UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Neurocomputing

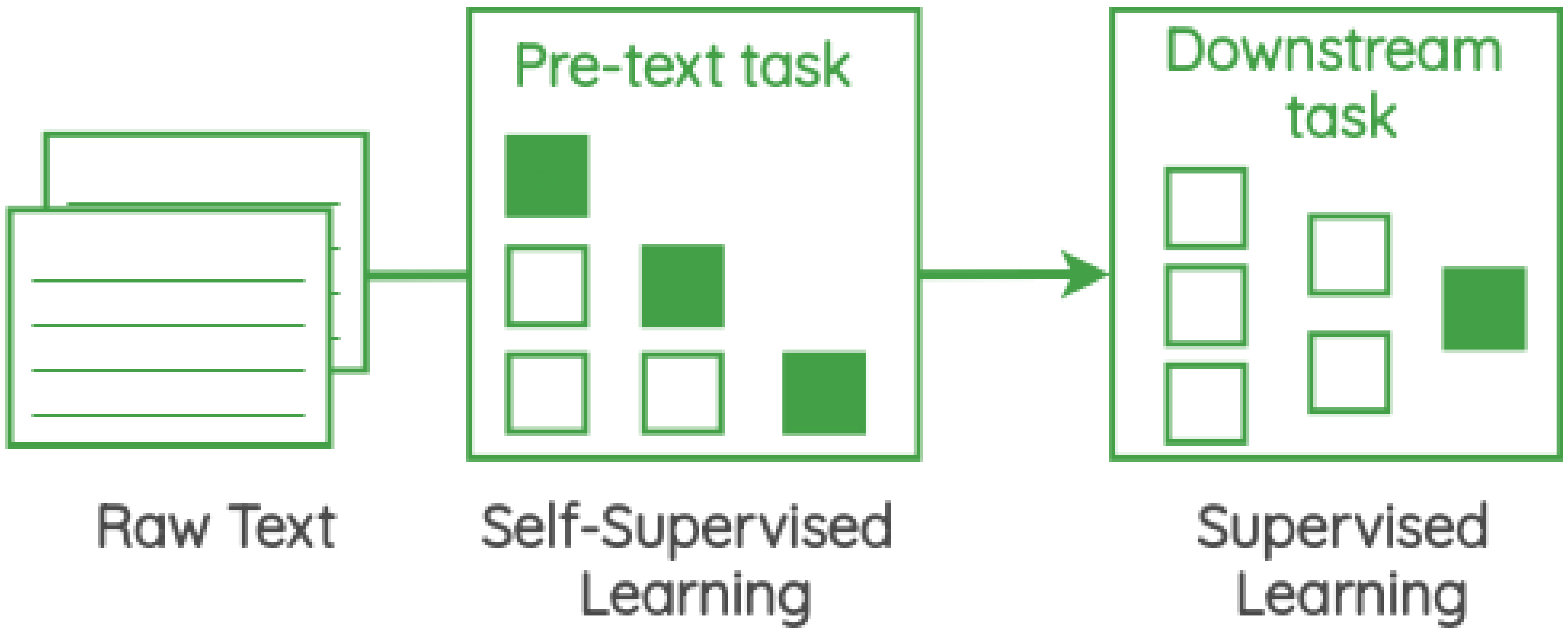
Contrastive learning

Julien Vitay
Professur für Künstliche Intelligenz - Fakultät für Informatik

1 - Self-supervised learning

Self-supervised learning

- **Supervised learning** uses a supervisory signal (e.g. human-annotated labels) to train a model (classification, regression).
- **Unsupervised learning** only relies on analysing the properties of the data (clustering, dimensionality reduction).
- **Semi-supervised learning** first extract features on raw data (e.g. autoencoder) and then fine-tunes a model on annotated data.
- **Self-supervised learning** creates its own supervisory signal from the raw data to extract features using a **pretext task** or **auxiliary task**. These features can then be used to learn a supervised learning problem (downstream task).

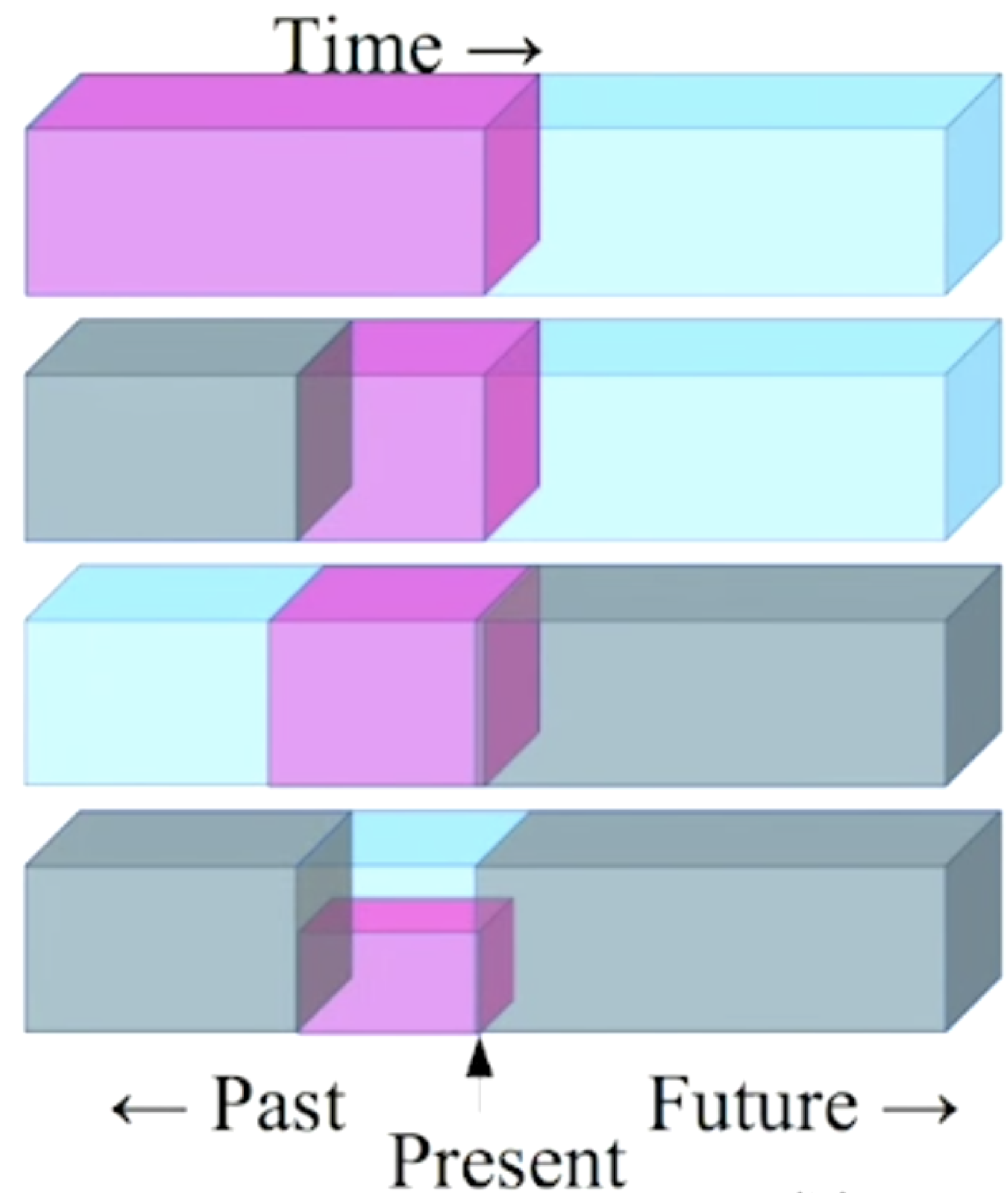


Source: https://amitness.com/2020/05/self-supervised-learning-nlp/

Self-supervised learning

- Pretext tasks can be easily and automatically derived from the existing data, such as predicting the future of a signal.

