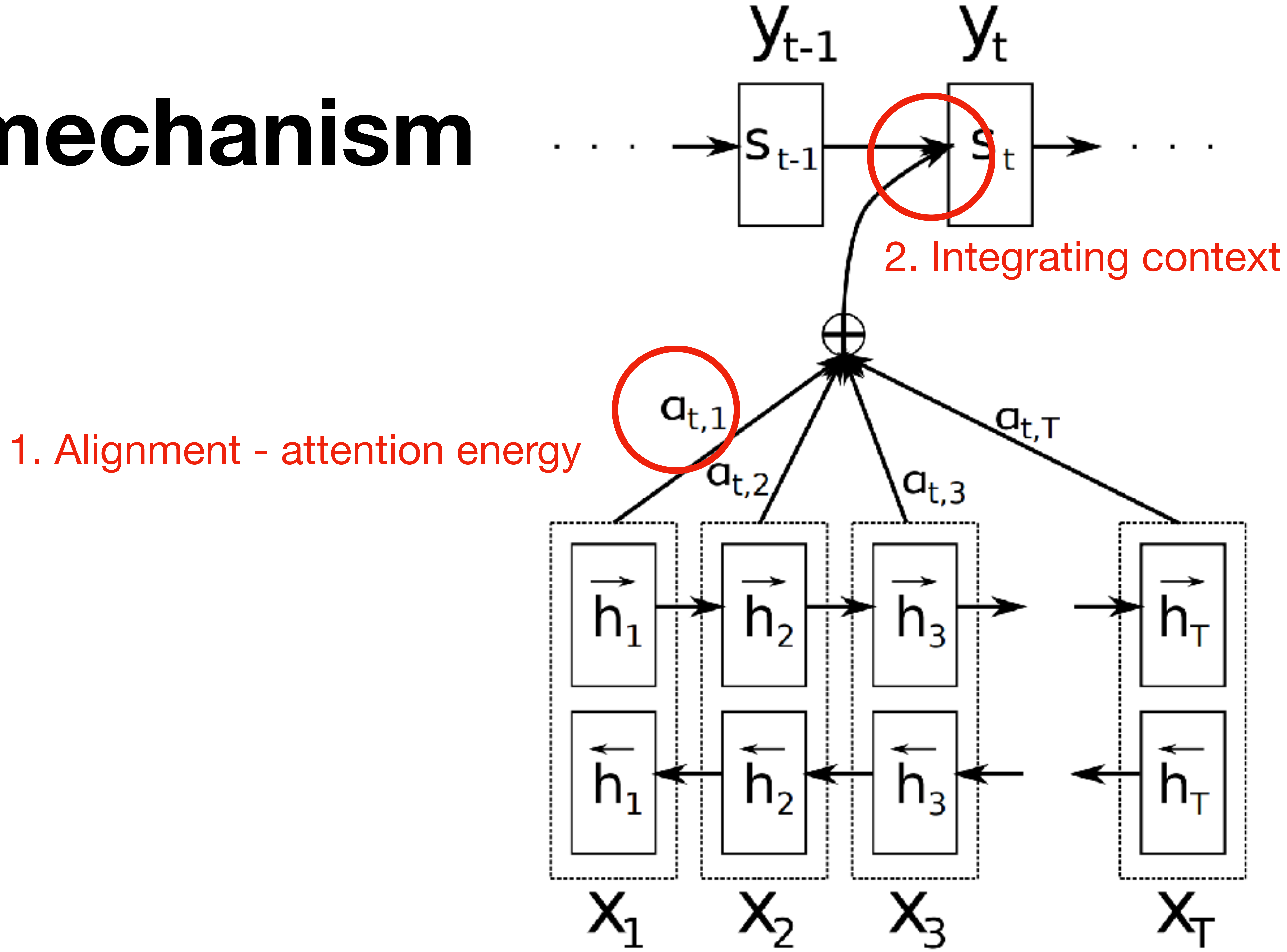

Figure 1: The graphical illustration of the proposed model trying to generate the t-th target word y_t given a source sentence $(x_1, x_2, \ldots, x_T)$.

NEURAL MACHINE TRANSLATION
BY JOINTLY LEARNING TO ALIGN AND TRANSLATE

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Alignment

Neural Machine Translation by Jointly Learning to Align and Translate
(https://arxiv.org/pdf/1409.0473.pdf)

A.1.2 ALIGNMENT MODEL

The alignment model should be designed considering that the model needs to be evaluated $T_x \times T_y$ times for each sentence pair of lengths T_x and T_y. In order to reduce computation, we use a single-layer multilayer perceptron such that

$$a(s_{i-1}, h_j) = v_a^\top \tanh \left(W_a s_{i-1} + U_a h_j \right),$$

where $W_a \in \mathbb{R}^{n \times n}, U_a \in \mathbb{R}^{n \times 2n}$ and $v_a \in \mathbb{R}^n$ are the weight matrices. Since $U_a h_j$ does not depend on i, we can pre-compute it in advance to minimize the computational cost.

Alignment

These are basically ***unnormalized scores*** of alignment between decoder state ***s*** and the hidden states H.

The mapping from $(\{h_i\}_{i \in [0,T]}, s_j)$ to the attention energies is known as the *alignment* model.

The idea of a global attentional model is to consider all the hidden states of the encoder when deriving the context vector c_t. In this model type, a variable-length alignment vector $\boldsymbol{a}_t$, whose size equals the number of time steps on the source side, is derived by comparing the current target hidden state $\boldsymbol{h}_t$ with each source hidden state $\bar{\boldsymbol{h}}_s$:

$$\begin{aligned} \boldsymbol{a}_t(s) &= \operatorname{align}(\boldsymbol{h}_t, \bar{\boldsymbol{h}}_s) \qquad (7) \\ &= \frac{\exp\left(\operatorname{score}(\boldsymbol{h}_t, \bar{\boldsymbol{h}}_s)\right)}{\sum_{s'} \exp\left(\operatorname{score}(\boldsymbol{h}_t, \bar{\boldsymbol{h}}_{s'})\right)} \end{aligned}$$

Effective Approaches to Attention-based Neural Machine Translation
(https://arxiv.org/pdf/1508.04025.pdf)

Alignment models

Here, score is referred as a *content-based* function for which we consider three different alternatives:

$$\operatorname{score}(\boldsymbol{h}_t, \bar{\boldsymbol{h}}_s) = \begin{cases} \boldsymbol{h}_t^\top \bar{\boldsymbol{h}}_s & \textit{dot} \\ \boldsymbol{h}_t^\top \boldsymbol{W}_a \bar{\boldsymbol{h}}_s & \textit{general} \\ \boldsymbol{v}_a^\top \tanh\left(\boldsymbol{W}_a[\boldsymbol{h}_t; \bar{\boldsymbol{h}}_s]\right) & \textit{concat} \end{cases}$$

Multiplicative model

Additive model

Effective Approaches to Attention-based Neural Machine Translation
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Multiplicative model

Additive model

Equivalent to

$$v_a^T \tanh\left(\mathbf{U}_a \mathbf{h}_t + \mathbf{W}_a \bar{\mathbf{h}}_s\right)$$

Effective Approaches to Attention-based Neural Machine Translation
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Alignment models

Multiplicative Models

$$score(h_i, s_j) = \begin{cases} h_i^T s_j & dot \\ h_t^T W_a s_j & general \end{cases}$$

Additive Models

$$score(h_i, s_j) = \begin{cases} v_a^T \tanh(u_a h_i + W_a s_j) & linear \\ v_a^T \tanh(W_a [h_i ; s_j]) & general \end{cases}$$

In general, the performance of multiplicative and additive functions are similar but the multiplicative function is faster and more space-efficient.

Integrating context

Specifically, given the target hidden state $\boldsymbol{h}_t$ and the source-side context vector $\boldsymbol{c}_t$, we employ a simple concatenation layer to combine the information from both vectors to produce an attentional hidden state as follows:

$$\tilde{\boldsymbol{h}}_t = \tanh(\boldsymbol{W_c}[\boldsymbol{c}_t; \boldsymbol{h}_t]) \tag{5}$$

The attentional vector $\tilde{\boldsymbol{h}}_t$ is then fed through the softmax layer to produce the predictive distribution formulated as:

