Deep Learning Architectures

Introduction to Machine Learning, Day 4

Gage DeZoort

Wintersession 2025 with PICSciE/RC

20 hours of machine learning training

Instructors

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Gage DeZoort, Postdoctoral Research Associate and Lecturer, Physics
Simon Park, Graduate Student, Computer Science and PLI
Abhishek Panigrahi, Graduate Student, Computer Science and PLI
Christian Jespersen, Graduate Student, Astrophysical Sciences
Rafael Pastrana, Graduate Student, Architecture
Quinn Gallagher, Graduate Student, Chemical and Biological Engineering
Holly Johnson, Graduate Student, Electrical and Computer Engineering

Introduction to Machine Learning for Humanists and Social Scientists → **A Hands-On Introduction to Machine Learning** → **Getting Started with LLMs with Princeton Language and Intelligence** / **Graph Neural Networks for Your Research** / **Machine Learning for the Physical Sciences**

Introduction to Machine Learning for Humanists and Social Scientists	Part 1	Mon Jan. 13	10 AM-12 PM
	Part 2	Tue Jan. 14	10 AM-12 PM
A Hands-On Introduction to Machine Learning	Part 1	Wed Jan. 15	2-4 PM
	Part 2	Thu Jan. 16	2-4 PM
	Part 3	Fri Jan. 17	2-4 PM
	Part 4	Tue Jan. 21	2-4 PM
Getting Started with LLMs with Princeton Language and Intelligence / Graph Neural Networks for Your Research / Machine Learning for the Physical Sciences	Part 1	Wed Jan. 22	2-4 PM
	Part 2	Thu Jan. 23	2-4 PM

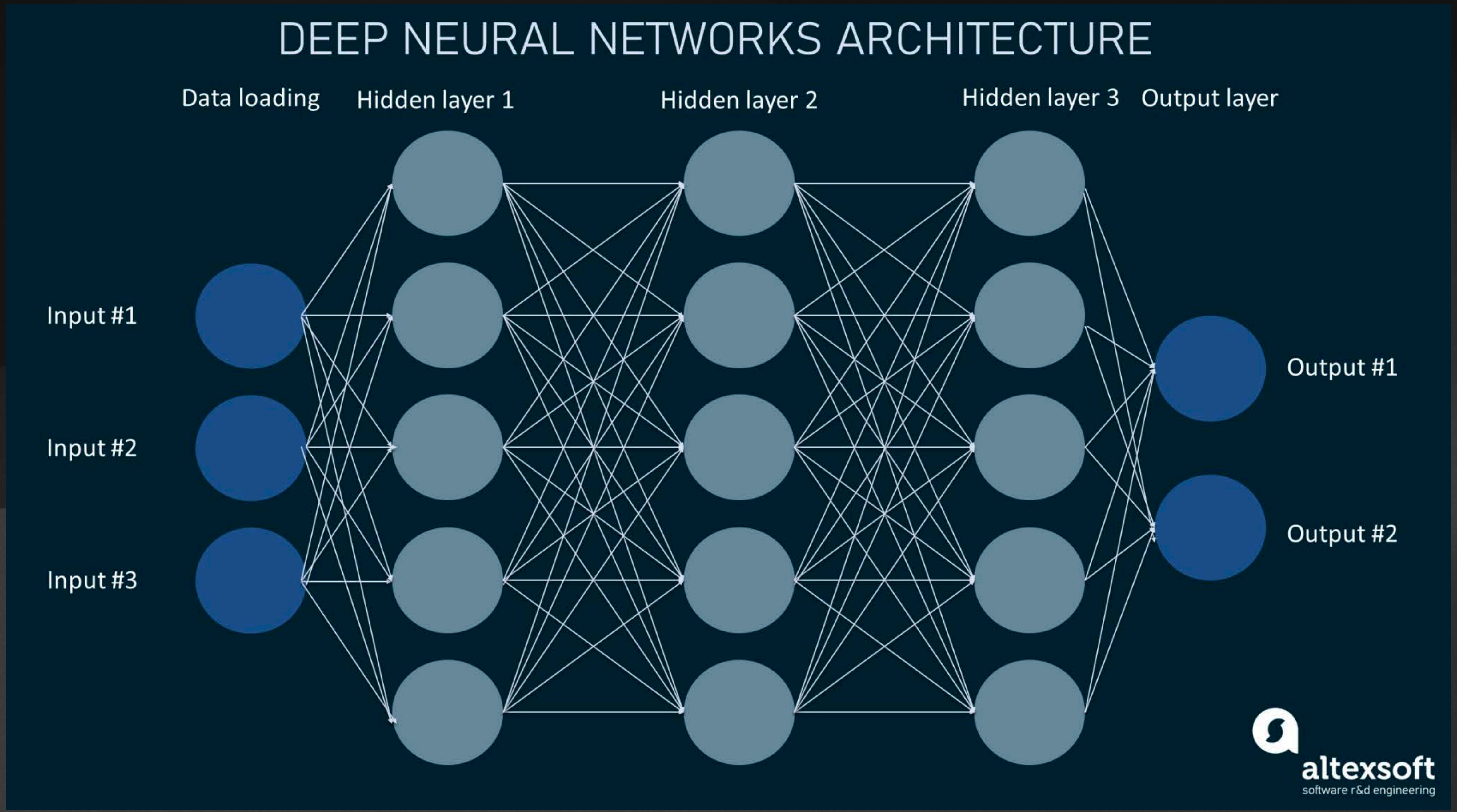
NATURAL & ARTIFICIAL MINDS

CENTER FOR STATISTICS AND MACHINE LEARNING

DataX — Accelerating Scientific Discovery at Princeton

PLi PRINCETON Language + Intelligence

https://researchcomputing.princeton.edu/workshops



- Forward pass:

$$z_i^{(\ell+1)} = \sum_{i=1}^{n_\ell} W_{ij}^{(\ell+1)} \sigma(z_j^{(\ell)}) + b_i^{(\ell+1)}$$

- Backward pass:

$$W_{ij}^{(\ell+1)} = W_{ij}^{(\ell)} - \gamma \frac{\partial L}{\partial W_{ij}}\Big|_{W_{ij}^{(\ell)}}$$