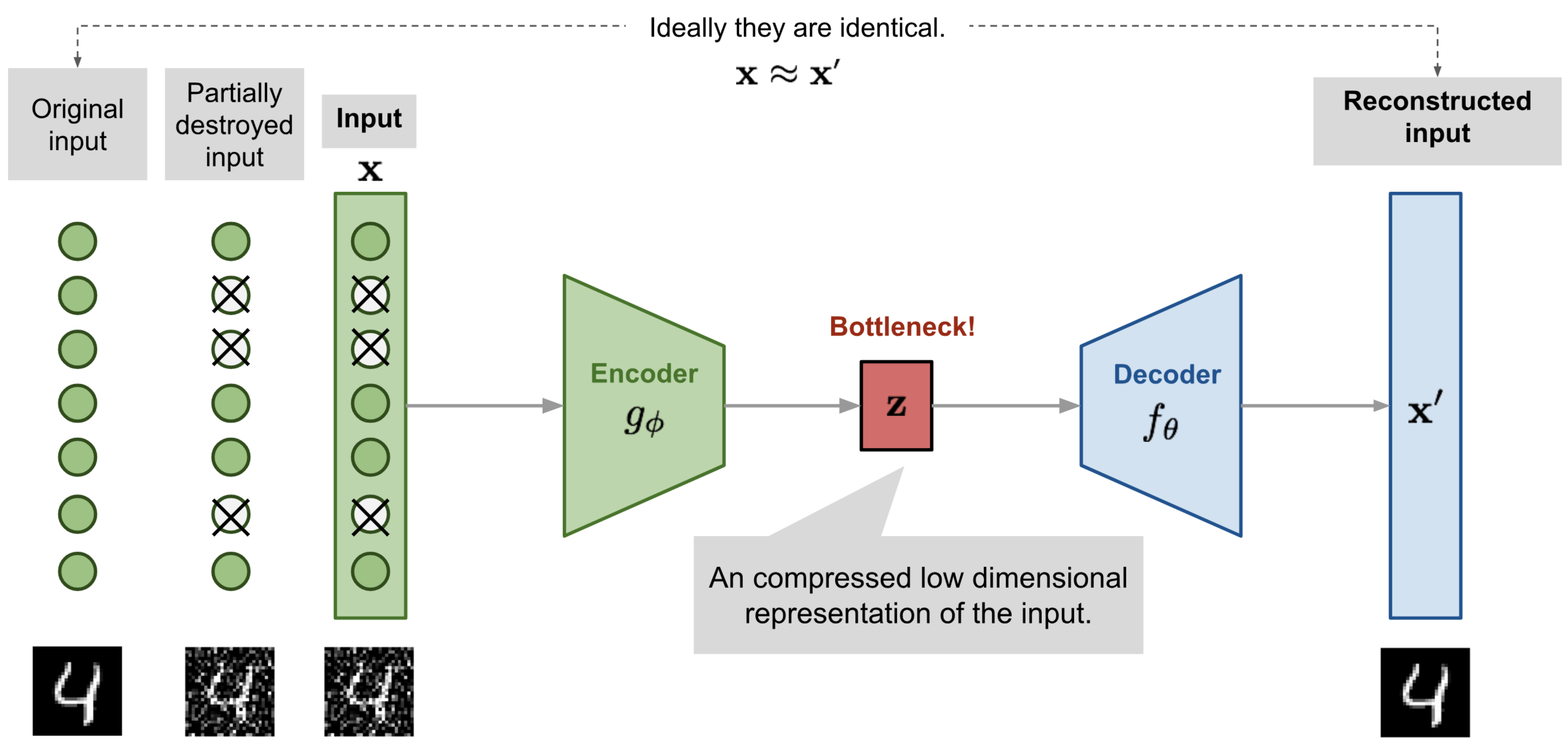
- Predict any part of the input from any other part.
- Predict the future from the past.
- Predict the future from the recent past.
- Predict the past from the present.
- Predict the top from the bottom.
- Predict the occluded from the visible
- Pretend there is a part of the input you don’t know and predict that.

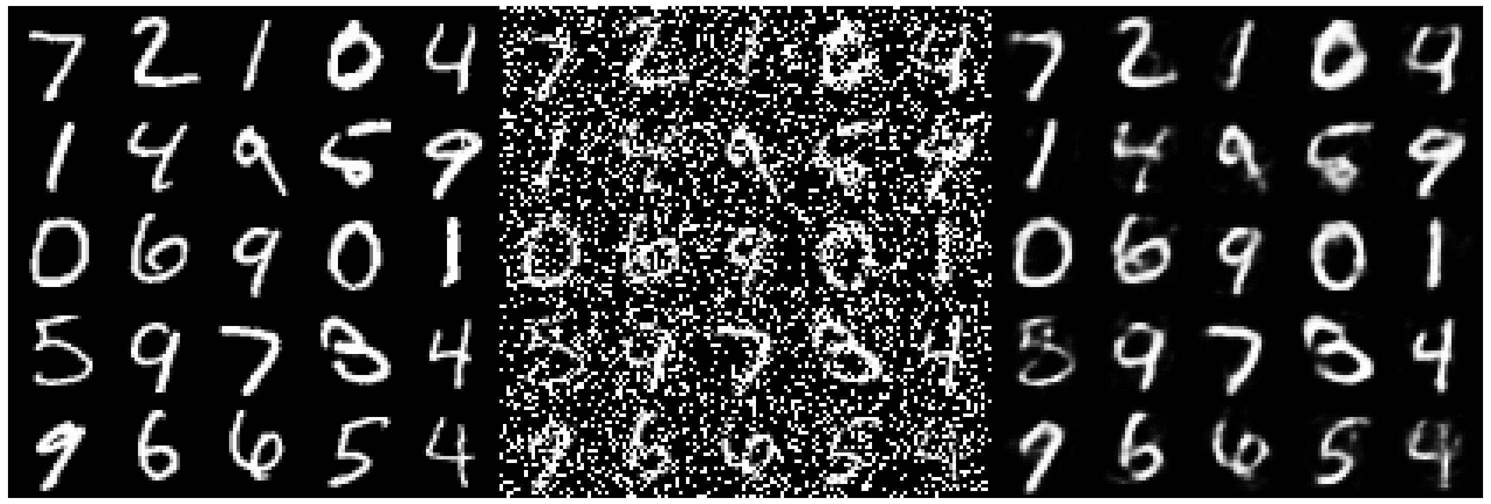


Slide: LeCun

Generative models

- Generative models (AE, GAN) are somehow self-supervised: reconstructing an image is just a pretext to learn a good latent representation, or to learn to remove noise (denoising AE).