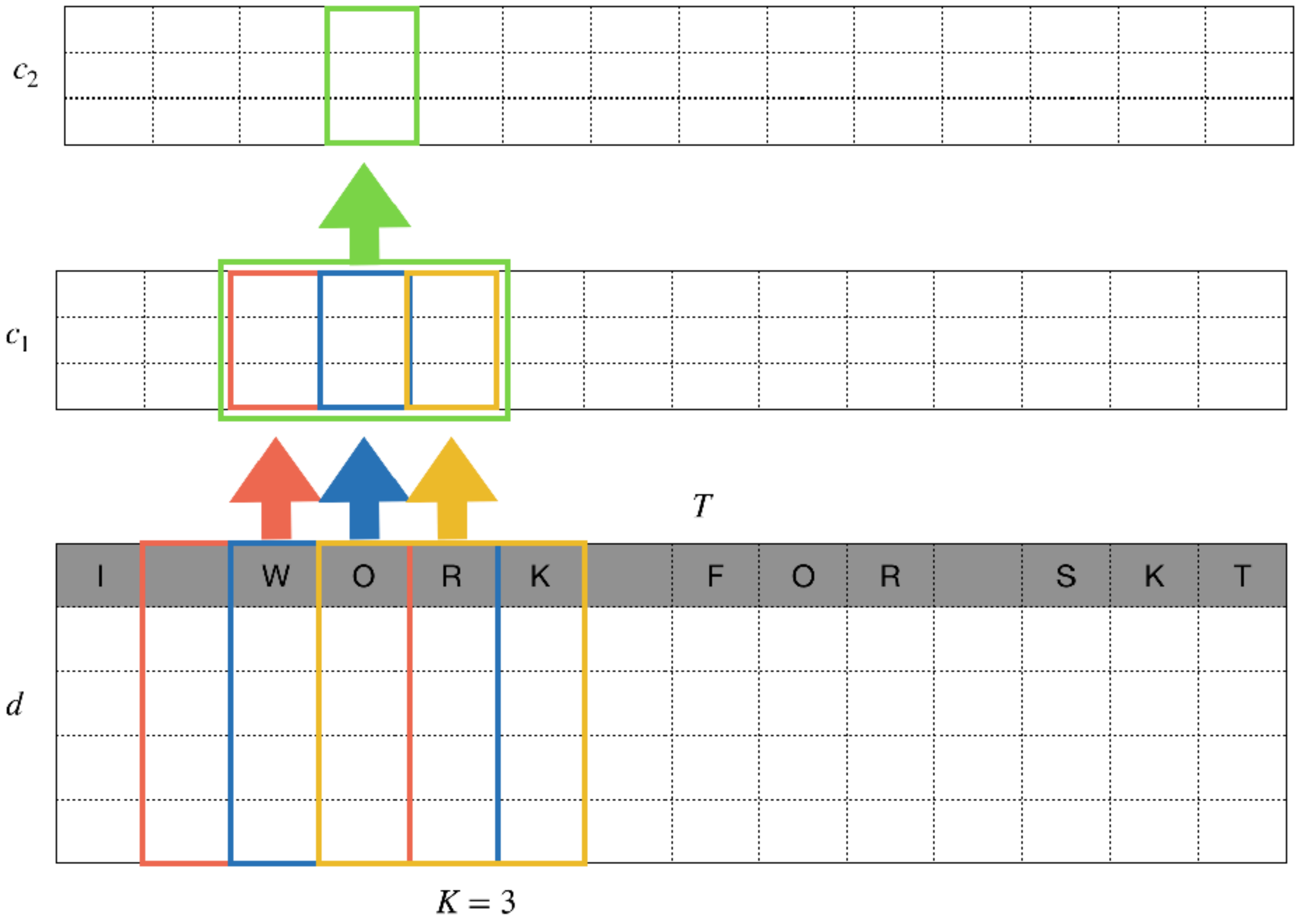
$$p(y_t|y_{<t}, x) = \mathrm{softmax}(\boldsymbol{W_s}\tilde{\boldsymbol{h}}_t) \tag{6}$$

We now detail how each model type computes the source-side context vector $\boldsymbol{c}_t$.

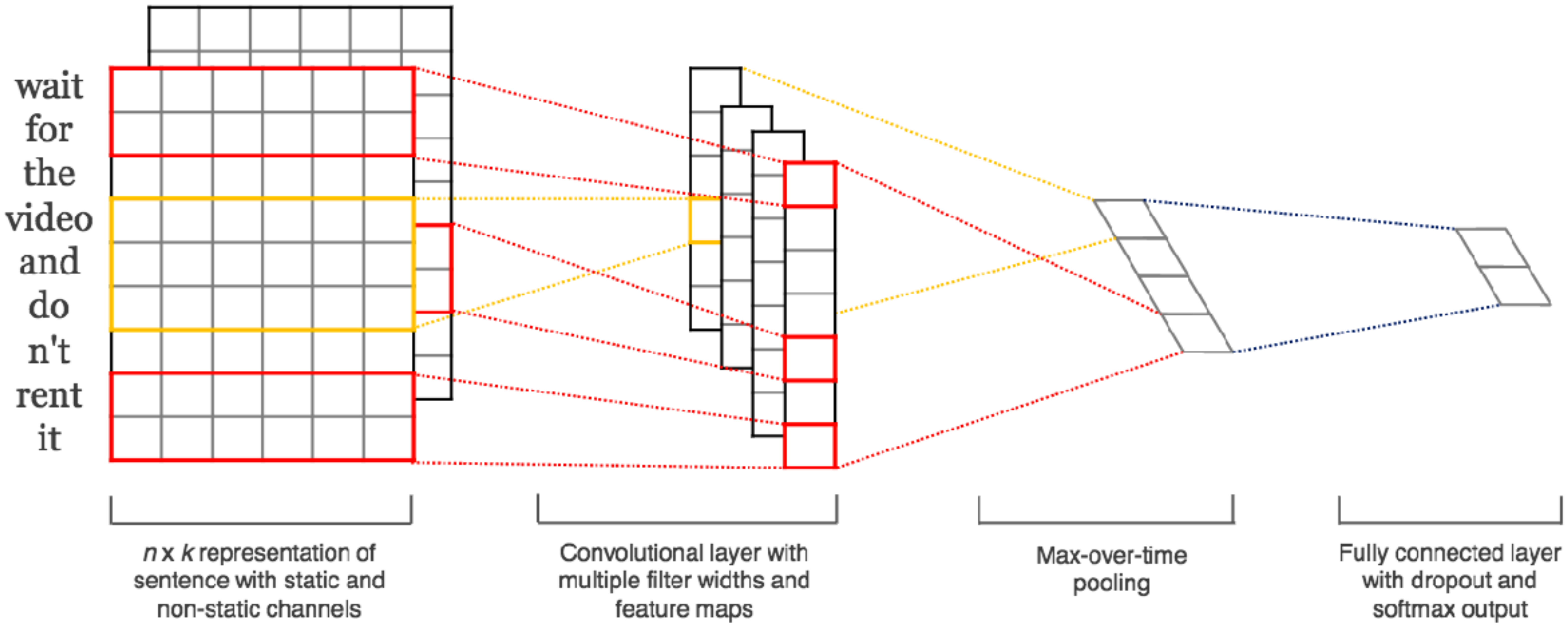
Self Attention

N-GRAM & CNN

***n*-gram is a contiguous sequence of *n* items from a given sample of text**



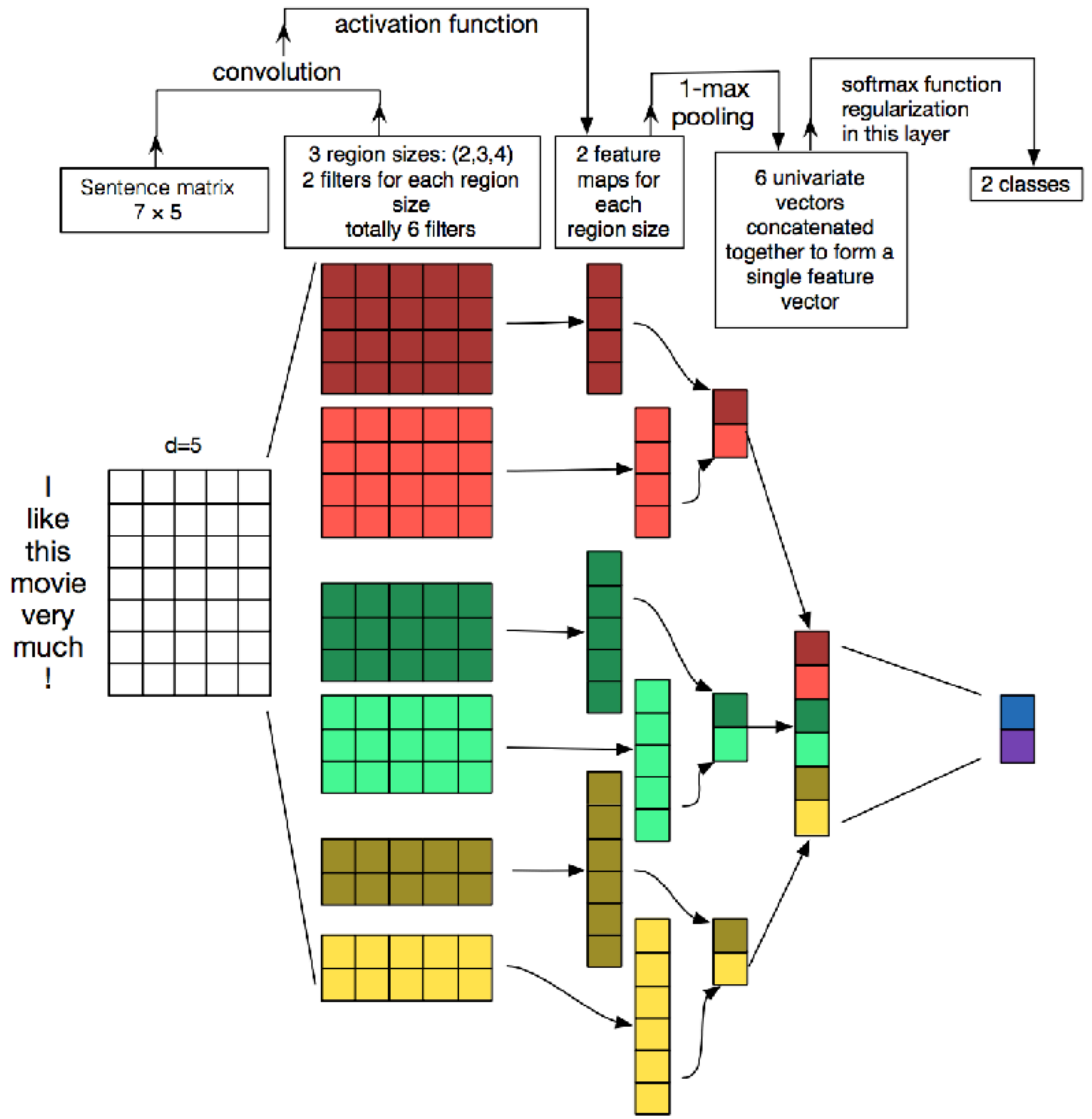
CNN for NLP



Yoon Kim (2014)