$$b_i^{(\ell+1)} = b_i^{(\ell)} - \gamma \frac{\partial L}{\partial b_i}\Big|_{b_i^{(\ell)}}$$

```python
class NeuralNetwork(nn.Module):
    def __init__(self):
        super().__init__()
        self.flatten = nn.Flatten()
        self.linear_relu_stack = nn.Sequential(
            nn.Linear(28*28, 512),
            nn.ReLU(),
            nn.Linear(512, 512),
            nn.ReLU(),
            nn.Linear(512, 10),
        )

    def forward(self, x):
        x = self.flatten(x)
        logits = self.linear_relu_stack(x)
        return logits
```

```python
def train_one_epoch(epoch_index, tb_writer):
    running_loss = 0.
    last_loss = 0.

    # Here, we use enumerate(training_loader) instead of
    # iter(training_loader) so that we can track the batch
    # index and do some intra-epoch reporting
    for i, data in enumerate(training_loader):
        # Every data instance is an input + label pair
        inputs, labels = data

        # Zero your gradients for every batch!
        optimizer.zero_grad()

        # Make predictions for this batch
        outputs = model(inputs)

        # Compute the loss and its gradients
        loss = loss_fn(outputs, labels)
        loss.backward()

        # Adjust learning weights
        optimizer.step()

        # Gather data and report
        running_loss += loss.item()
        if i % 1000 == 999:
            last_loss = running_loss / 1000 # loss per batch
            print('  batch {} loss: {}'.format(i + 1, last_loss))
            tb_x = epoch_index * len(training_loader) + i + 1
            tb_writer.add_scalar('Loss/train', last_loss, tb_x)