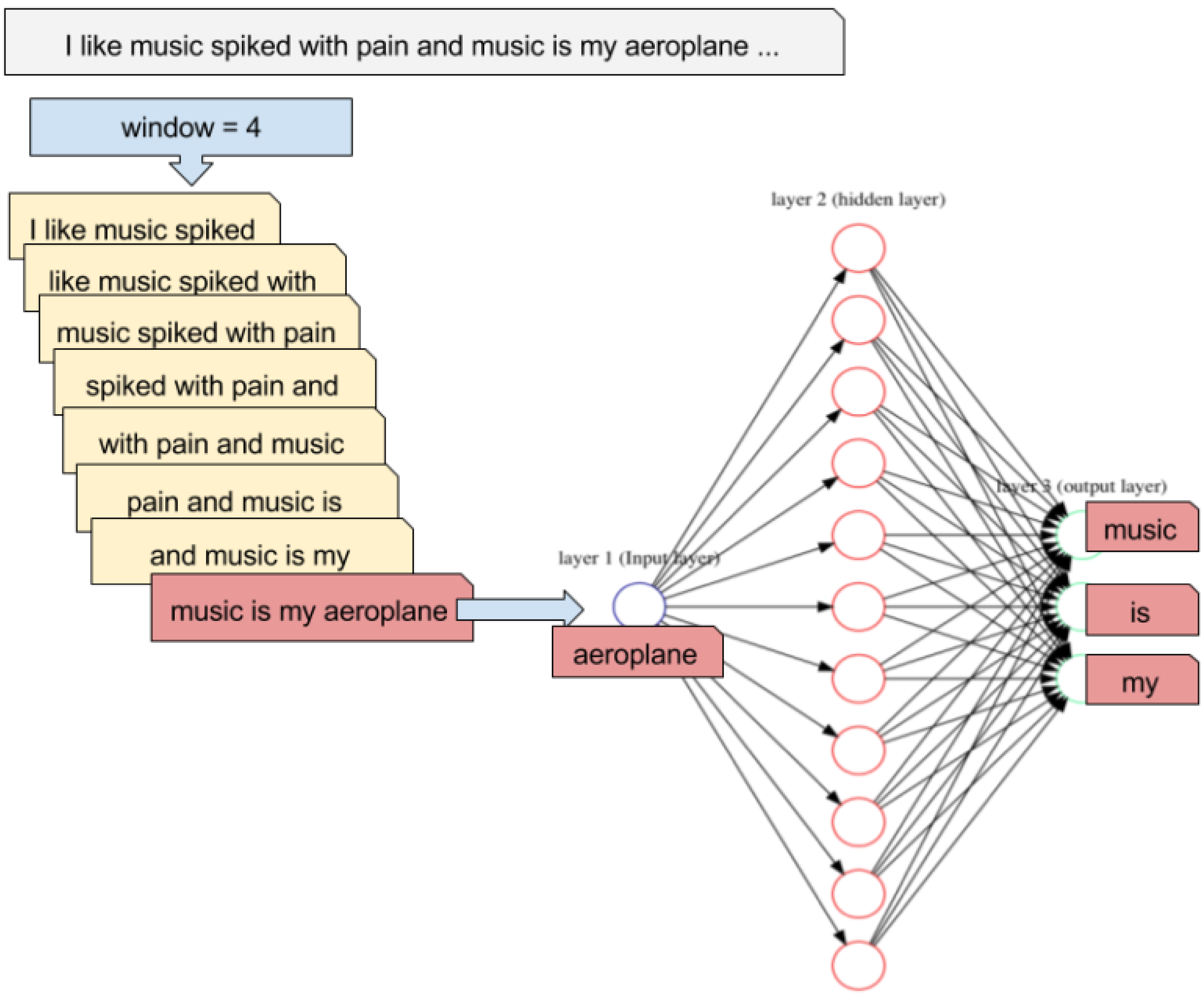


Source : https://lilianweng.github.io/lil-log/2018/08/12/from-autoencoder-to-beta-vae.html

Vincent et al. (2010) Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion. JMLR, 38.

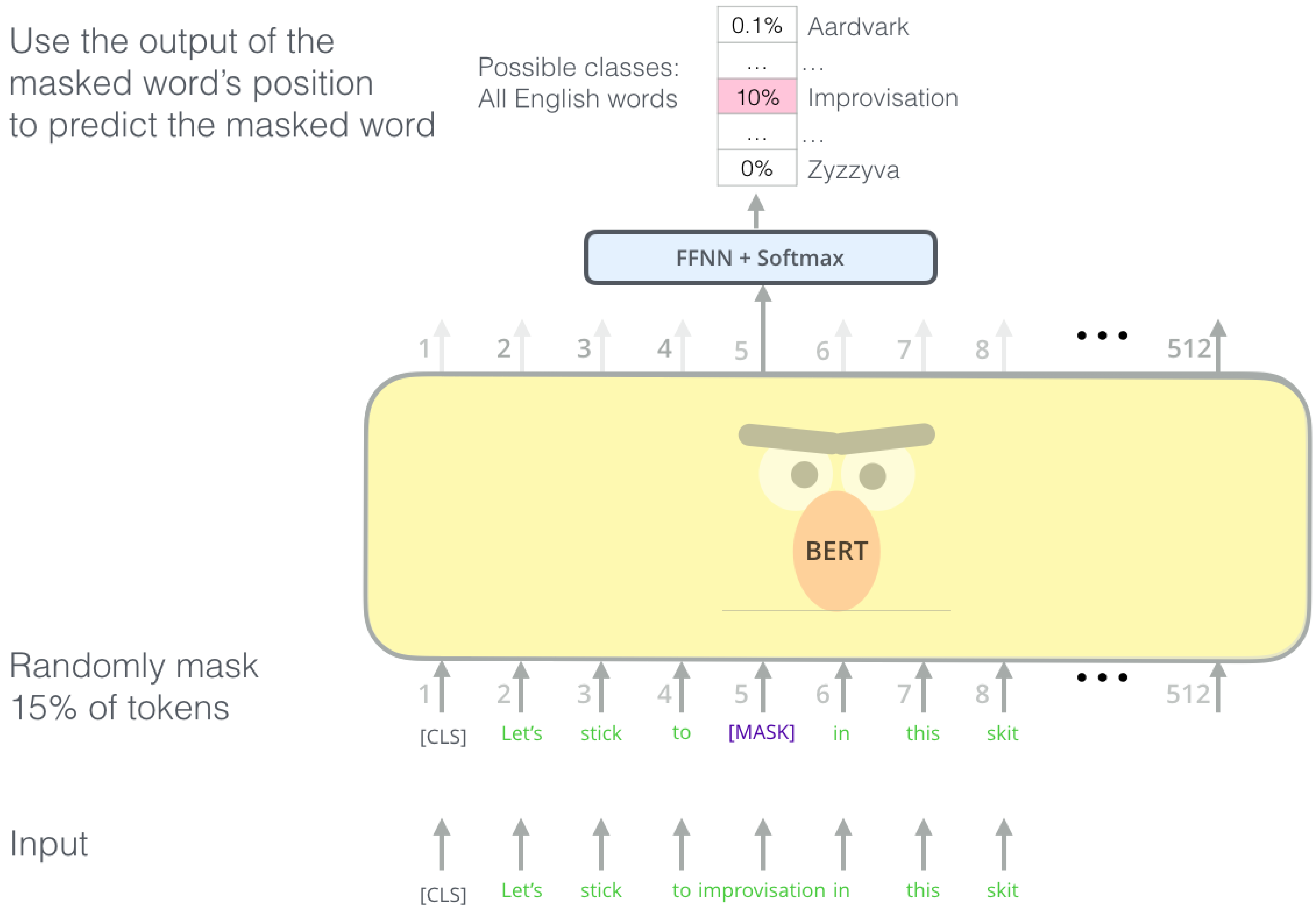
word2vec

- word2vec is trained using the pretext task of predicting the surrounding words in a sentence.



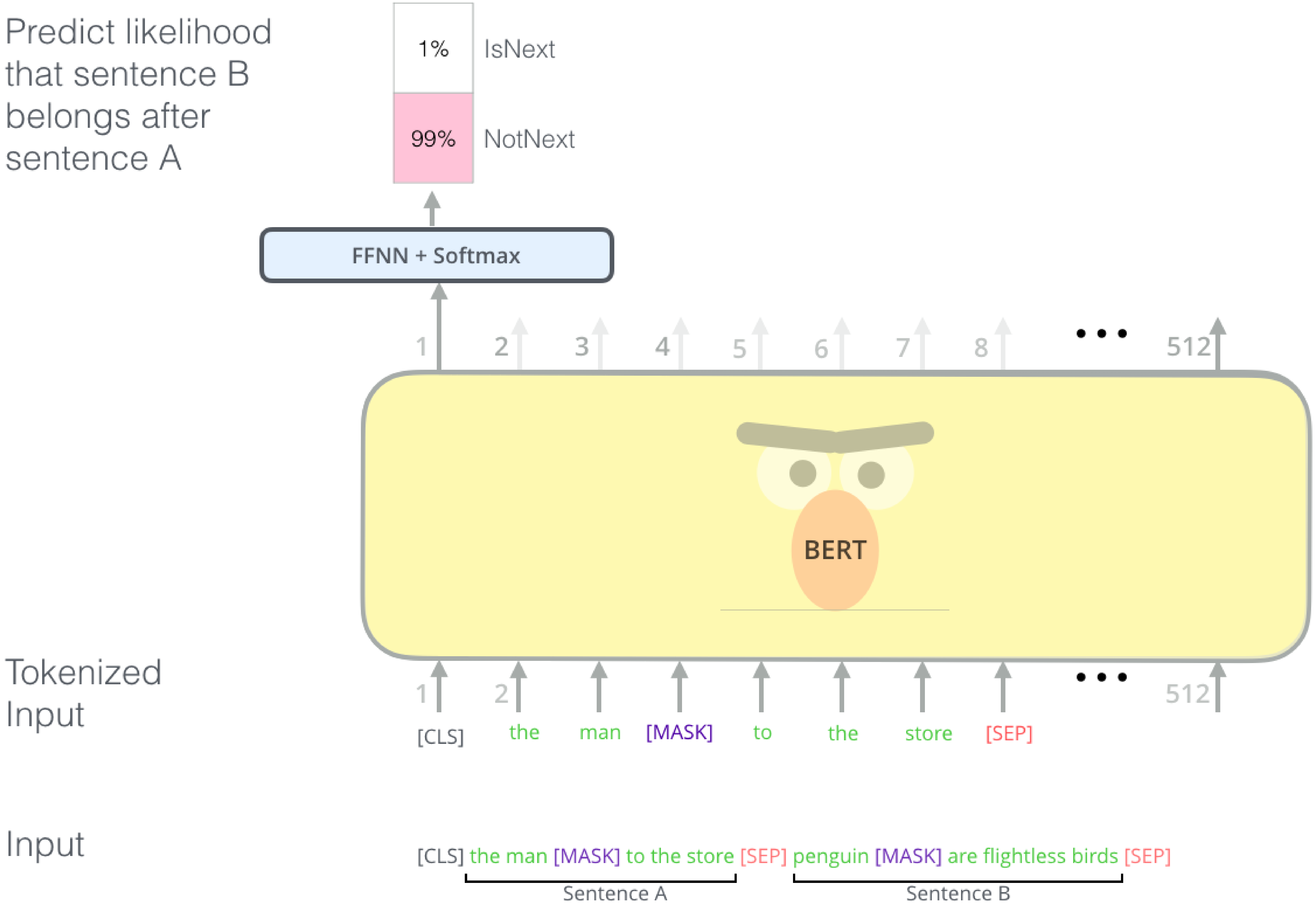
Source: https://jaxenter.com/deep-learning-search-word2vec-147782.html