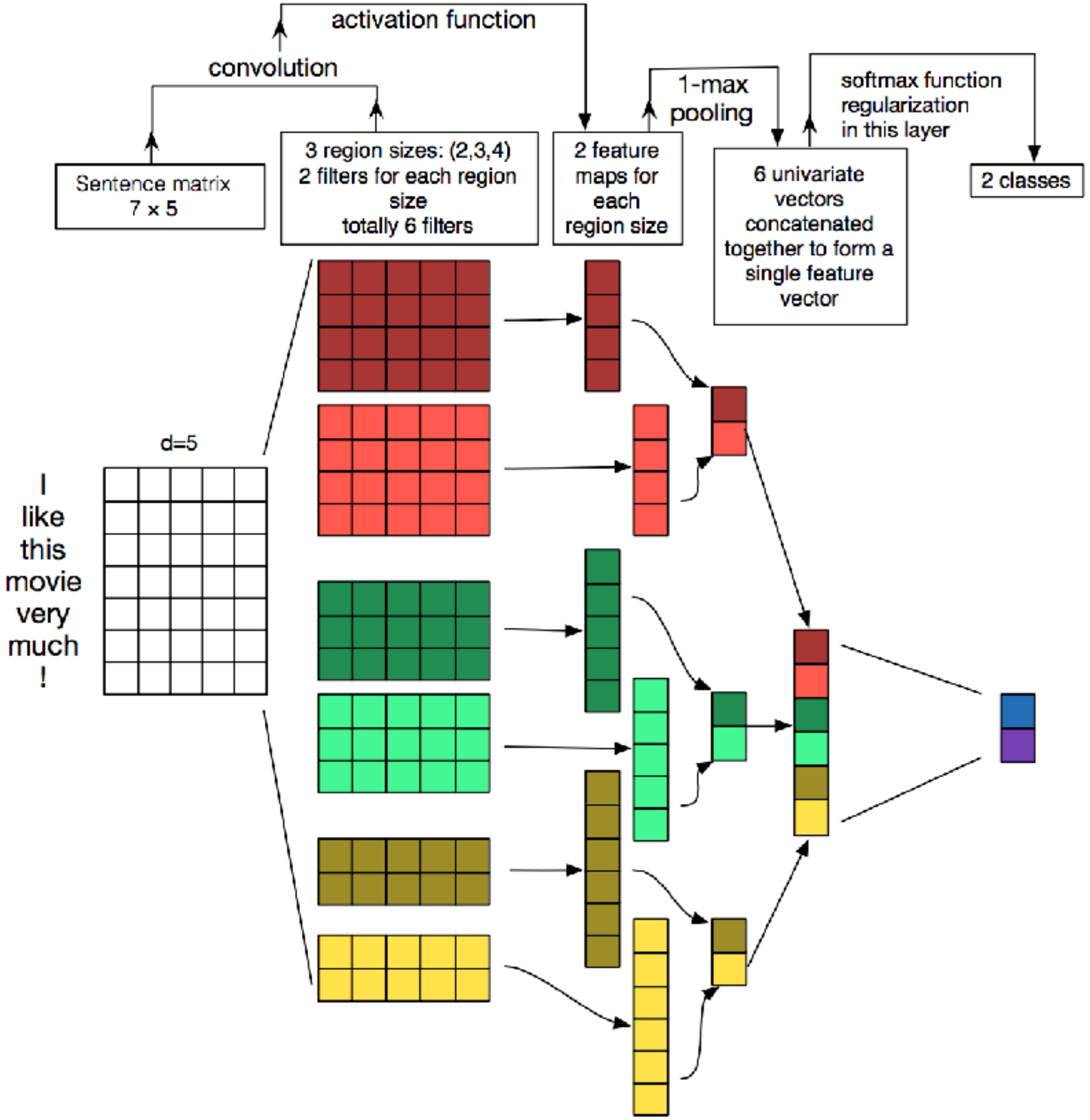
https://arxiv.org/abs/1408.5882

CNN for NLP



[A Sensitivity Analysis of (and Practitioners' Guide to) Convolutional Neural Networks for Sentence Classification]

CNN for NLP

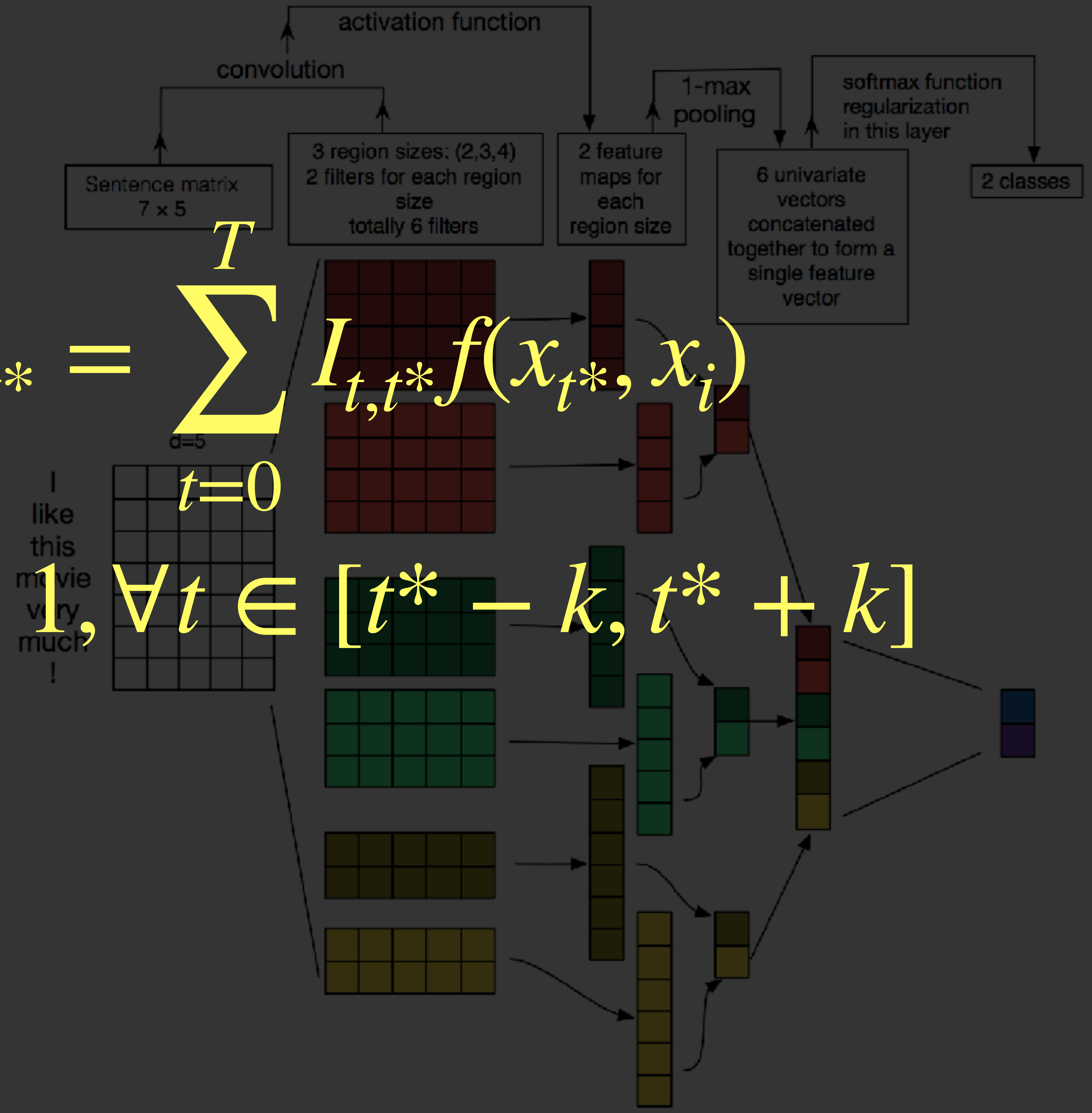


Wants to increase Receptive fields?