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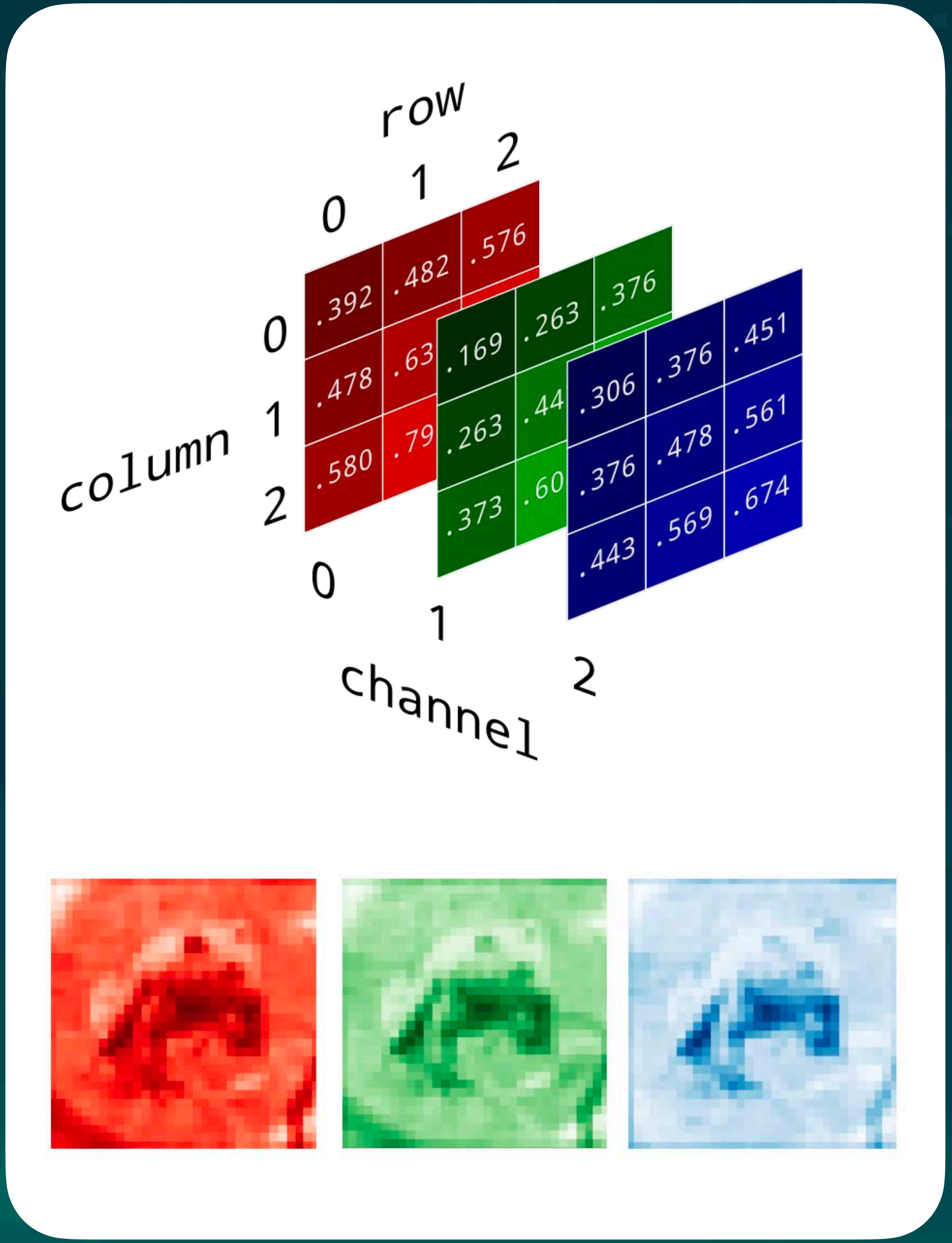
Beyond Simple DNNs

Survey of Deep Learning Architectures

- Deep NN (DNN) $\leftrightarrow$ Feed-Forward NN (FFNN) $\leftrightarrow$ Fully-Connected NN (FCNN)
- Many other architectures exist:
    - Recurrent NNs (RNNs): process sequential data
    - Convolutional NNs (CNNs): process data on a grid
    - Graph Neural Networks (GNNs): process data on a graph / attention
    - Generative Models: produce new data
    - … and more!

Convolutional Neural Networks (CNNs)

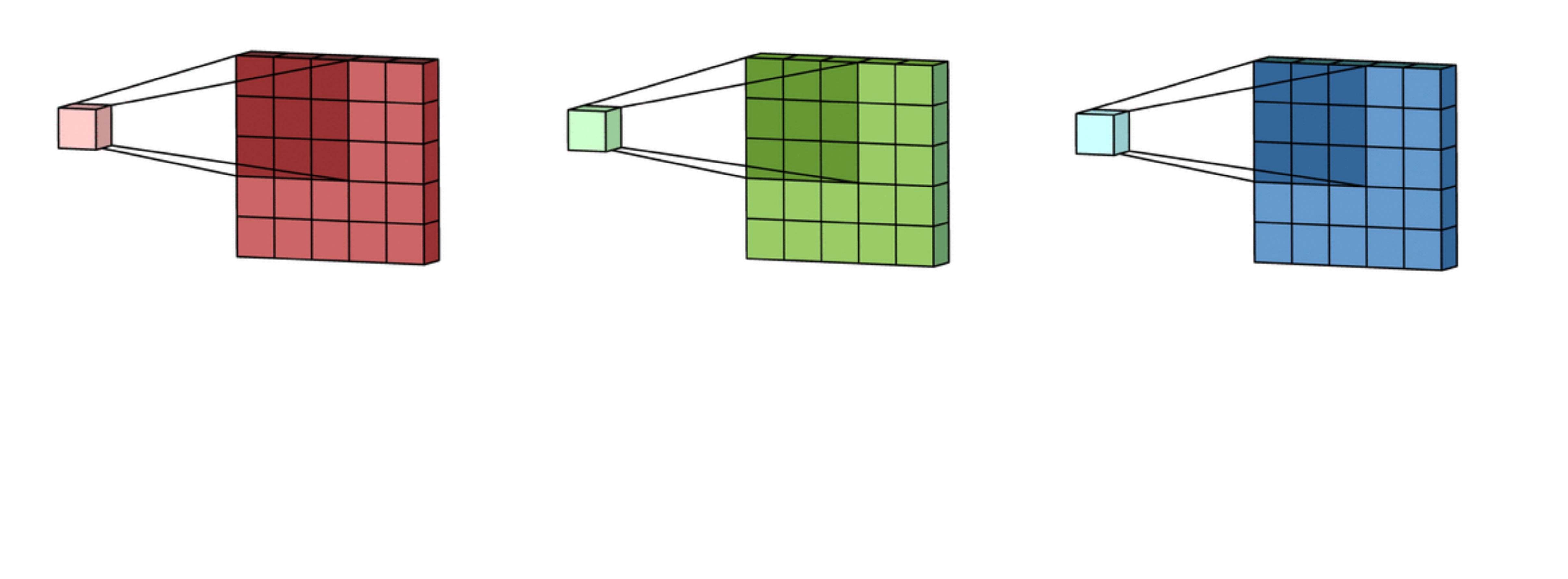
- Deep learning applied to images (data on a grid)
  - For square images, inputs are $I \in \mathbb{R}^{n_{\text{pixels}} \times n_{\text{pixels}} \times n_{\text{features}}}$

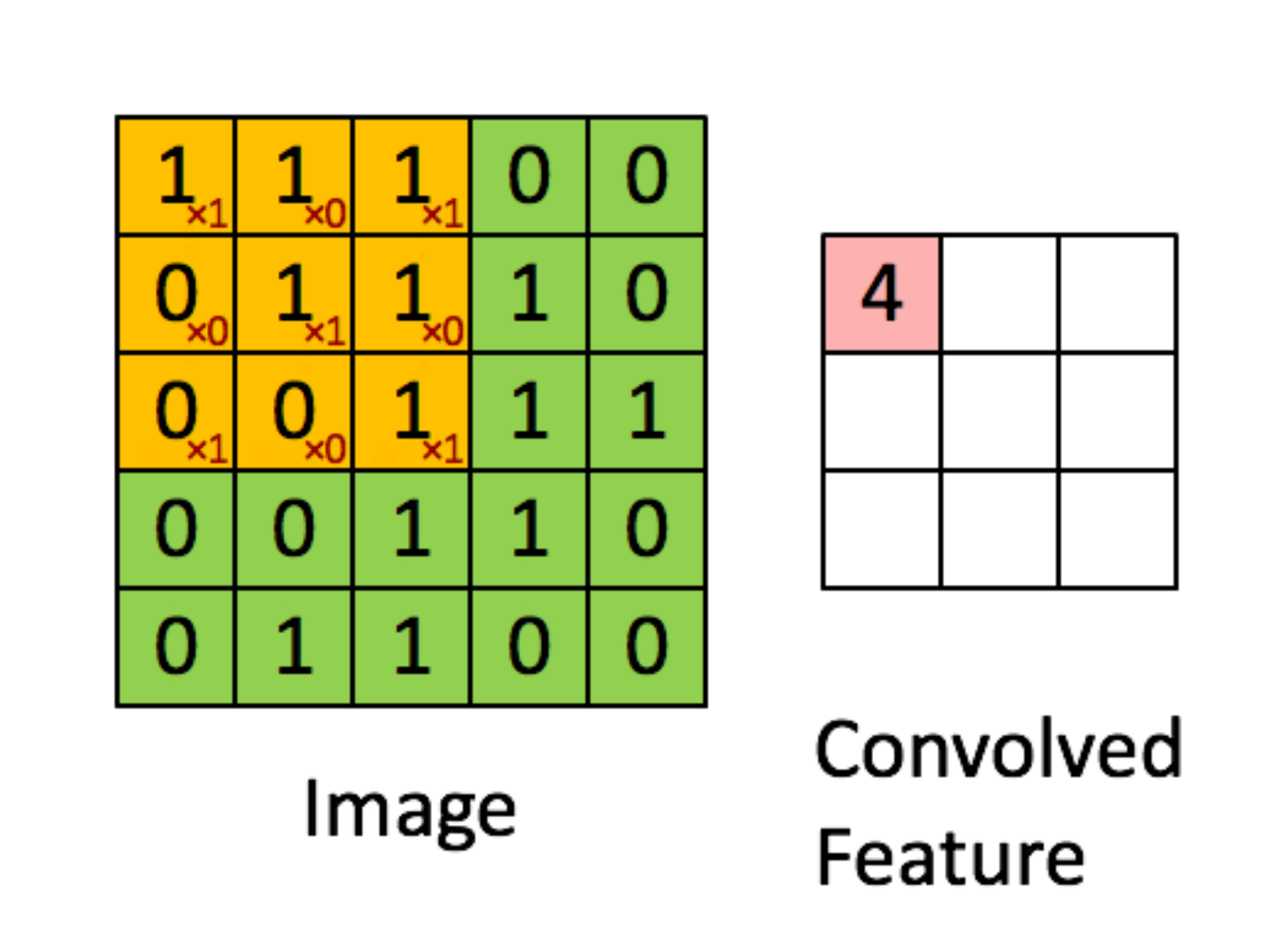