Masked word prediction



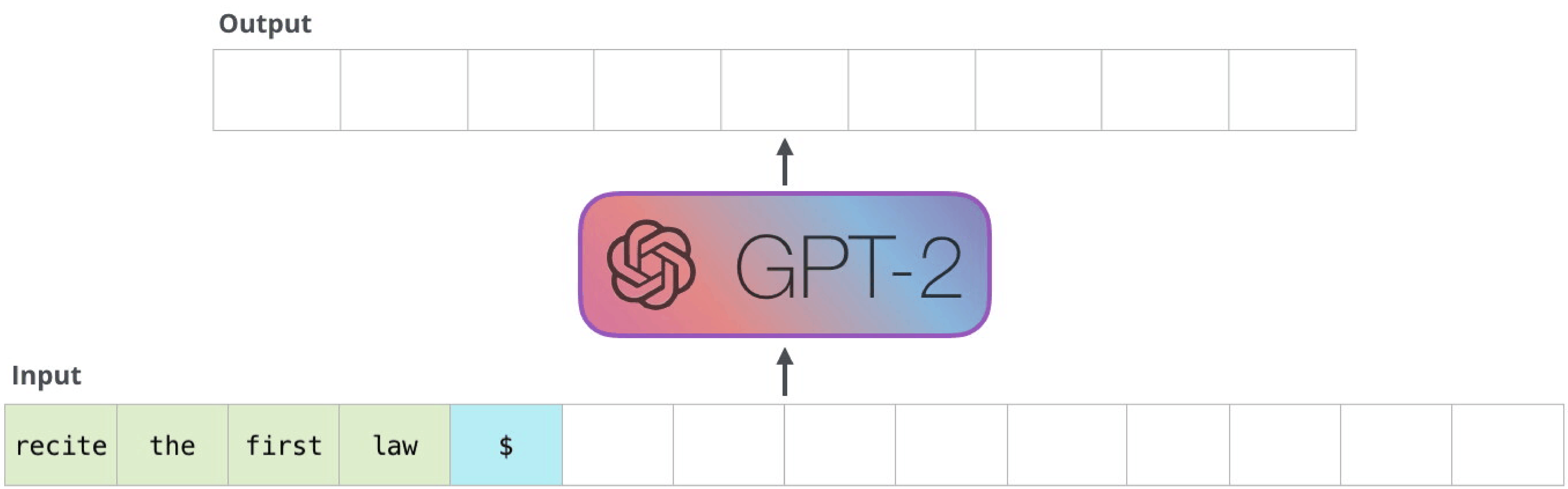
Source: https://jalammar.github.io/illustrated-bert/

Next sentence prediction



Source: https://jalammar.github.io/illustrated-bert/

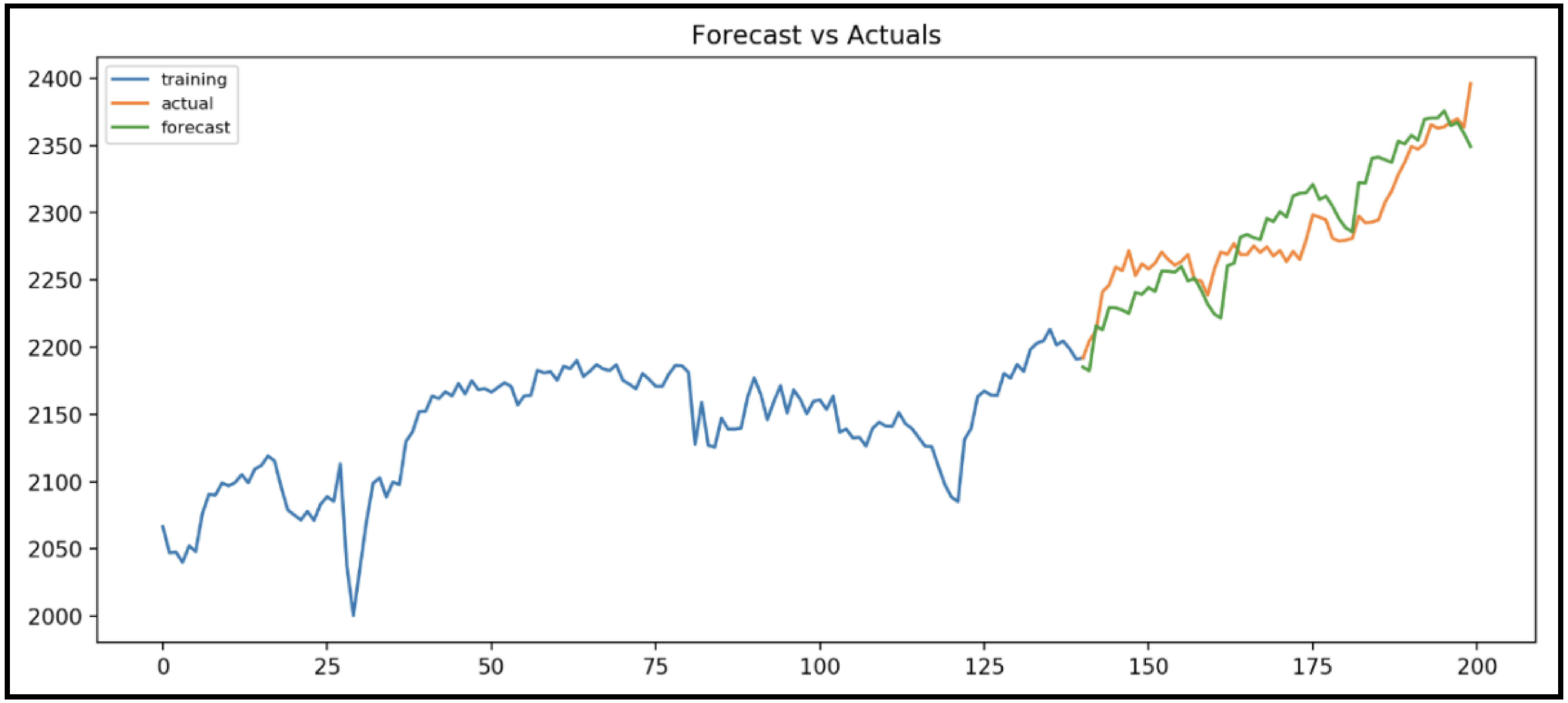
Next word prediction



Source: https://jalammar.github.io/illustrated-gpt2/

Autoregression

- Autoregressive models (RNN) are trained to predict the next value $\mathbf{x}_{t+1}$ of a (multivariate) signal based on its history $(\mathbf{x}_{t-T}, \dots, \mathbf{x}_t)$.
- At inference time, they can “unroll” the future by considering their prediction as the future “ground truth”.
- Useful for forecasting: weather, share values, predictive maintenance, etc.