Dilated convolution (wavenet)

[A Sensitivity Analysis of (and Practitioners' Guide to) Convolutional Neural Networks for Sentence Classification]

CNN for NLP



$$h_{t^*} = \sum_{t=0}^{T} I_{t,t^*} f(x_{t^*}, x_i)$$

$$I_{t,t^*} = 1, \forall t \in [t^* - k, t^* + k]$$

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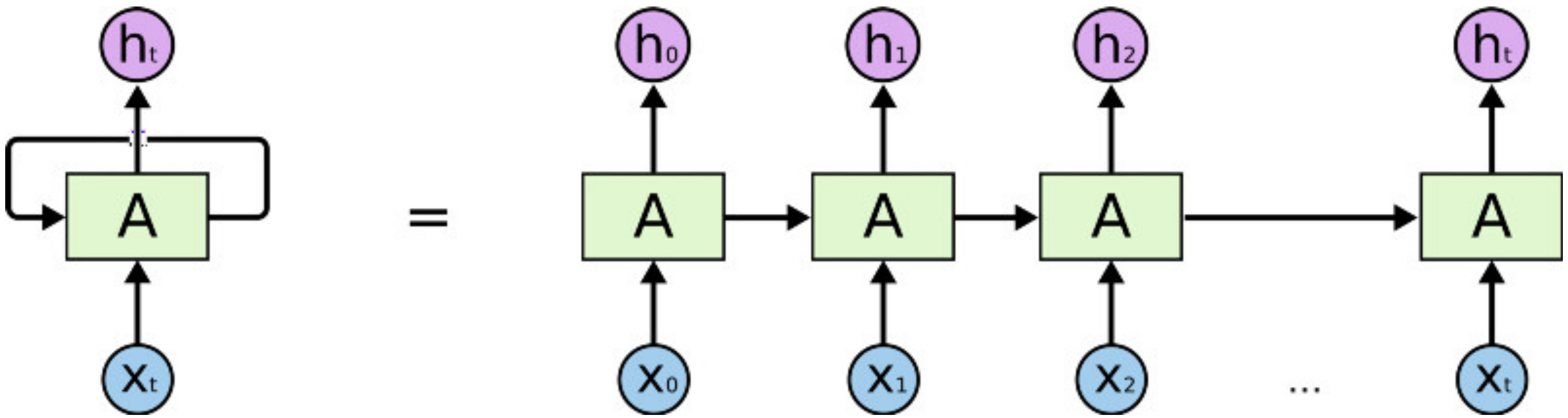
RNN for NLP

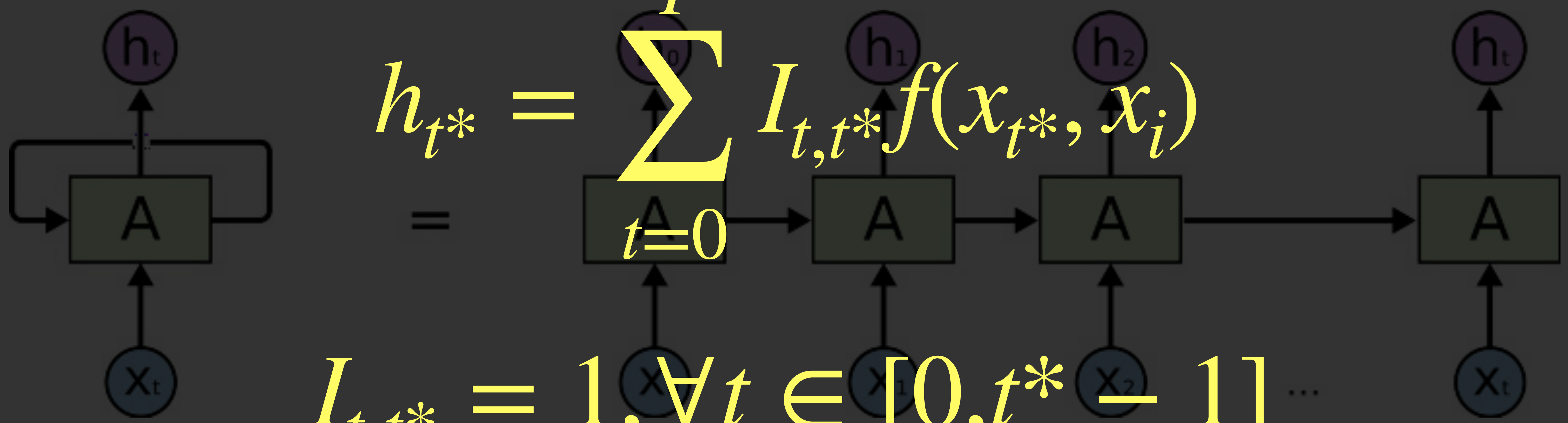
Unfolding **Computational Graphs**



$$h^{(t)} = f(h^{(t-1)}, x^{(t)}; \theta)$$

RNN for NLP

Unfolding **Computational Graphs**



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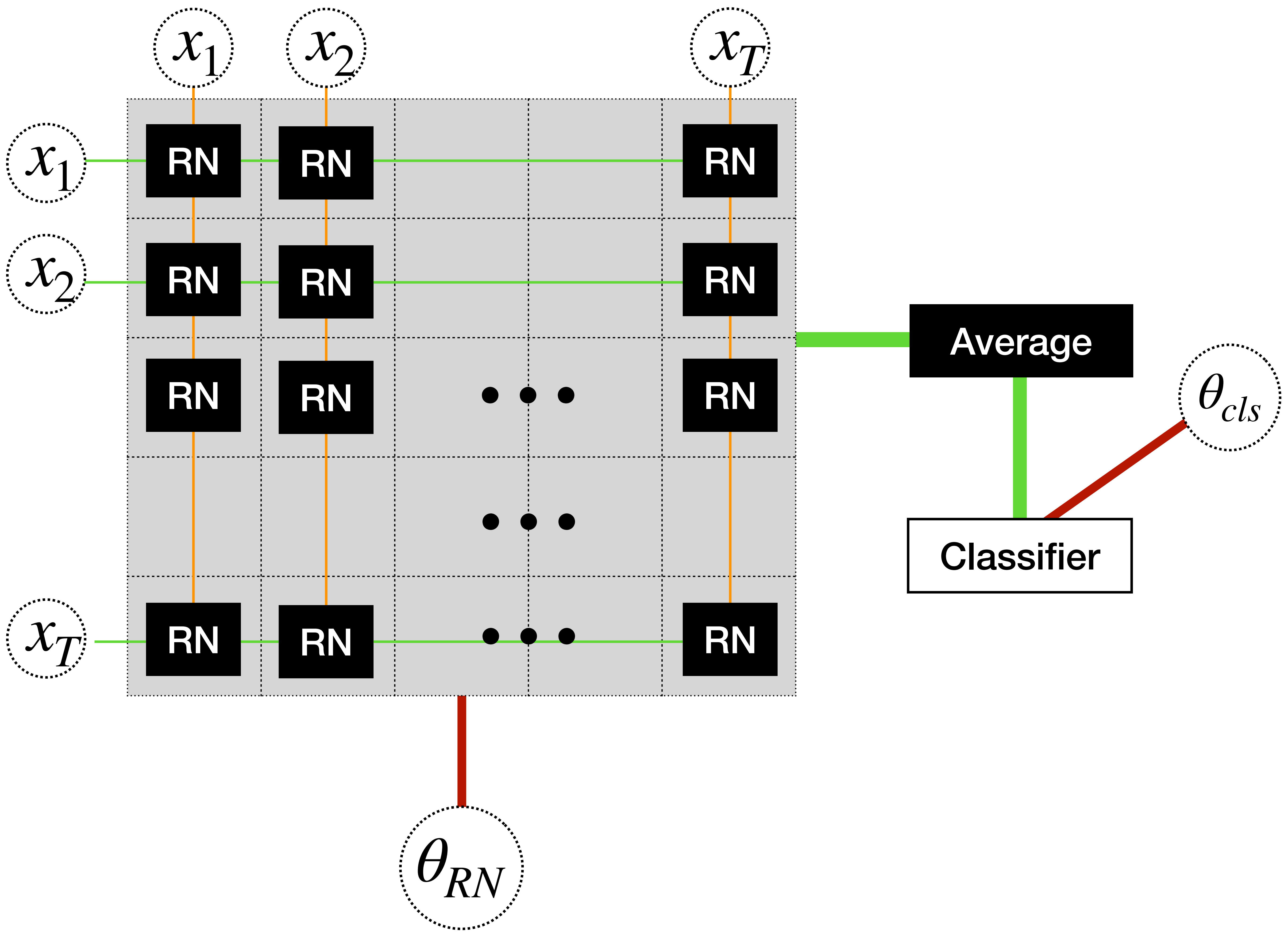
Relation Network (Skip bigram)