https://ai.plainenglish.io/complete-guide-image-classification-on-cifar-10-chapter-i-multiclass-logistic-regression-525daee0775b

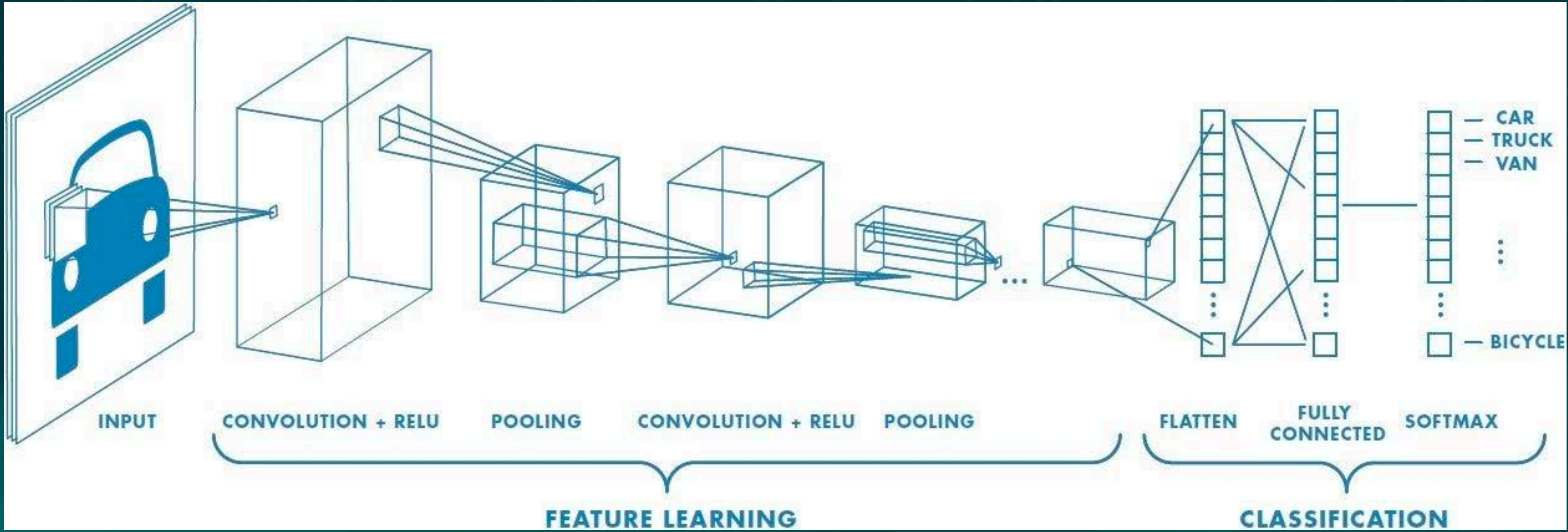
Convolutional Neural Networks (CNNs)

- Very similar approach to DNNs (non-sequential inputs, feed-forward approach), except now we use *convolutional* layers
  - Convolution: filter is *convolved* (weighted sum with learnable weights) with the input image
  - Again, parameter sharing!



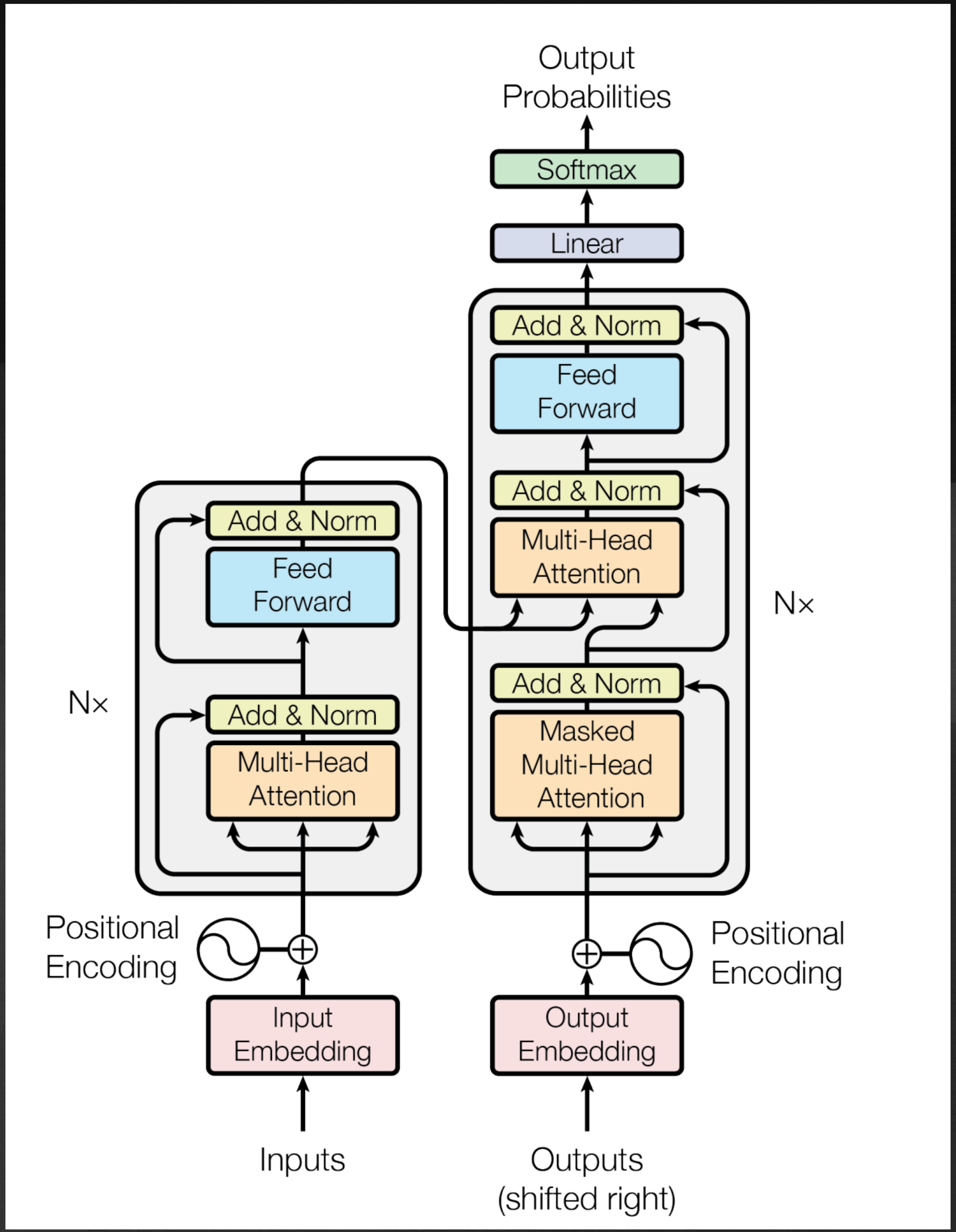


Convolutional Neural Networks (CNNs)



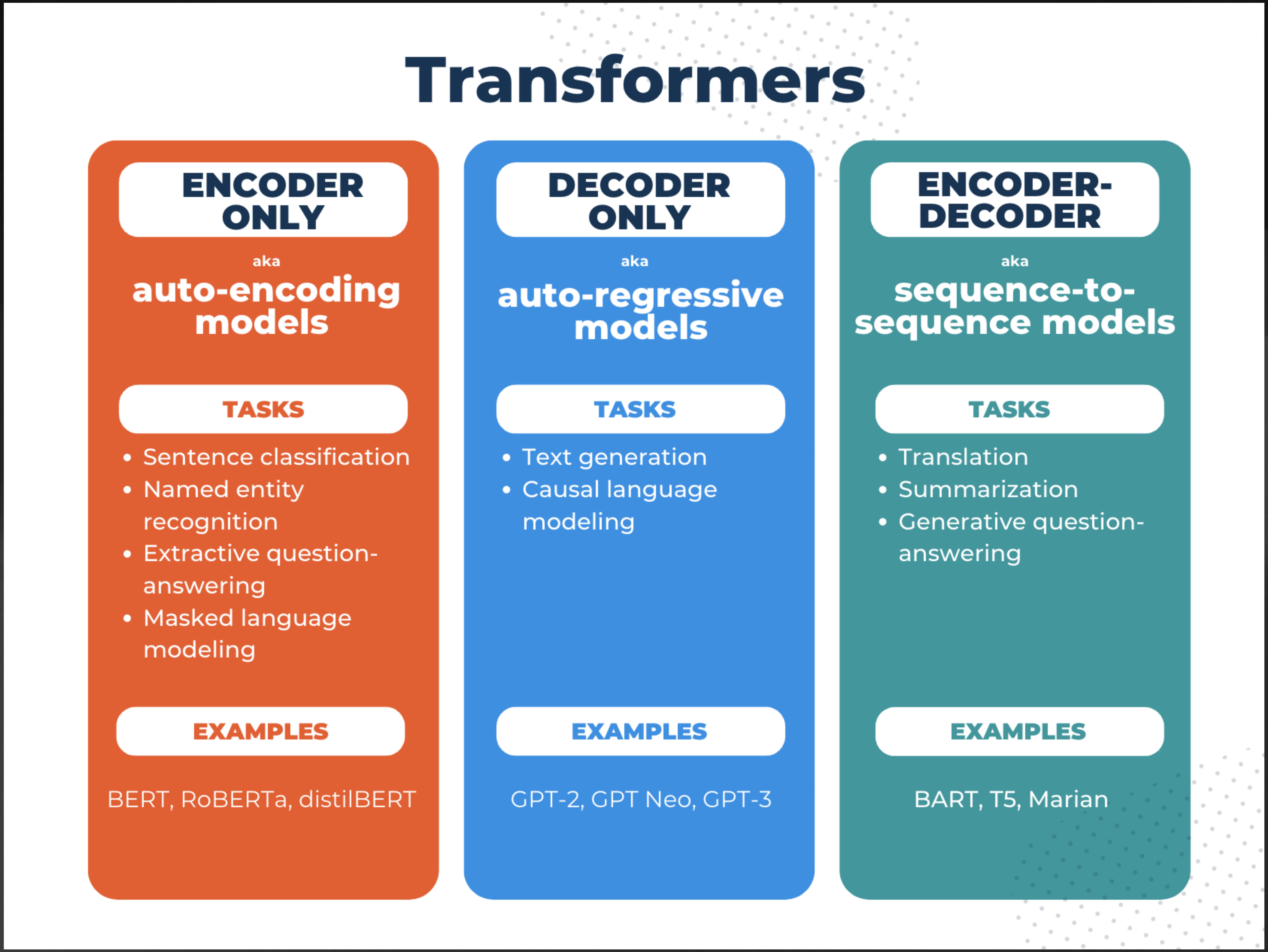
https://miro.medium.com/v2/resize:fit:1358/1*vkQ0hXDaQv57sALXAJquxA.jpeg

Transformers



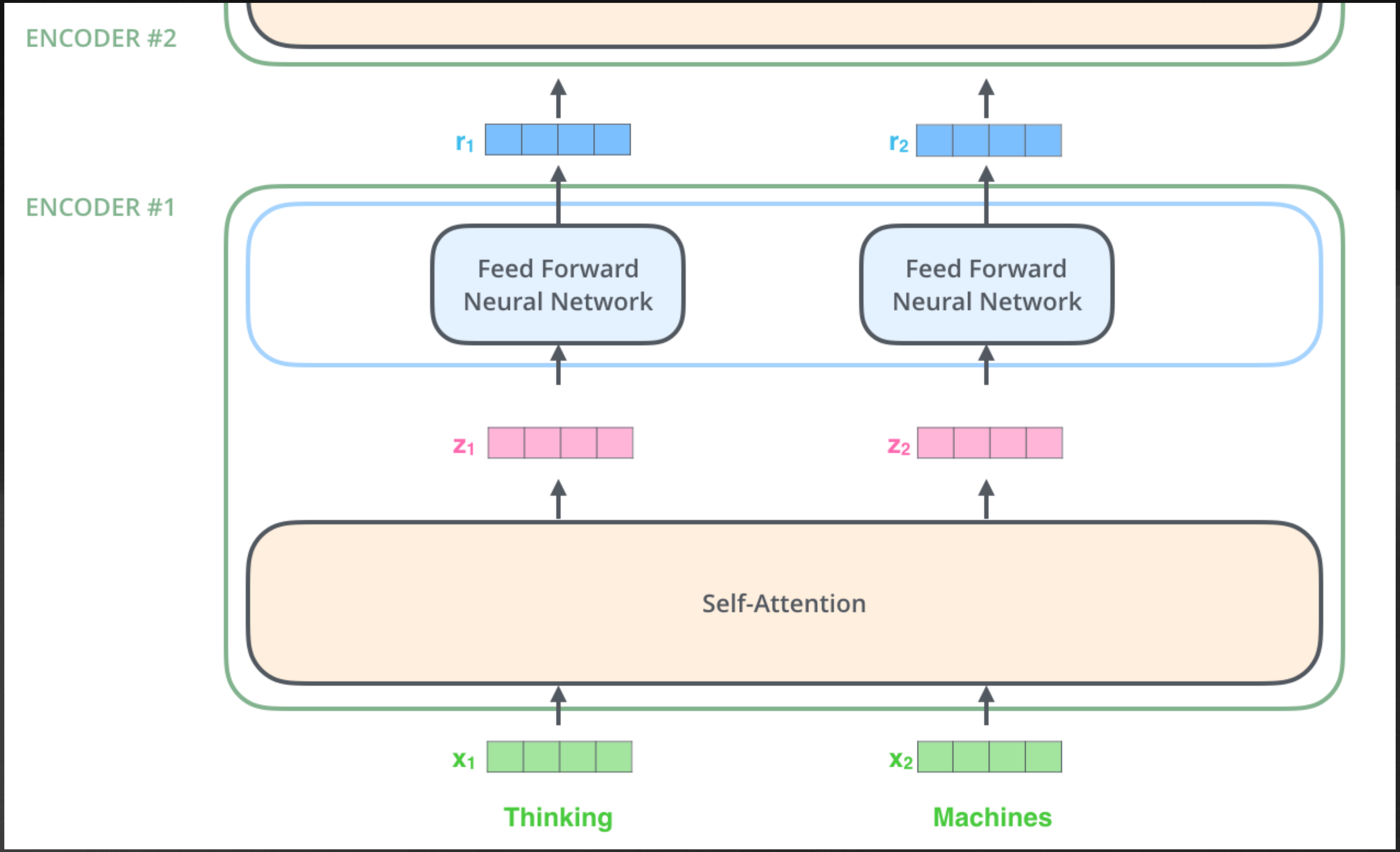
Attention is All You Need (Google, 2017)
https://arxiv.org/pdf/1706.03762