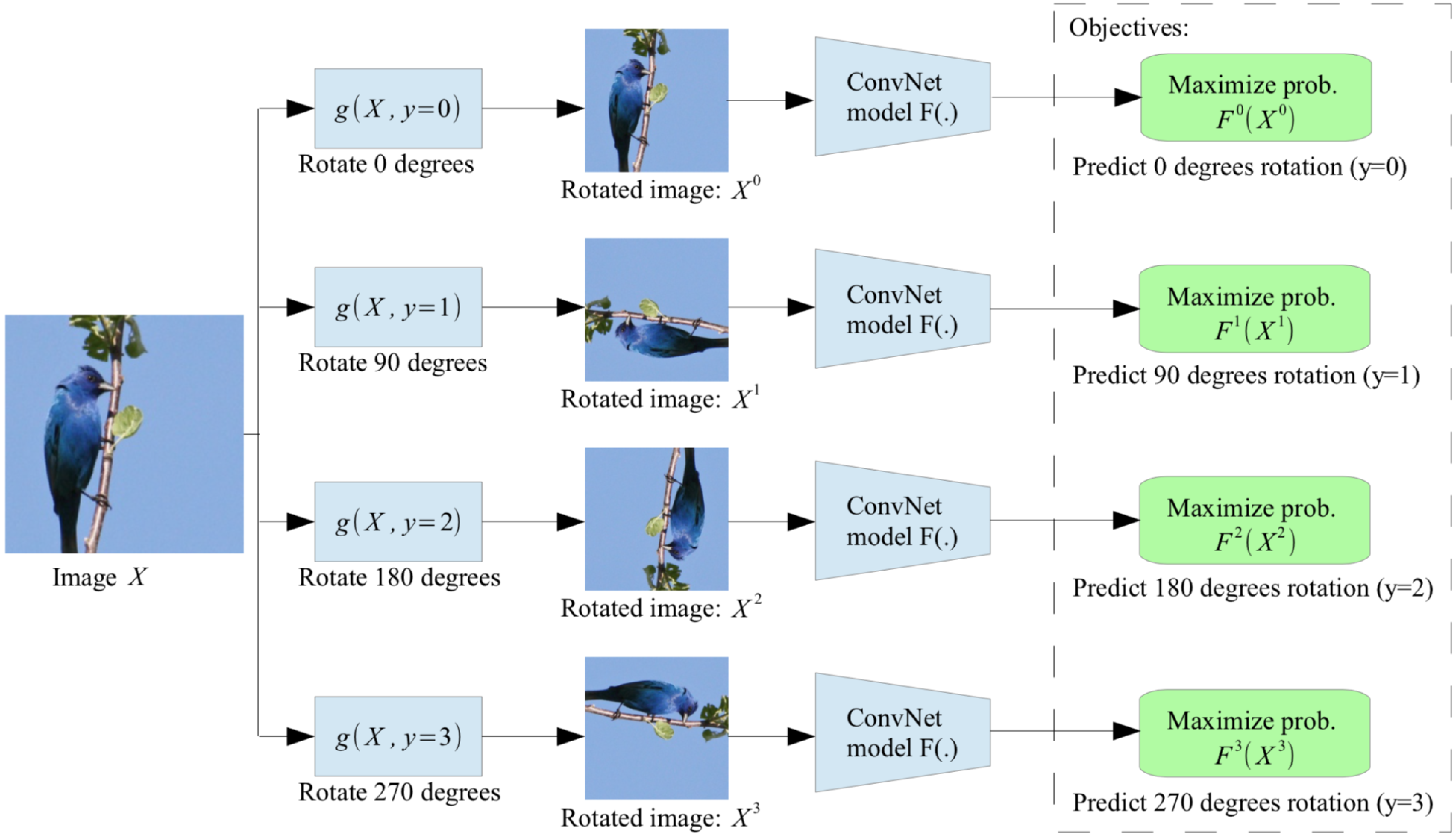



```
Test RMSE: 23.580
Test Percentage Error: 0.010%
```

Source: https://saas.berkeley.edu/rp/arima

Rotation prediction

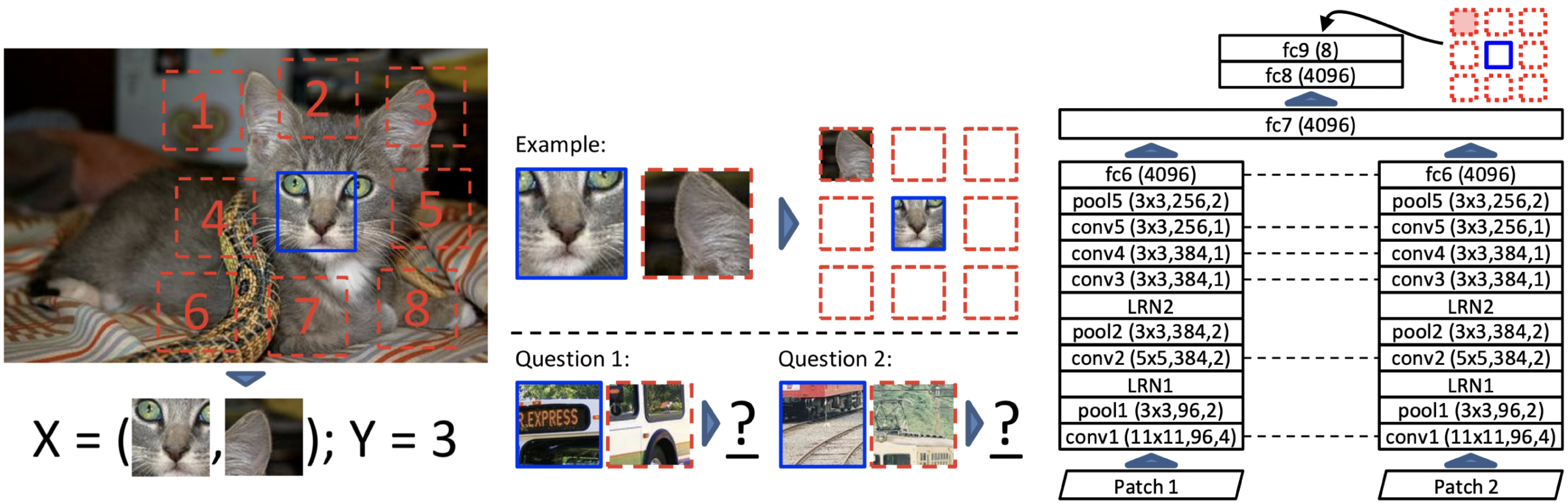
- Rotations are applied to an image and the CNN has to guess which one has been applied.
- By doing so, it has to learn visual features that "understand" what the regular position of an object is.



Gidaris et al. (2018) Unsupervised Representation Learning by Predicting Image Rotations. doi:10.48550/arXiv.1803.07728.