To summarize sentence based on pairwise relationship



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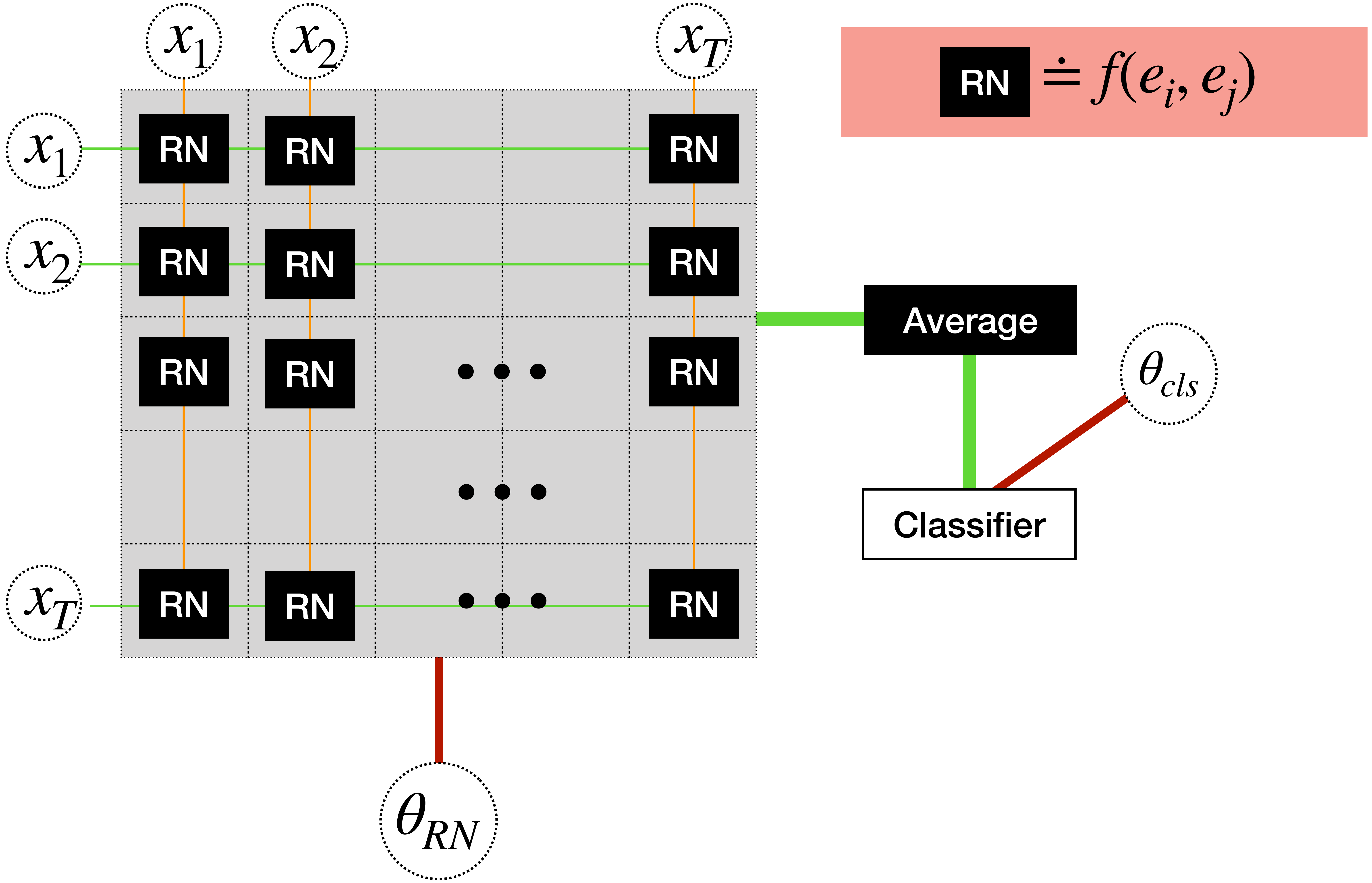

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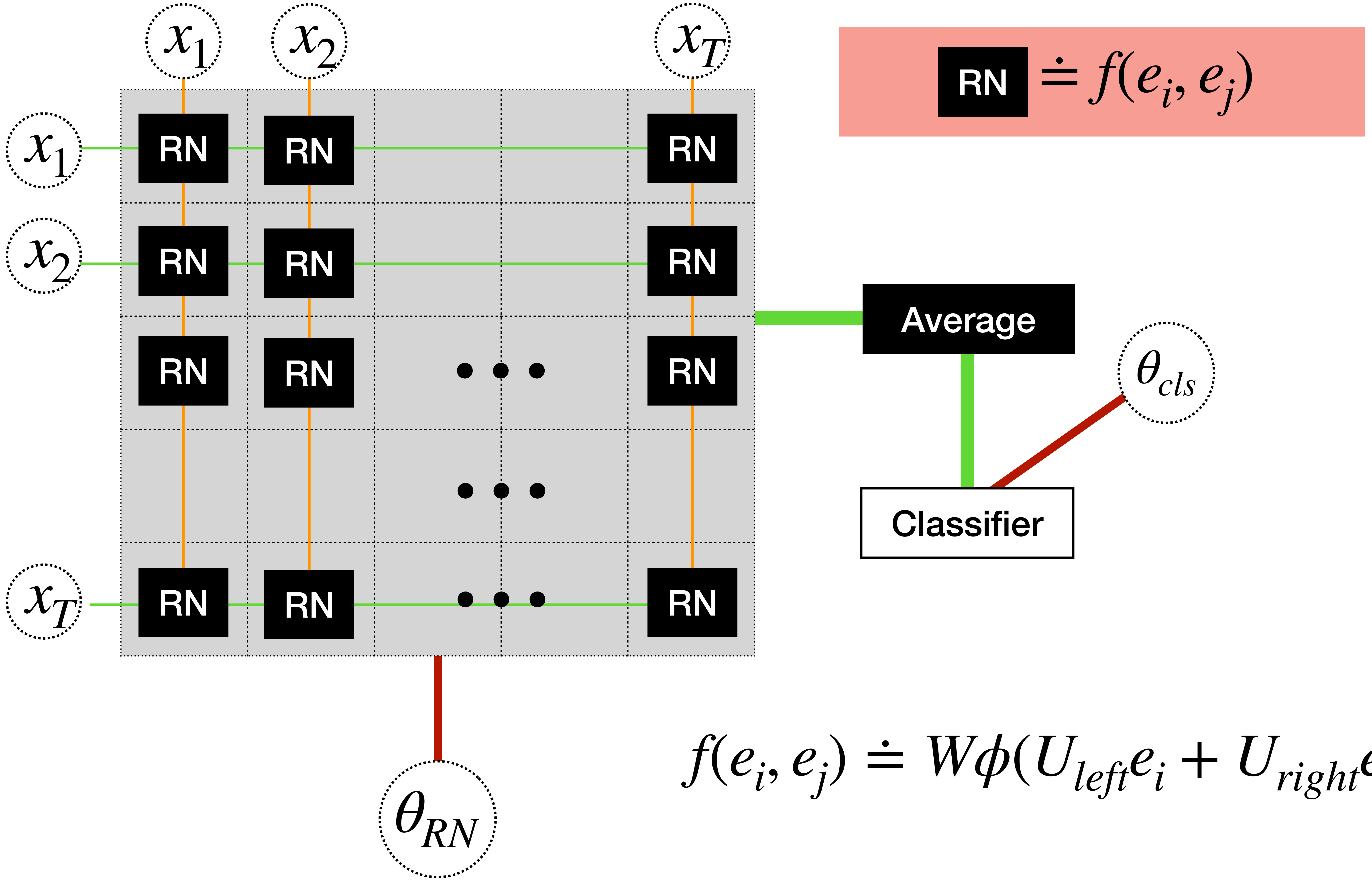
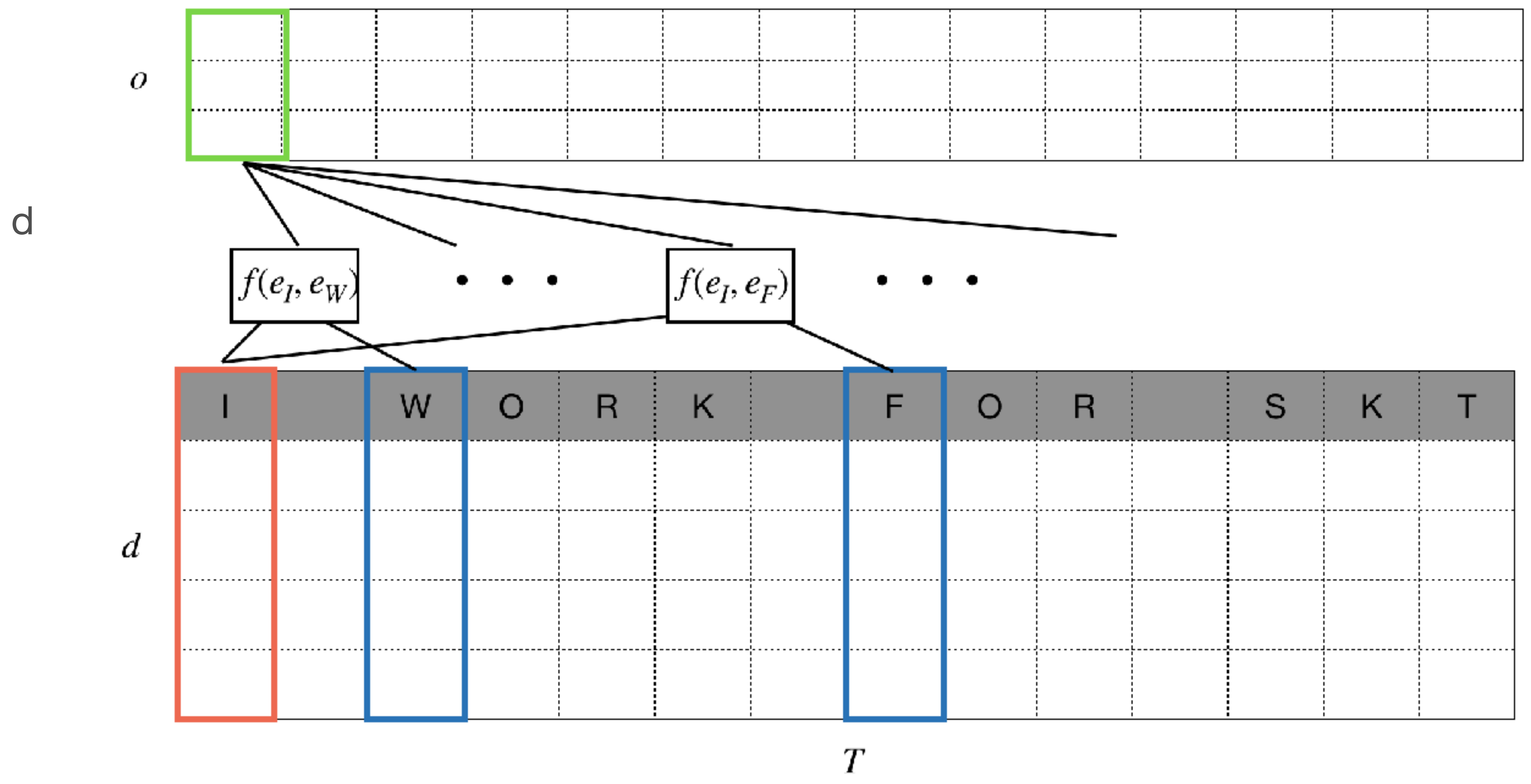


$$f(e_i, e_j) \doteq W\phi(U_{left}e_i + U_{right}e_j)$$

Skip bigram - Relation Net

A pair of words may give us more clear information about the sentence.
ex) ‘like’ in ‘I like’ vs ‘like’ in ‘like this’