Transformers



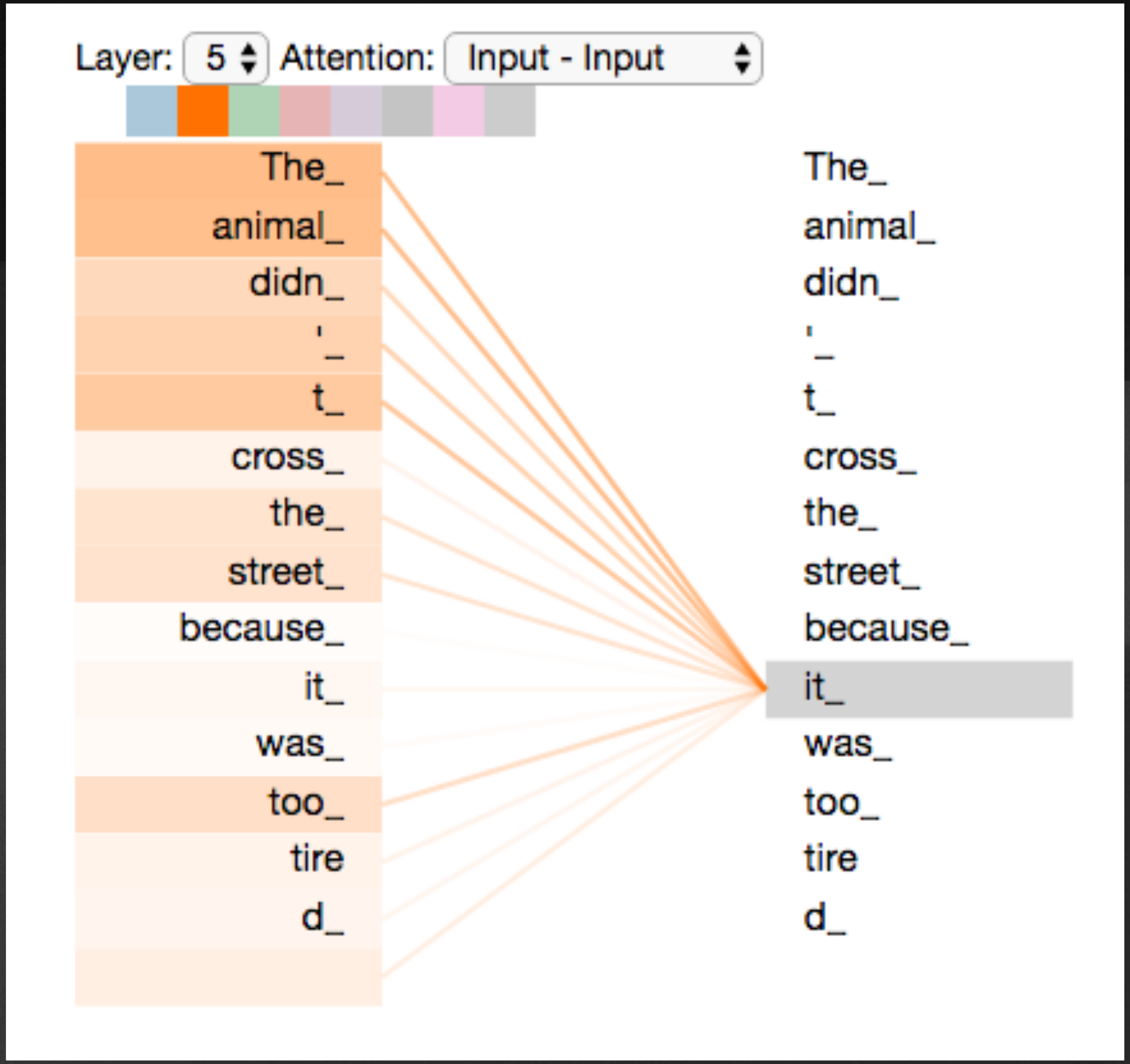
https://www.comet.com/site/blog/explainable-ai-for-transformers/

Transformers



https://jalammar.github.io/illustrated-transformer/

Transformers



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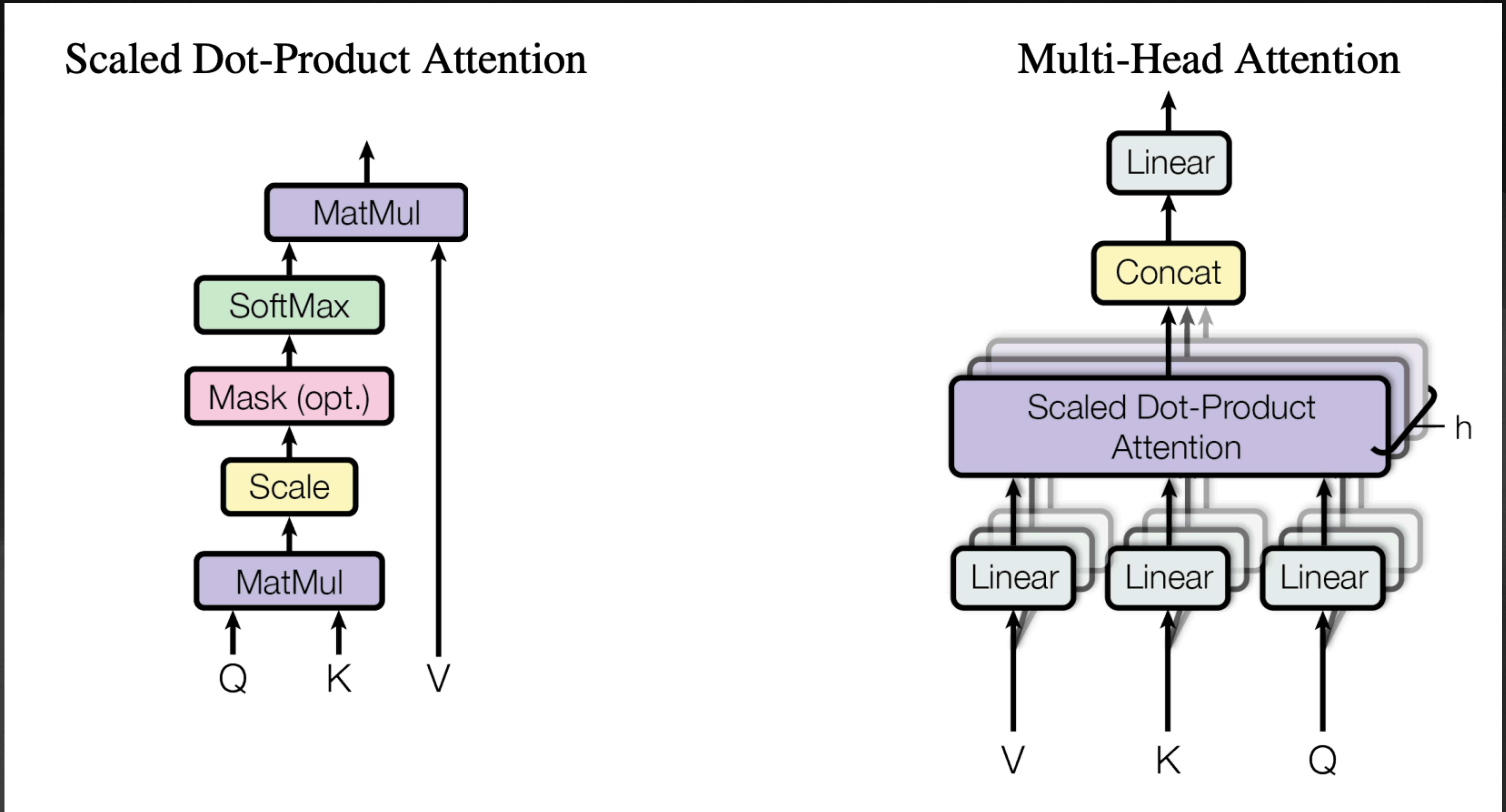
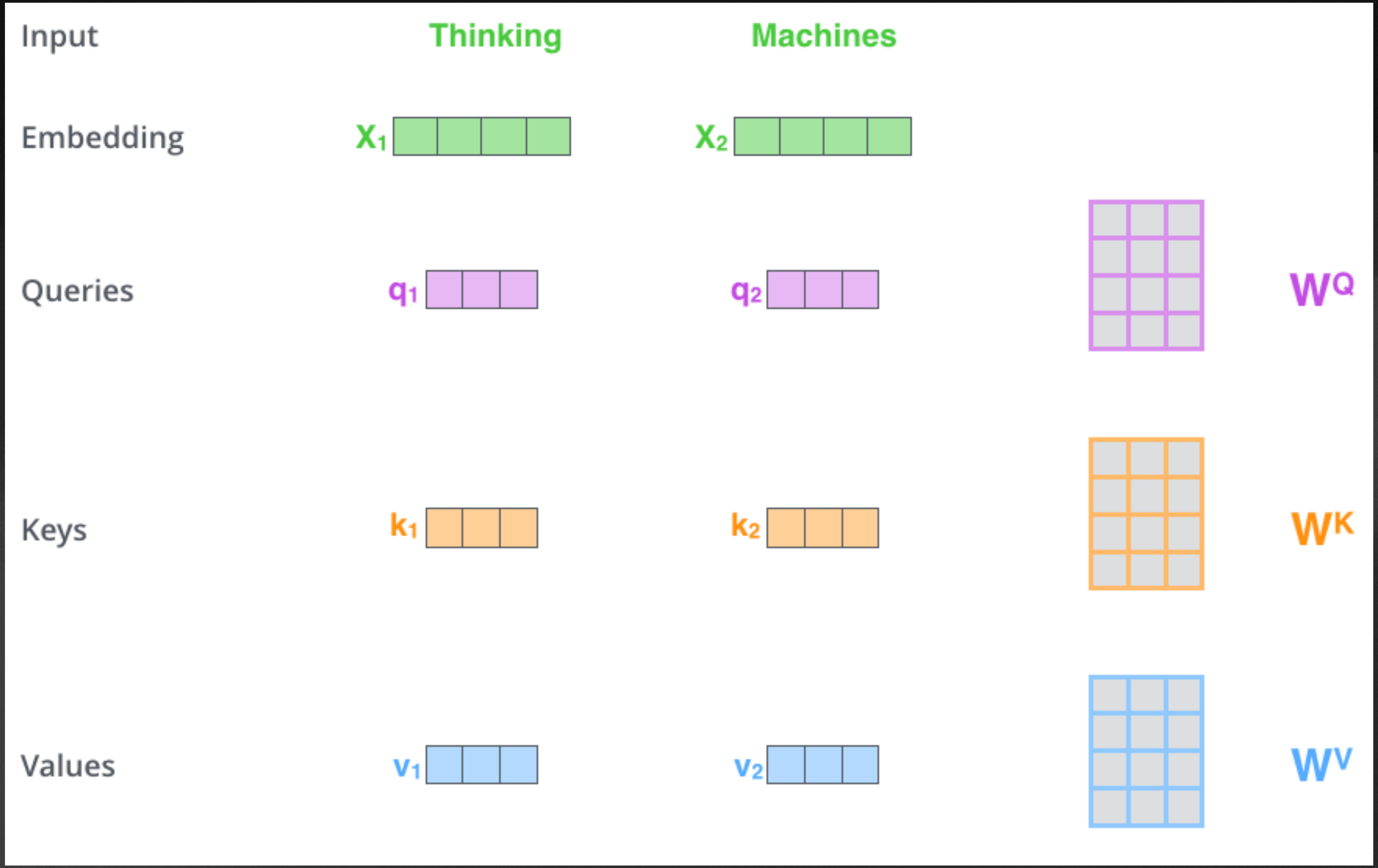


$$\mathrm{Attention}(Q, K, V) = \mathrm{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$$

$$\mathrm{MultiHead}(Q, K, V) = \mathrm{Concat}(\mathrm{head_1}, ..., \mathrm{head_h})W^O$$
$$\text{where } \mathrm{head_i} = \mathrm{Attention}(QW_i^Q, KW_i^K, VW_i^V)$$

Attention is All You Need
https://arxiv.org/pdf/1706.03762

Transformers



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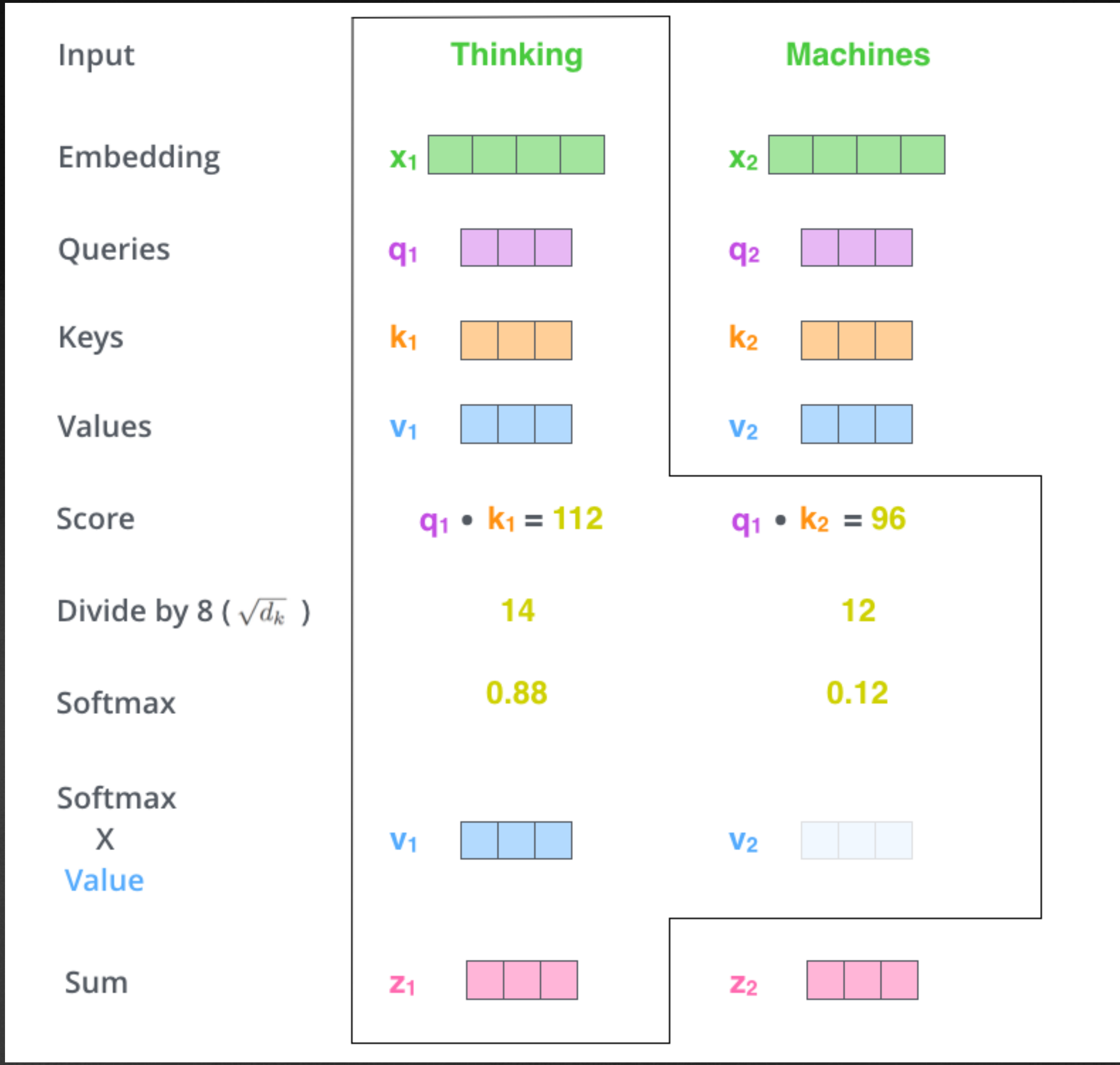