Relative position of image patches

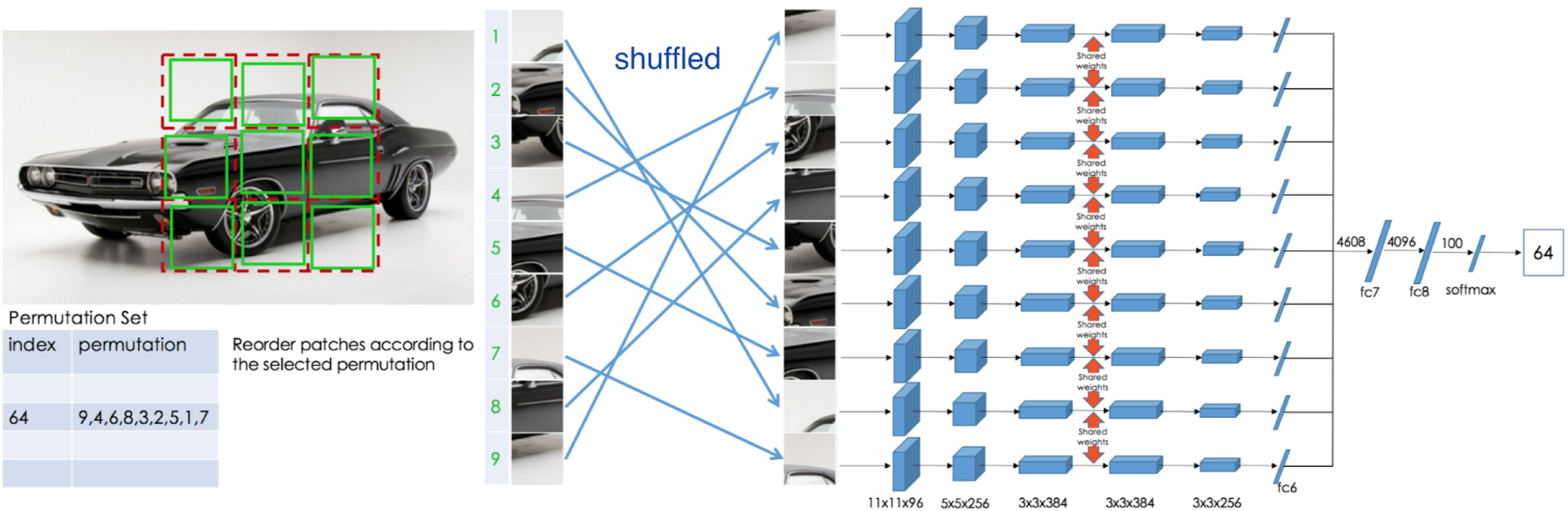
- One can also cut two patches of an image and ask the CNN to predict their relative position on a grid.
- The task is easier when the CNN "understands" the content of the patches, i.e. has learned good features.
- Note that the two patches go through the **same** CNN, but the two outputs are concatenated before the classification layers.



Doersch et al. (2016) Unsupervised Visual Representation Learning by Context Prediction. doi:10.48550/arXiv.1505.05192.

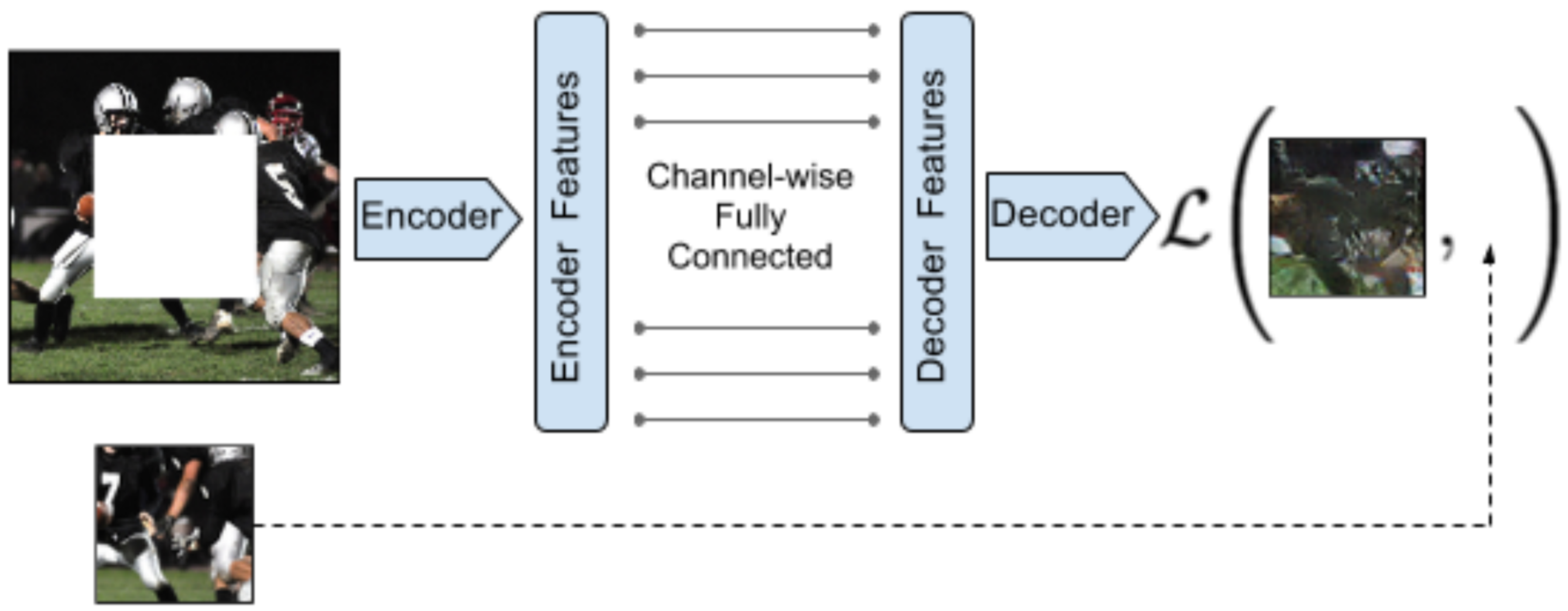
Jigsaw puzzle

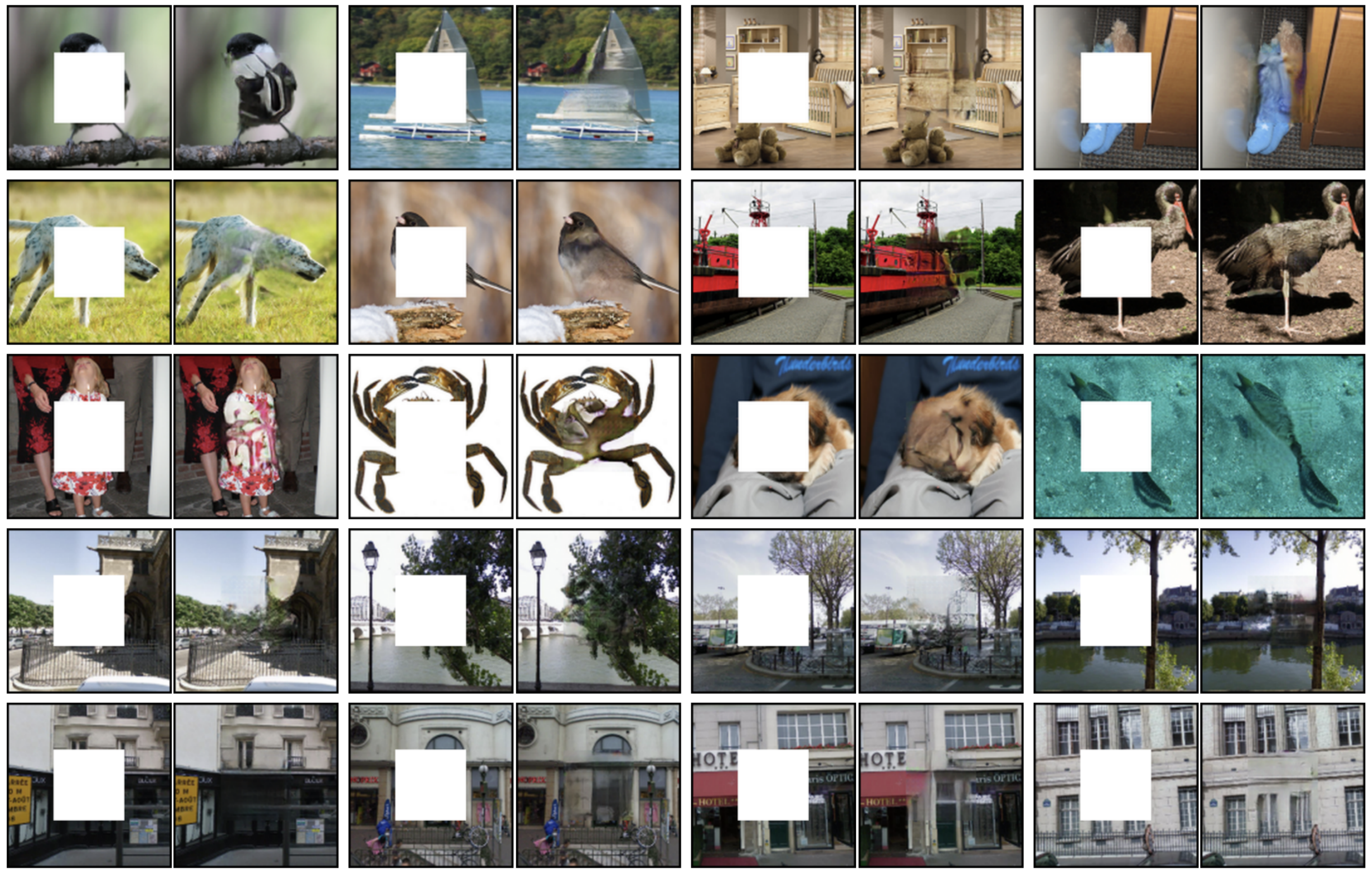
- One can also shuffle patches of an image according to a specific permutation, and have the network predict which permutation was applied.