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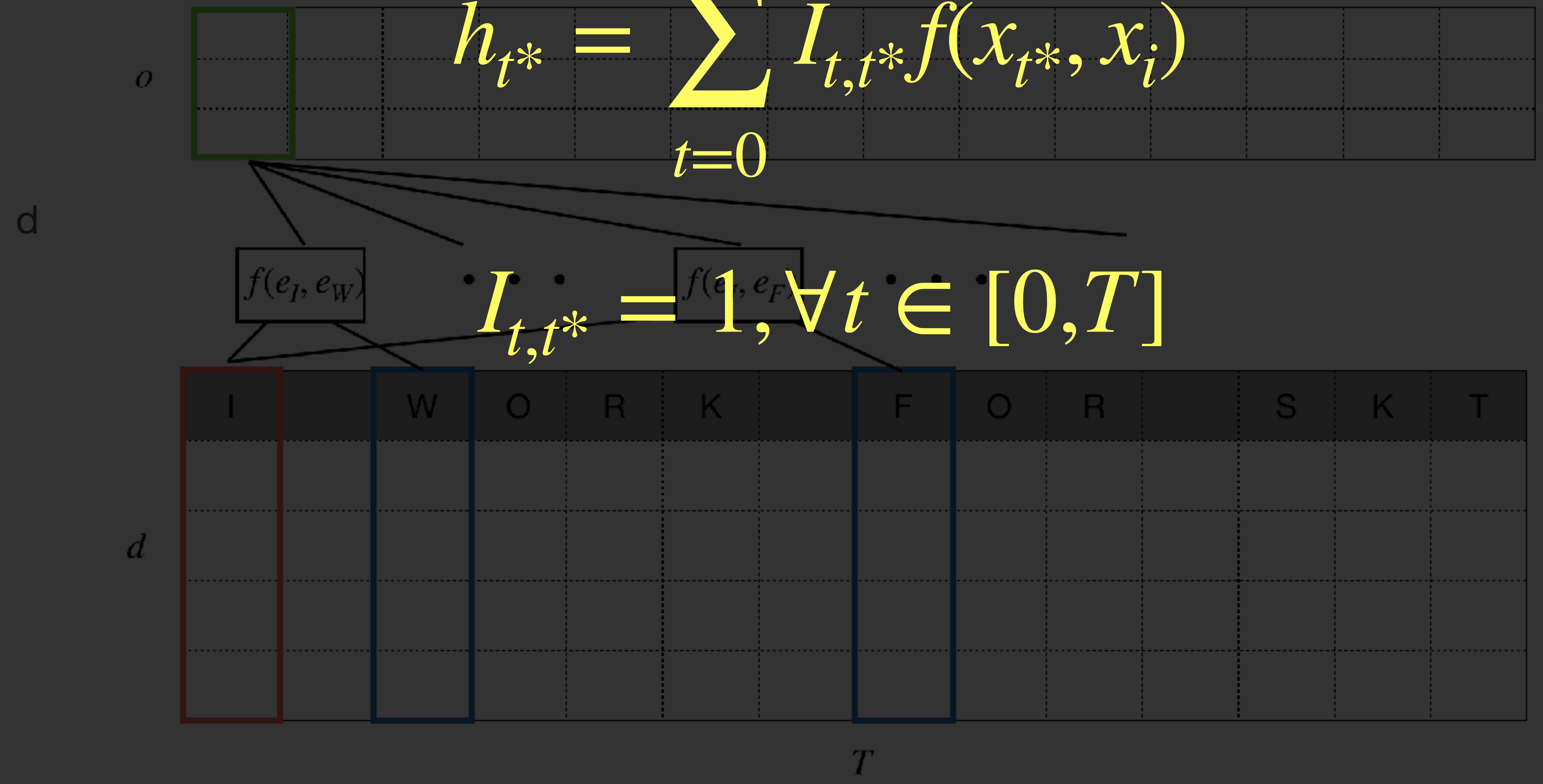
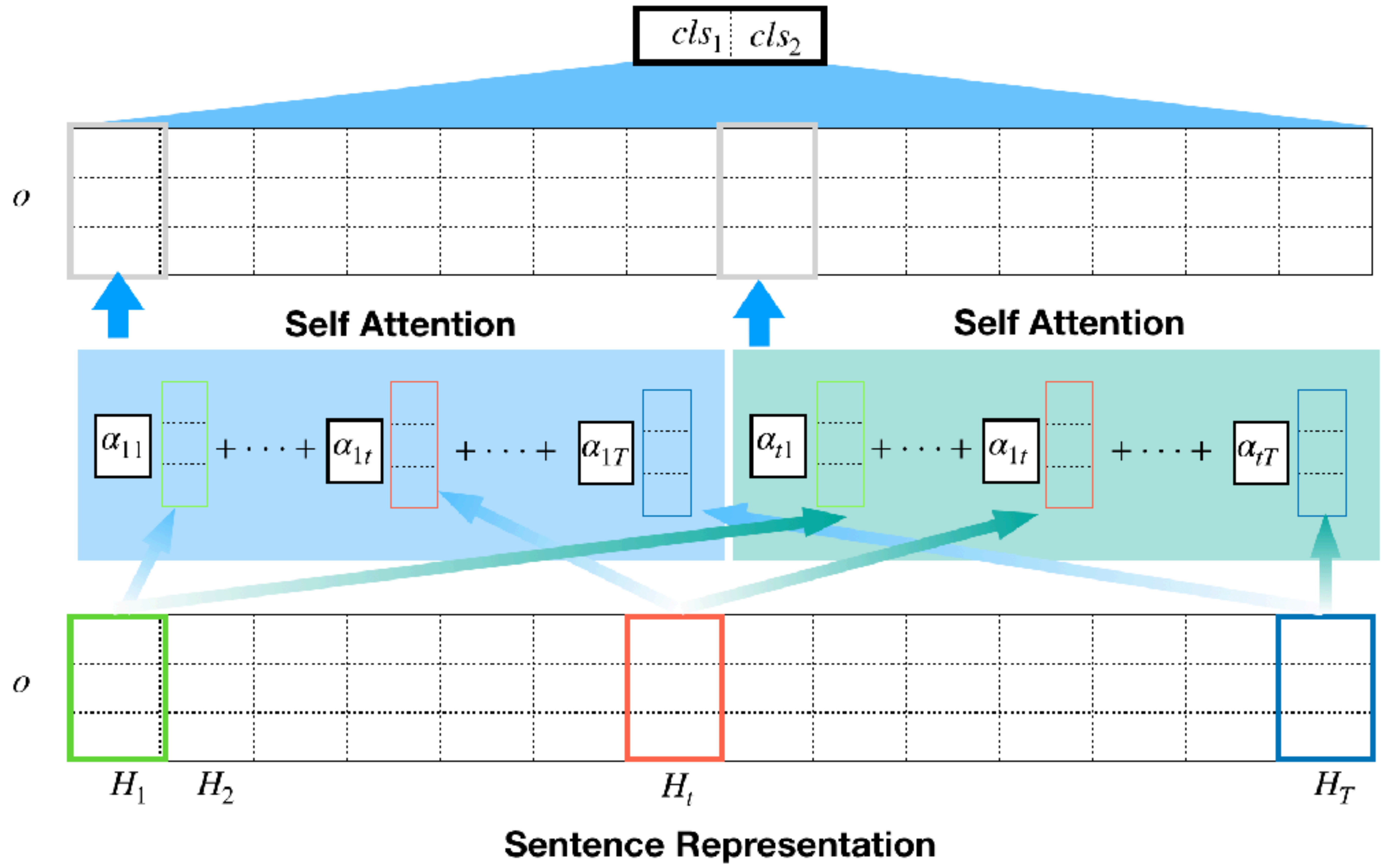


Idea of Self Attention

Why don’t we have more generator function than just indicator?