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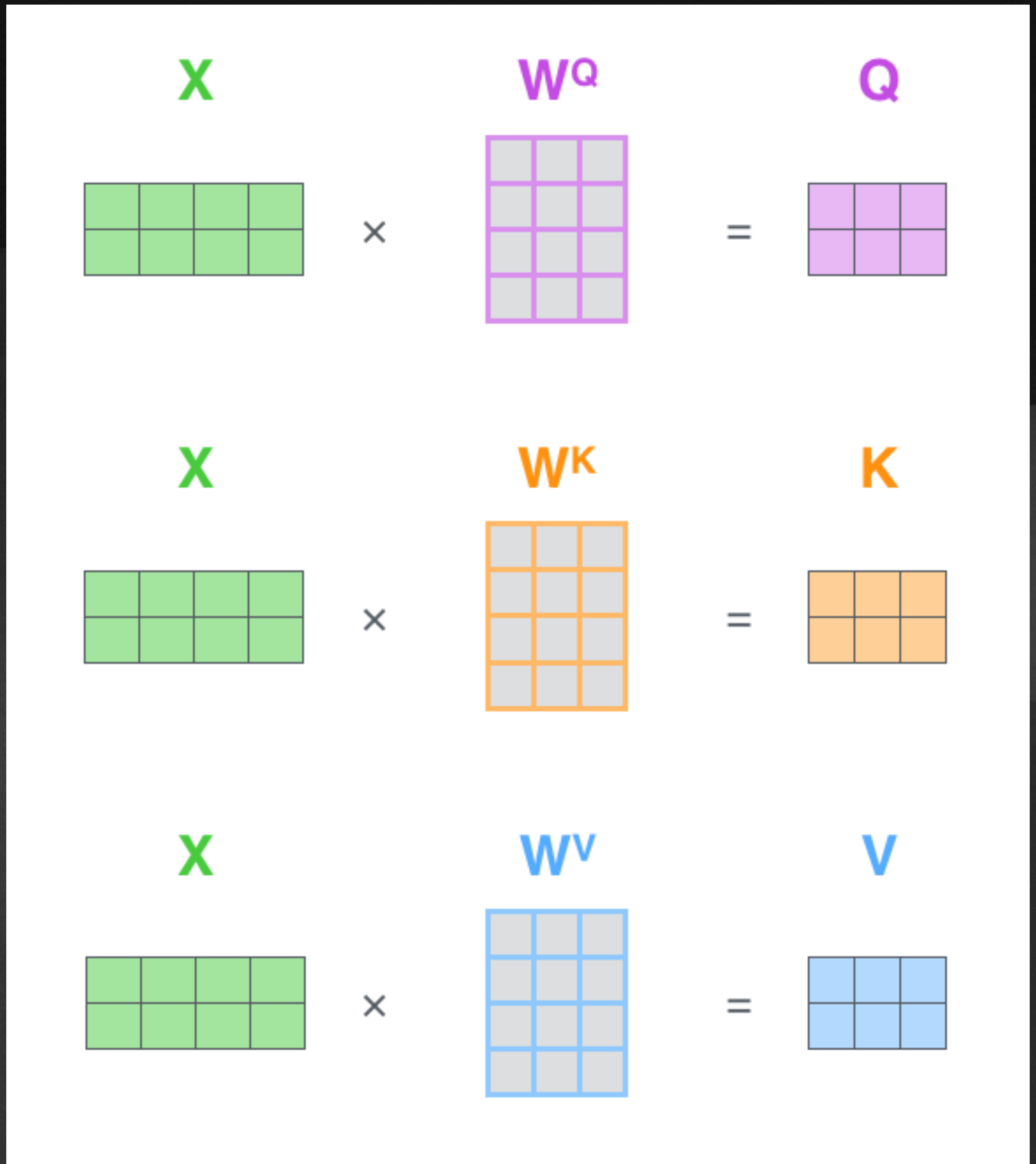

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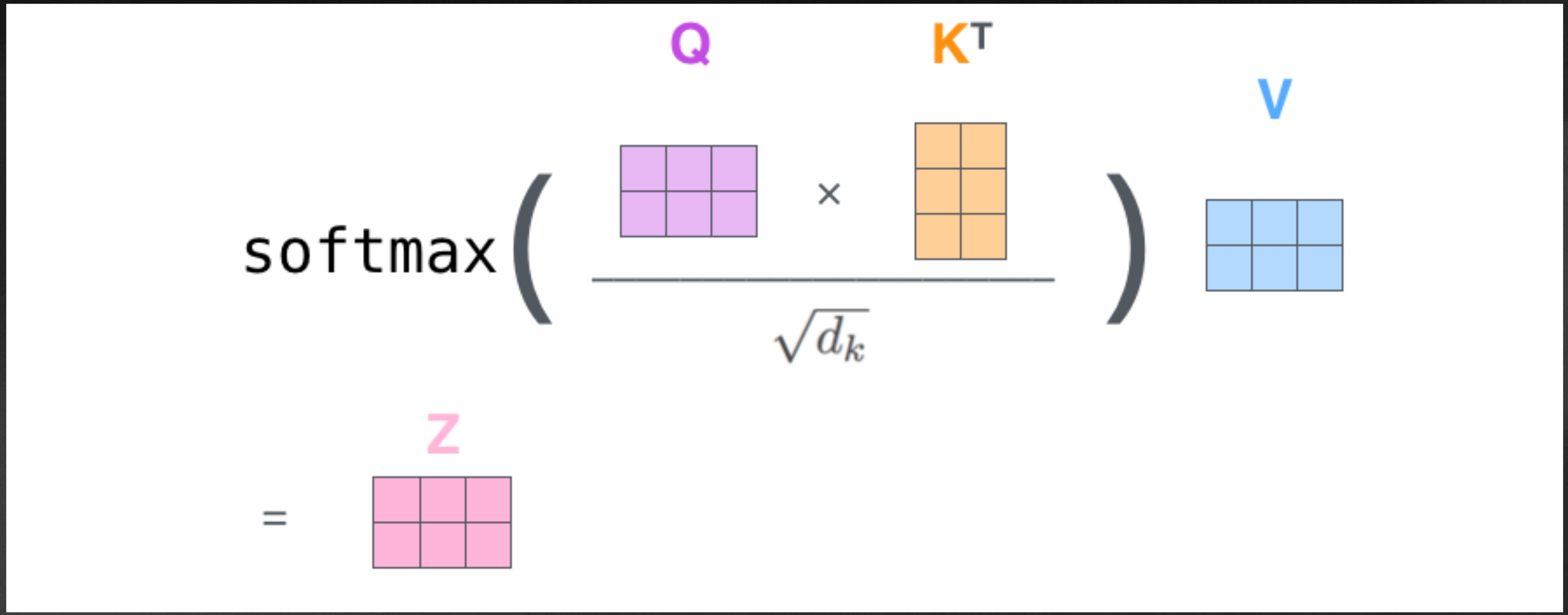
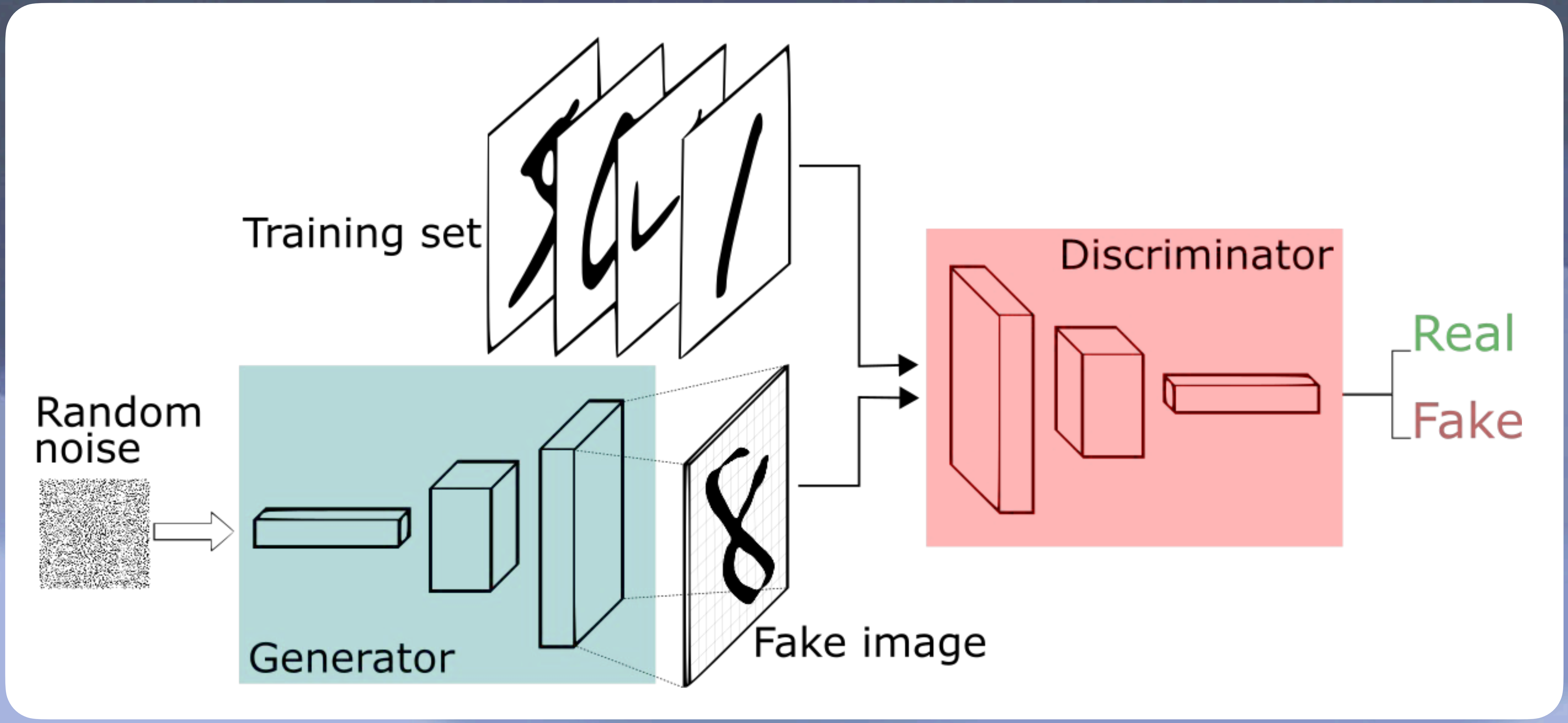


https://jalammar.github.io/illustrated-transformer/

Generative Adversarial Networks (GANs)

Survey of Deep Learning Architectures

- “Generative” AI: use ML to create new images, sounds, etc.
- GANs: two agents (the *generator* and the *discriminator*) are given competing tasks:

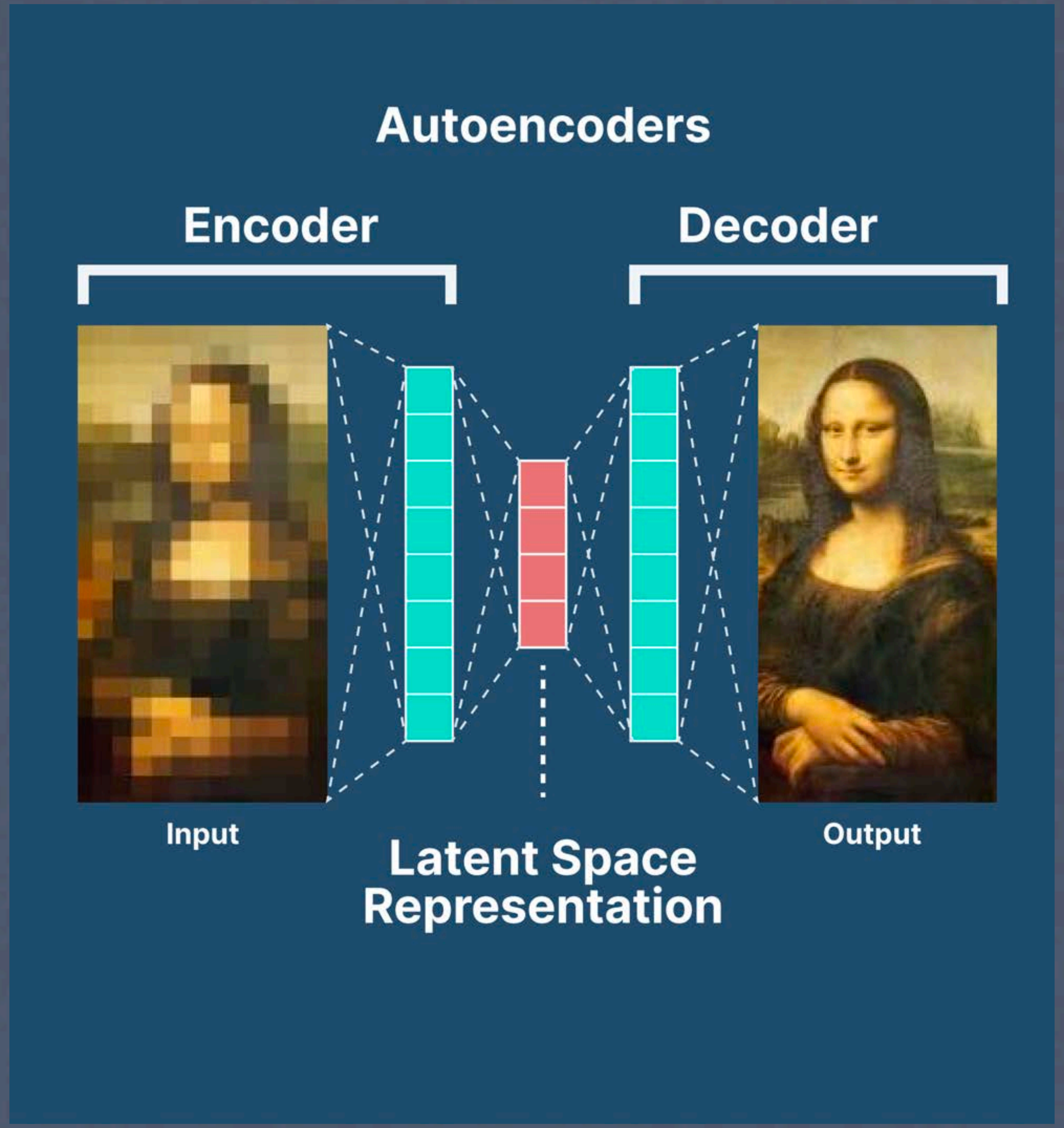


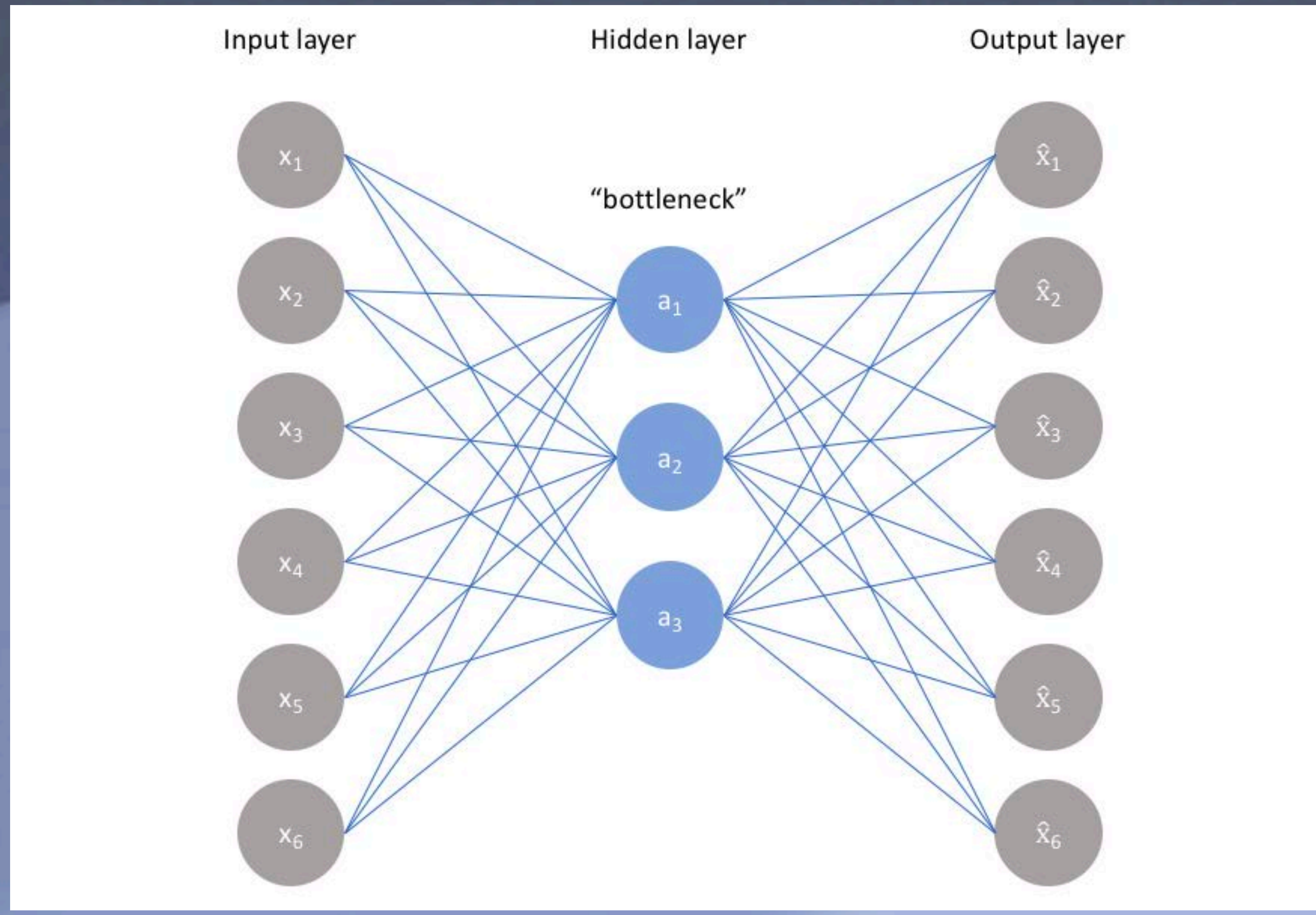
https://sthalles.github.io/intro-to-gans/

Autoencoders

Learning Efficient Codings

- Autoencoders are used to produce compressed data representations
  - **Encoder**: produces a lower-dimensional (compressed) “latent” representation of the input data