Context encoder

- As with denoising autoencoders, **context encoders** can be trained to generate the contents of an arbitrary image region based on its surroundings.
- The loss function is the sum of the reconstruction loss and an adversarial loss (as in GANs).
- Useful for in-paintings. The encoder part can be fine-tuned on classification tasks.

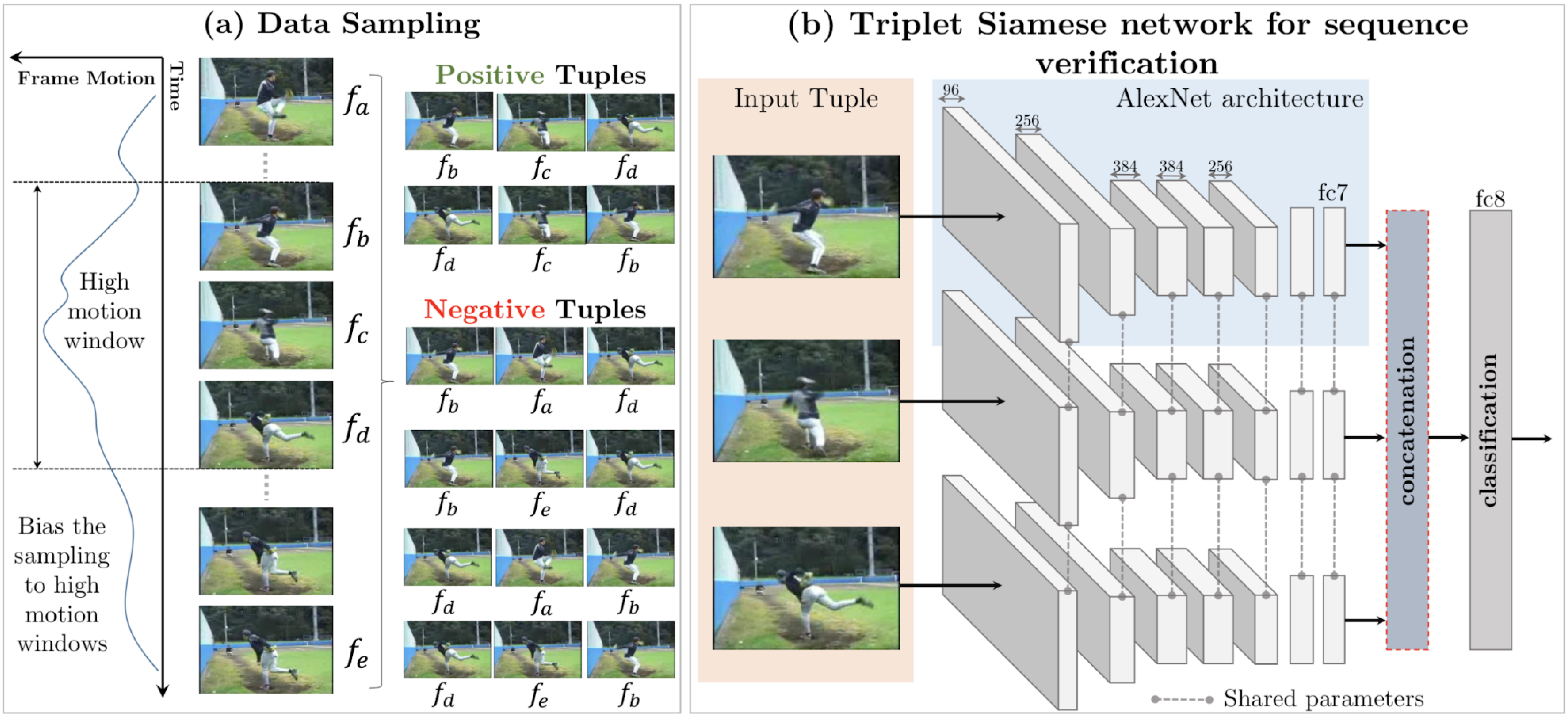




Pathak et al. (2016)

Frame order validation

- Triplet siamese networks have to guess whether three frames are consecutive in a video sequence or not.

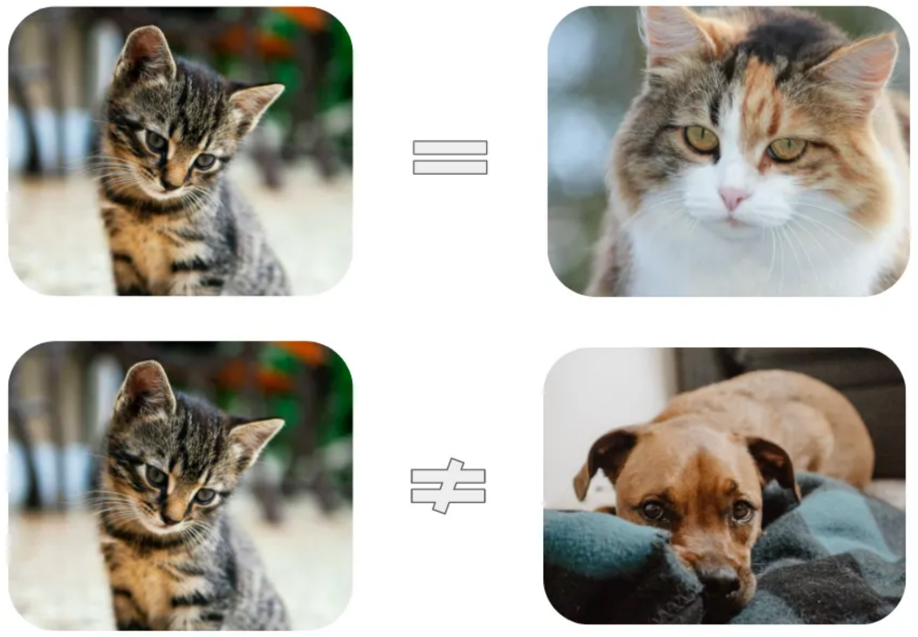


Misra et al. (2016) Shuffle and Learn: Unsupervised Learning using Temporal Order Verification. doi:10.48550/arXiv.1603.08561.