$$h_{t*} = \sum_{t=0}^{T} g(t, t^*) \cdot f(x_t, x_{t^*})$$

Self - Attention



Self - Attention

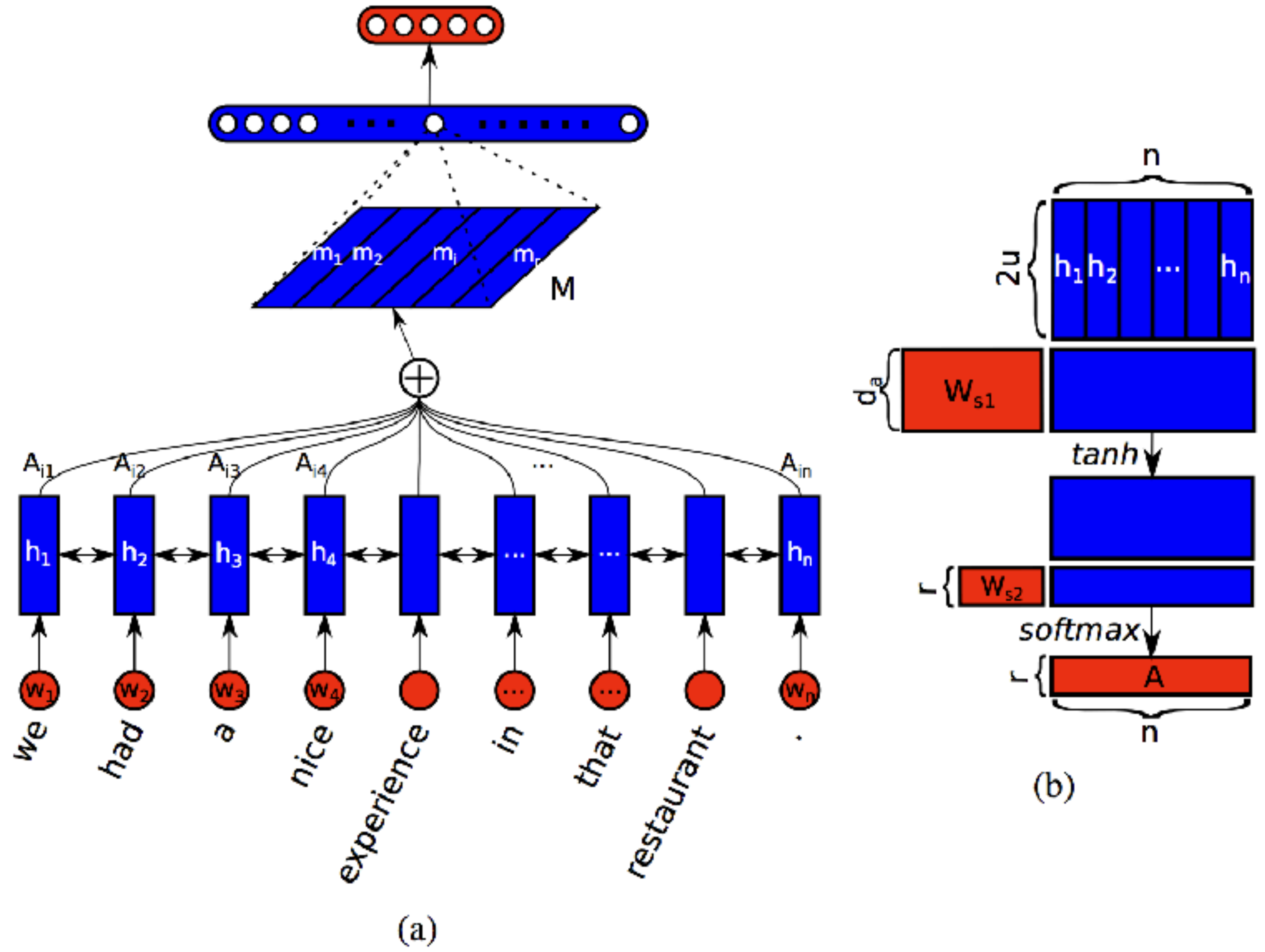


Figure 1: A sample model structure showing the sentence embedding model combined with a fully connected and softmax layer for sentiment analysis (a). The sentence embedding M is computed as multiple weighted sums of hidden states from a bidirectional LSTM ($\mathbf{h_1}, ..., \mathbf{h_n}$), where the summation weights ($A_{i1}, ..., A_{in}$) are computed in a way illustrated in (b). Blue colored shapes stand for hidden representations, and red colored shapes stand for weights, annotations, or input/output.

Transformer

Sorely based on attention-mechanism without underlying RNNs

RNNs are ***slow***, especially for LSTM and ***loose long-term dependency***

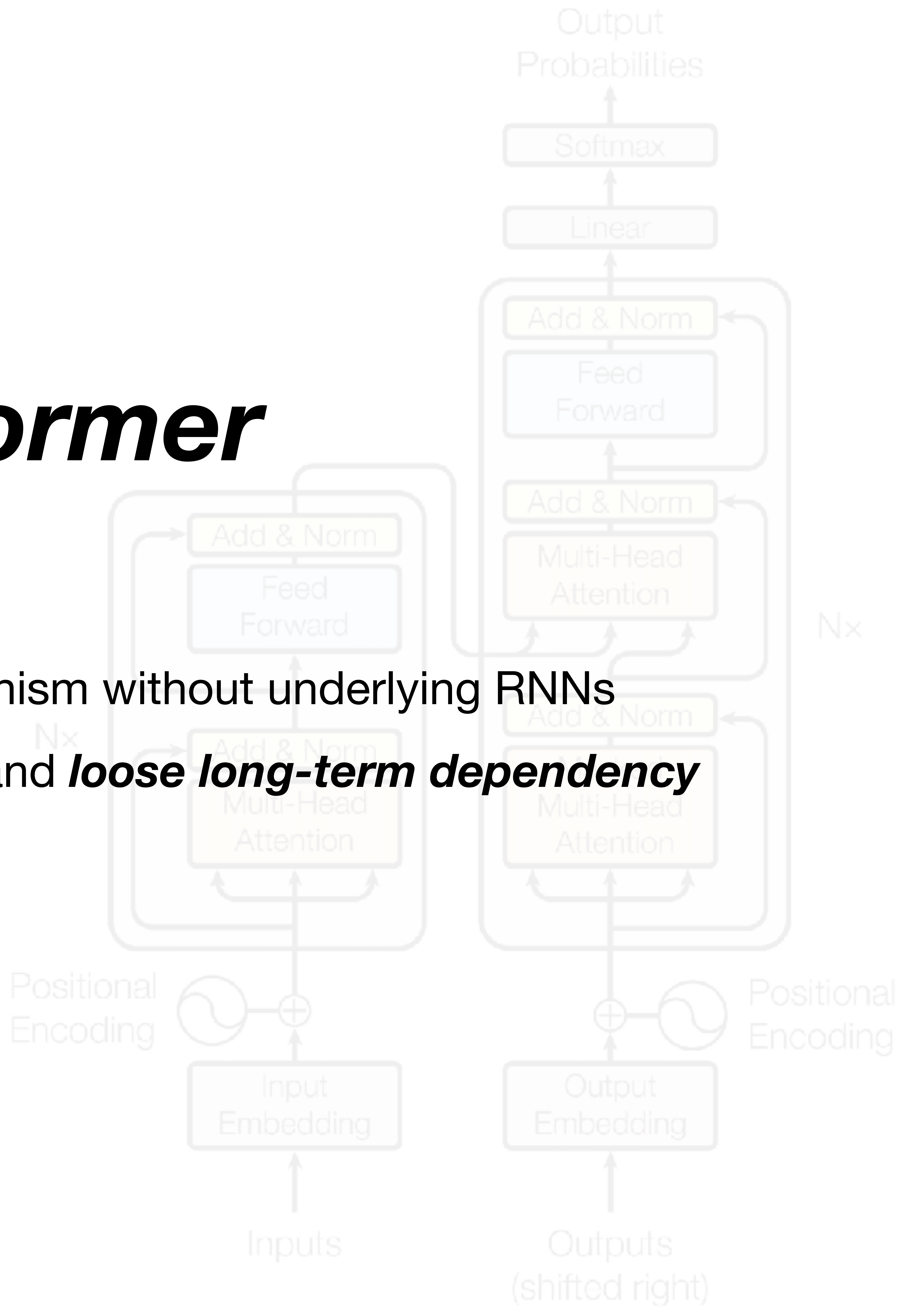


Figure 1: The Transformer - model architecture.