  - **Decoder**: given the compressed representation, reconstruct the original data
- Decoded representations typically less noisy,
- Uses: efficient encoding, image denoting, generative modeling, anomaly detection



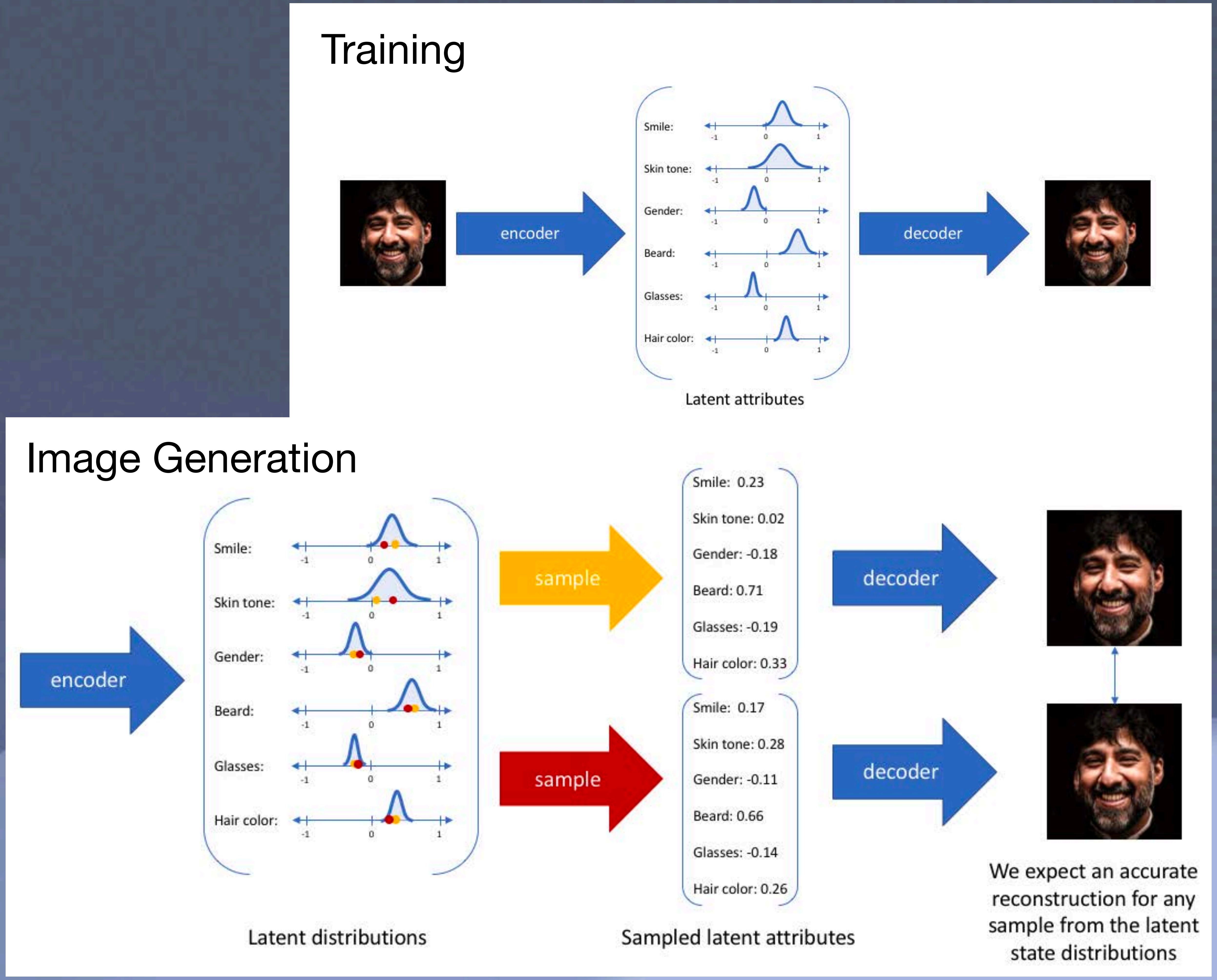


https://www.v7labs.com/blog/autoencoders-guide#:~:text=An%20autoencoder%20is%20an%20unsupervised,even%20generation%20of%20image%20data.

Variational Autoencoder (VAEs)

Generative Modeling via Autoencoders

- Generate realistic images from random noise
  - **Encoder**: predict means and standard deviations of a *probability distribution* over the latent features
  - **Decoder:** given a random sample from the latent distributions, produce the corresponding output



https://www.jeremyjordan.me/variational-autoencoders/

SCAN ME