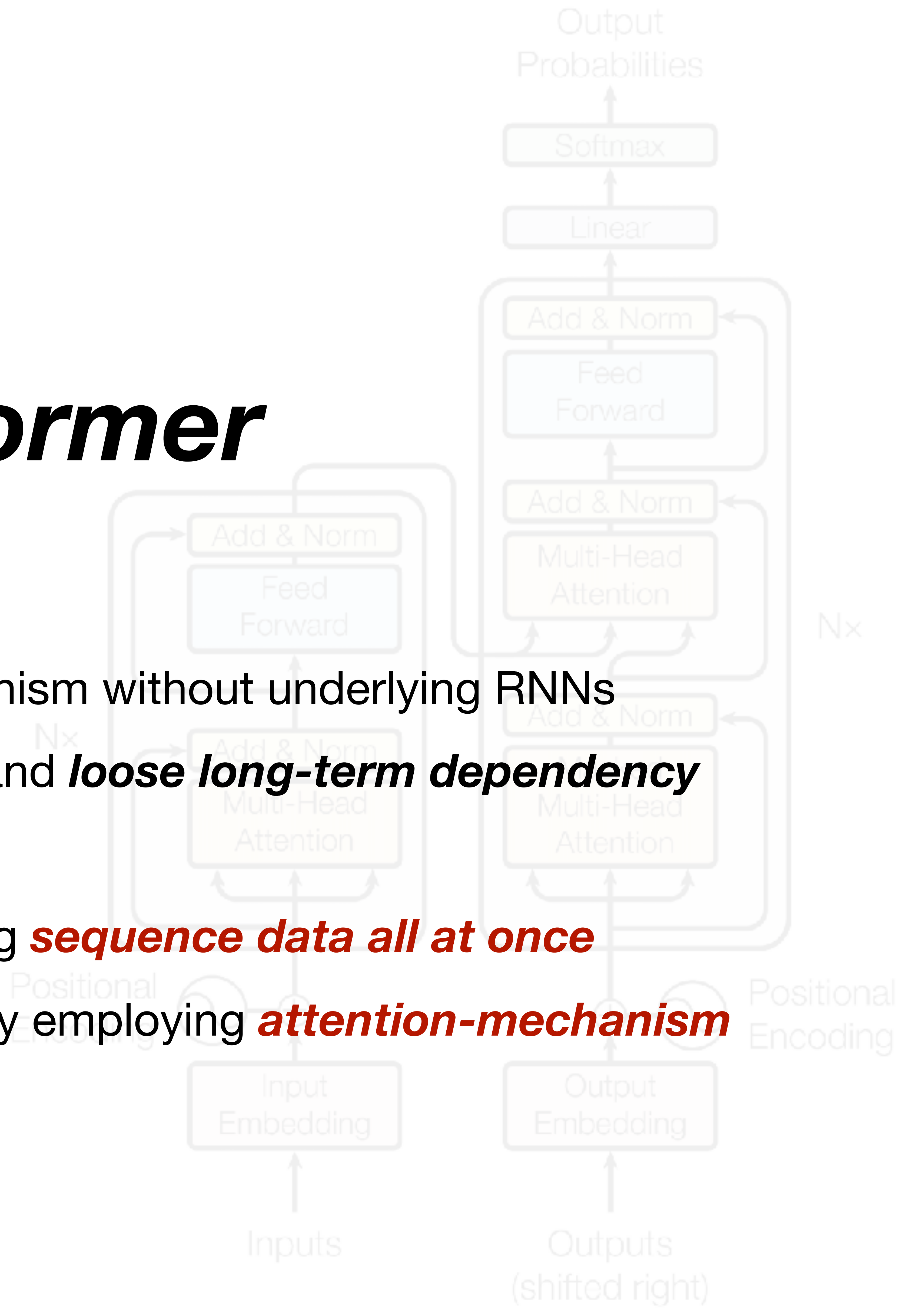
Transformer

Sorely based on attention-mechanism without underlying RNNs

RNNs are ***slow***, especially for LSTM and ***loose long-term dependency***

Much ***faster*** than RNN by putting ***sequence data all at once***

Can capture ***long-term dependency*** by employing ***attention-mechanism***



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Much ***faster*** than RNN by putting ***sequence data all at once***

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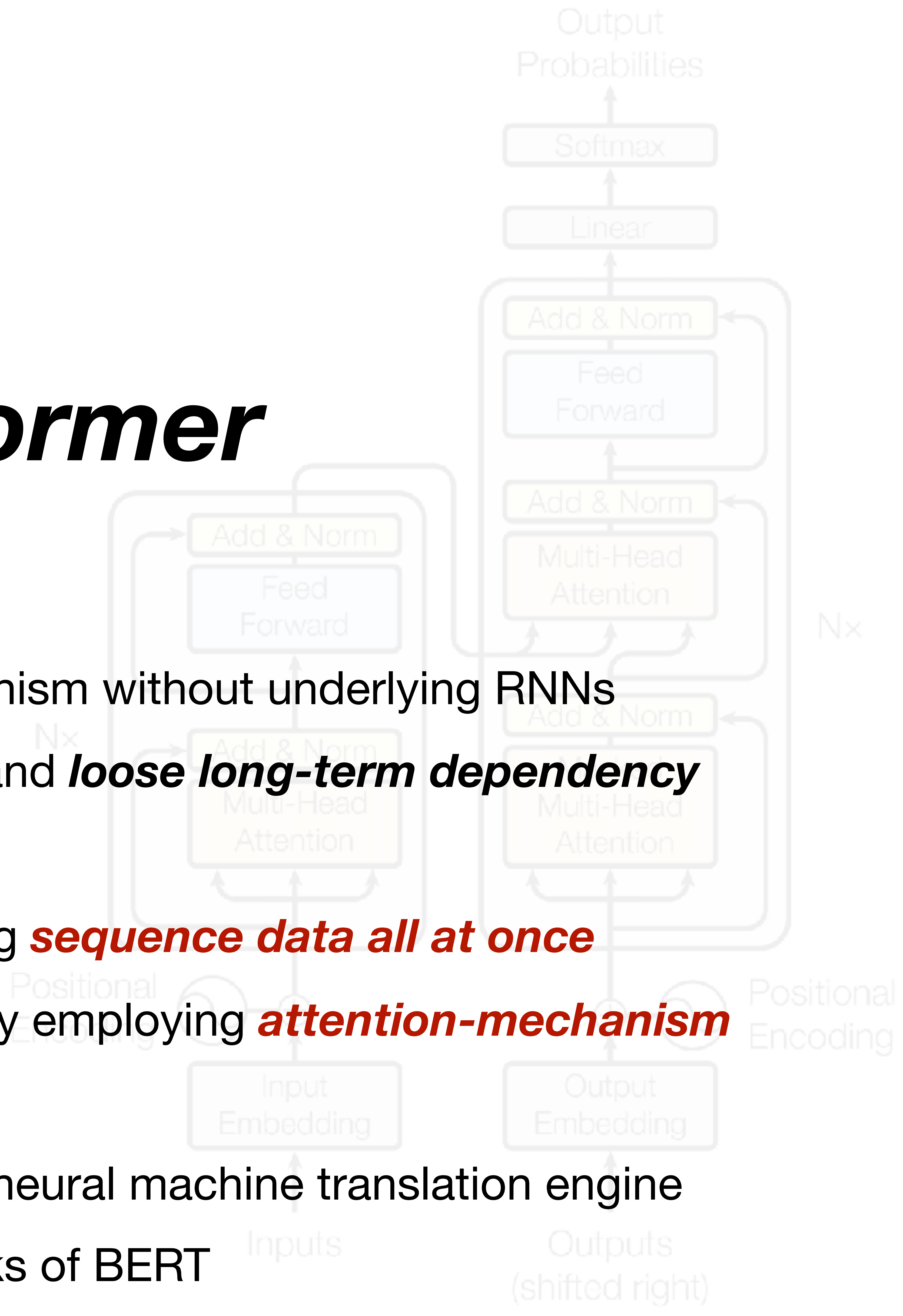
Known as the core engine for STOA neural machine translation engine

Building blocks of BERT



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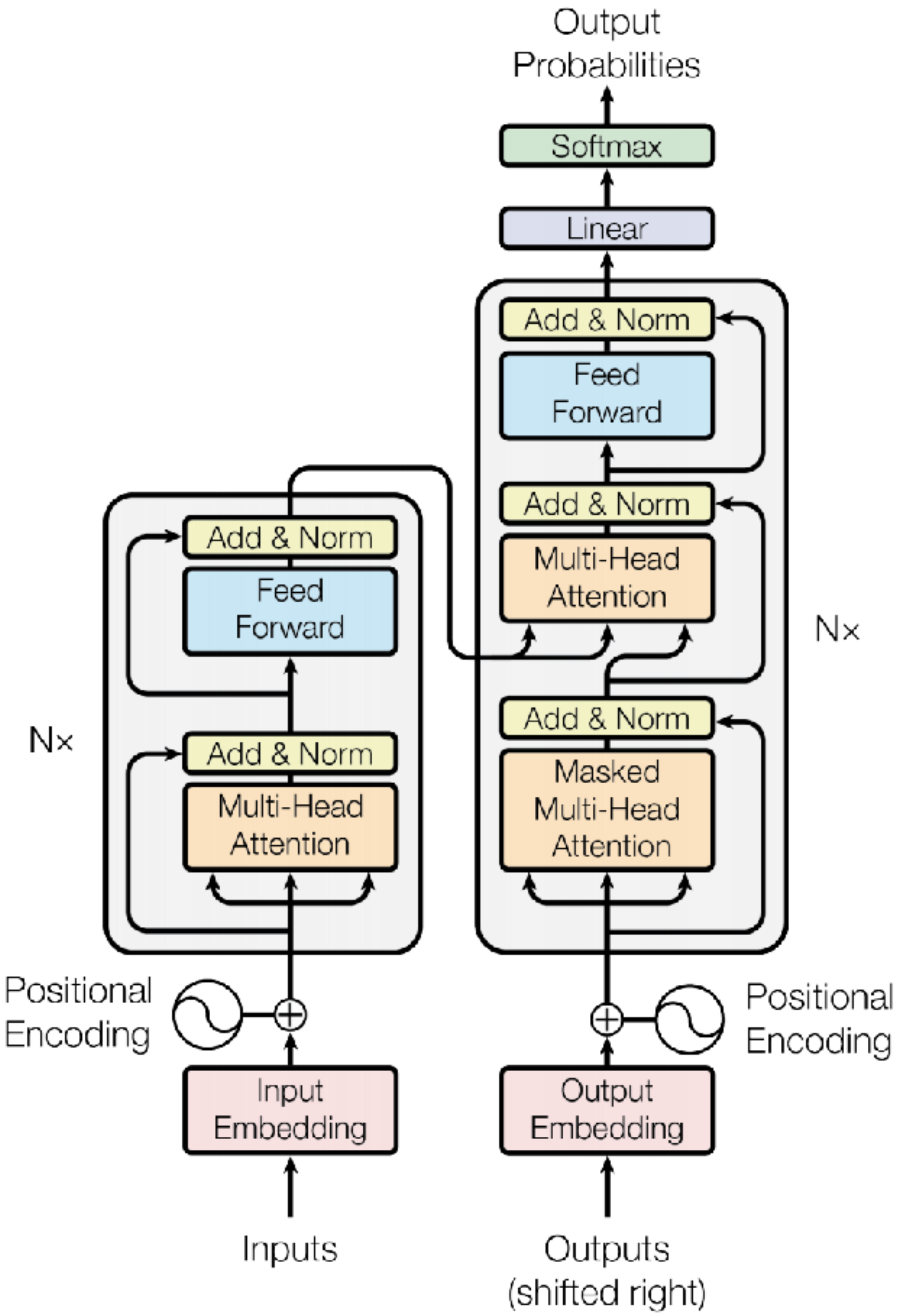
Transformer Architecture



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