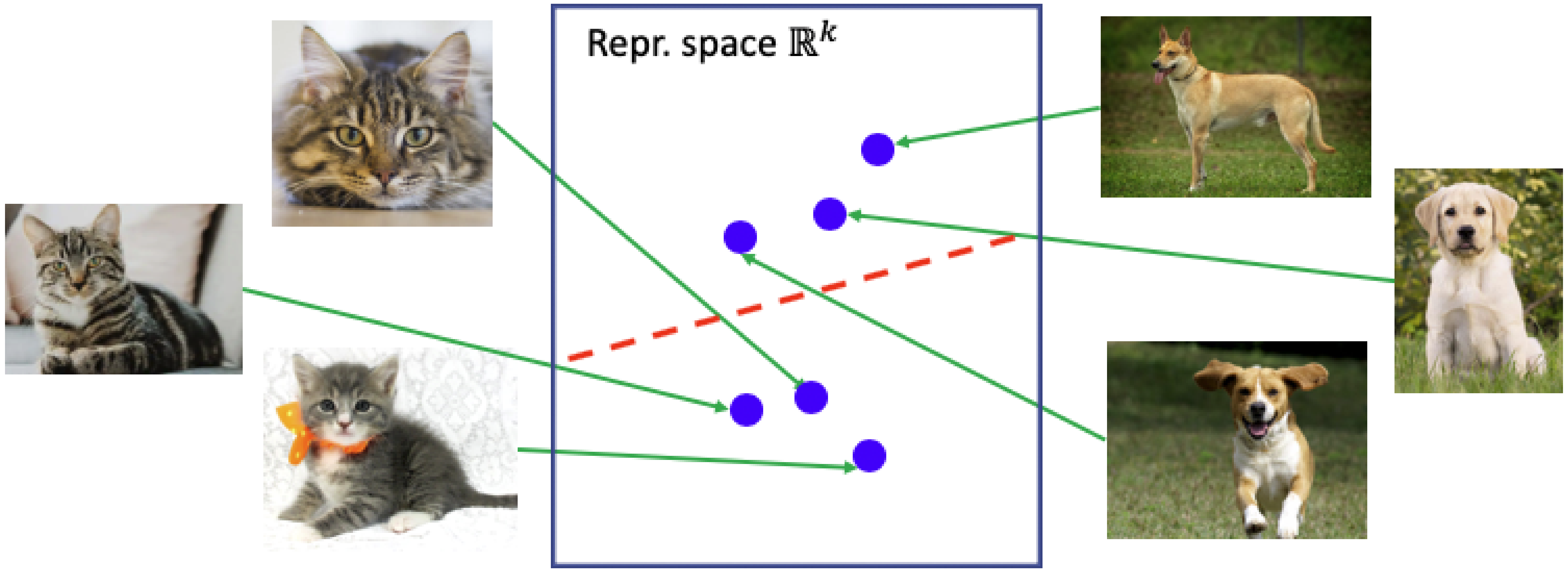
2 - Contrastive learning

Contrastive learning

- The idea of **contrastive learning** is to force a neural network to learn similar representations for similar images (e.g. cats), and different representations for different images (cats vs. dogs).
- In supervised learning, this is achieved by forcing the output layer to **linearly** separate the classes, so the last FC layer must group its representation of cats together and separate it from dogs.
- But how could we do this without the labels?



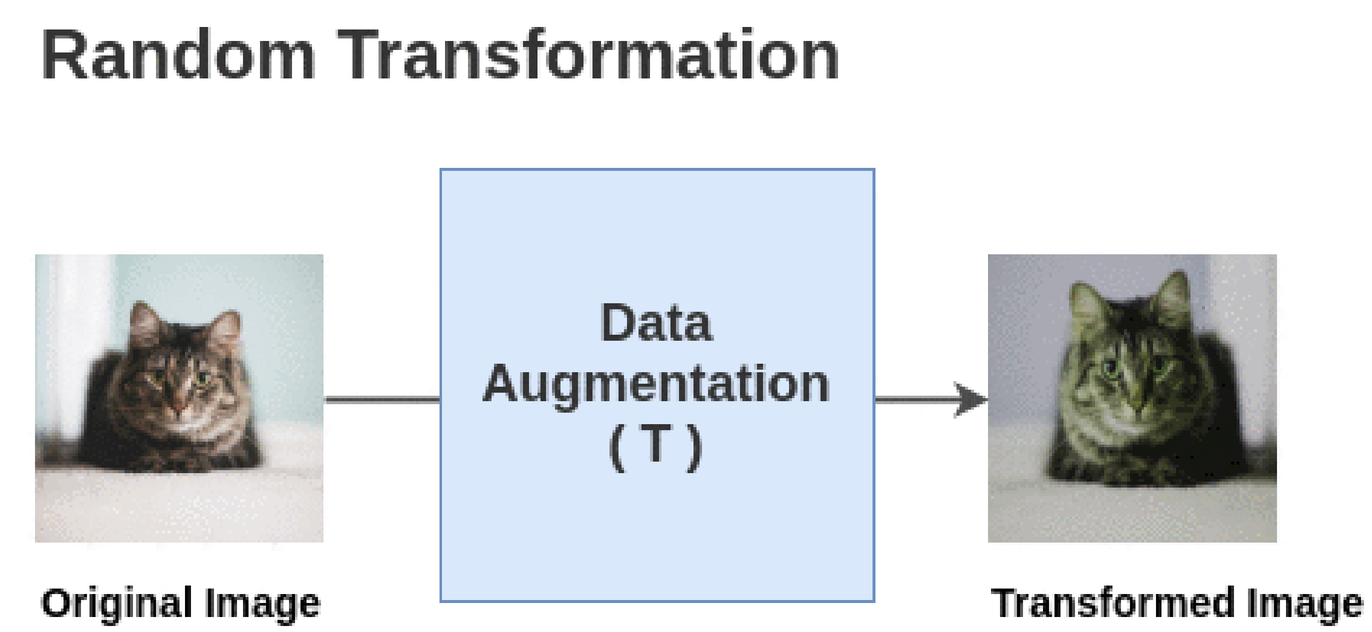
Source: https://towardsdatascience.com/understanding-contrastive-learning-d5b19fd96607



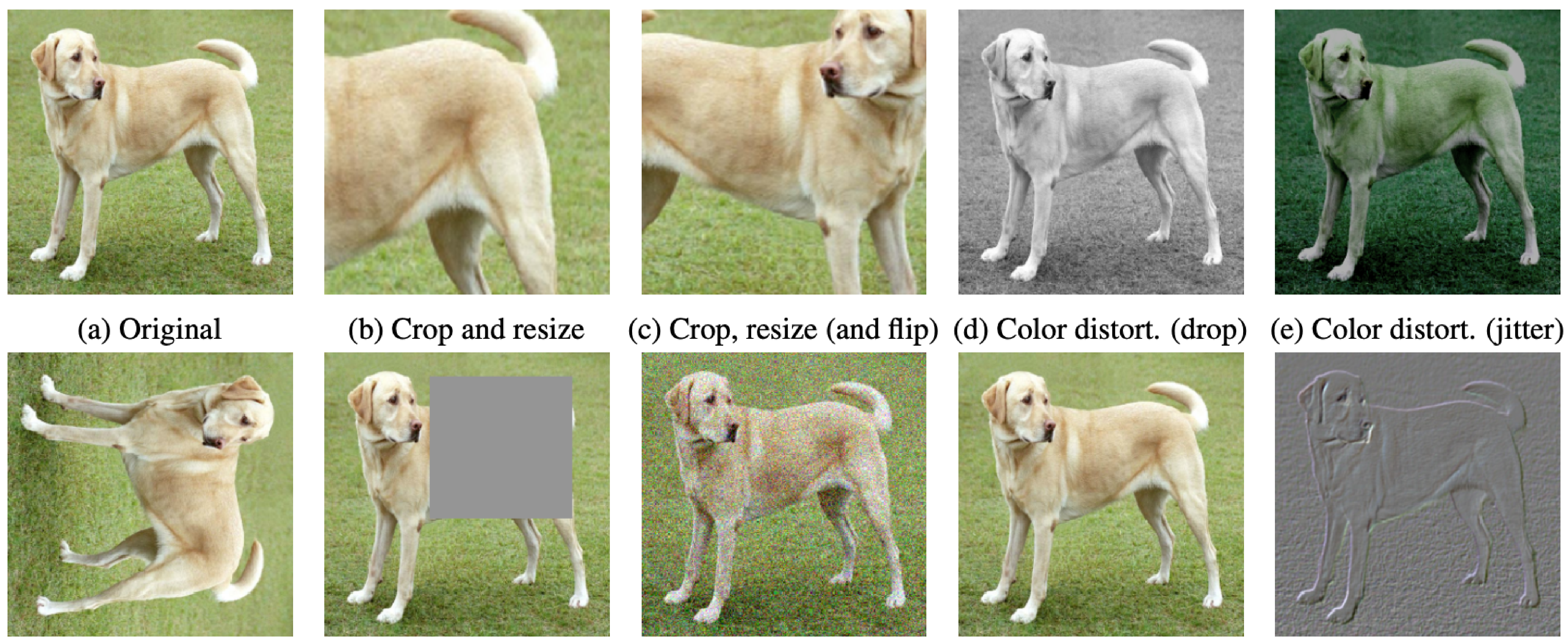
Source: https://ai.stanford.edu/blog/understanding-contrastive-learning/

Data augmentation

- A cheap and easy to obtain similar instances of the same class without labels is to perform **data augmentation** on the same image:
    - crop, resize, flip, blur, color distortion....
- Ideally, the representation for these augmented images should be similar at the end of the neural network.



Source: https://amitness.com/2020/03/illustrated-simclr/



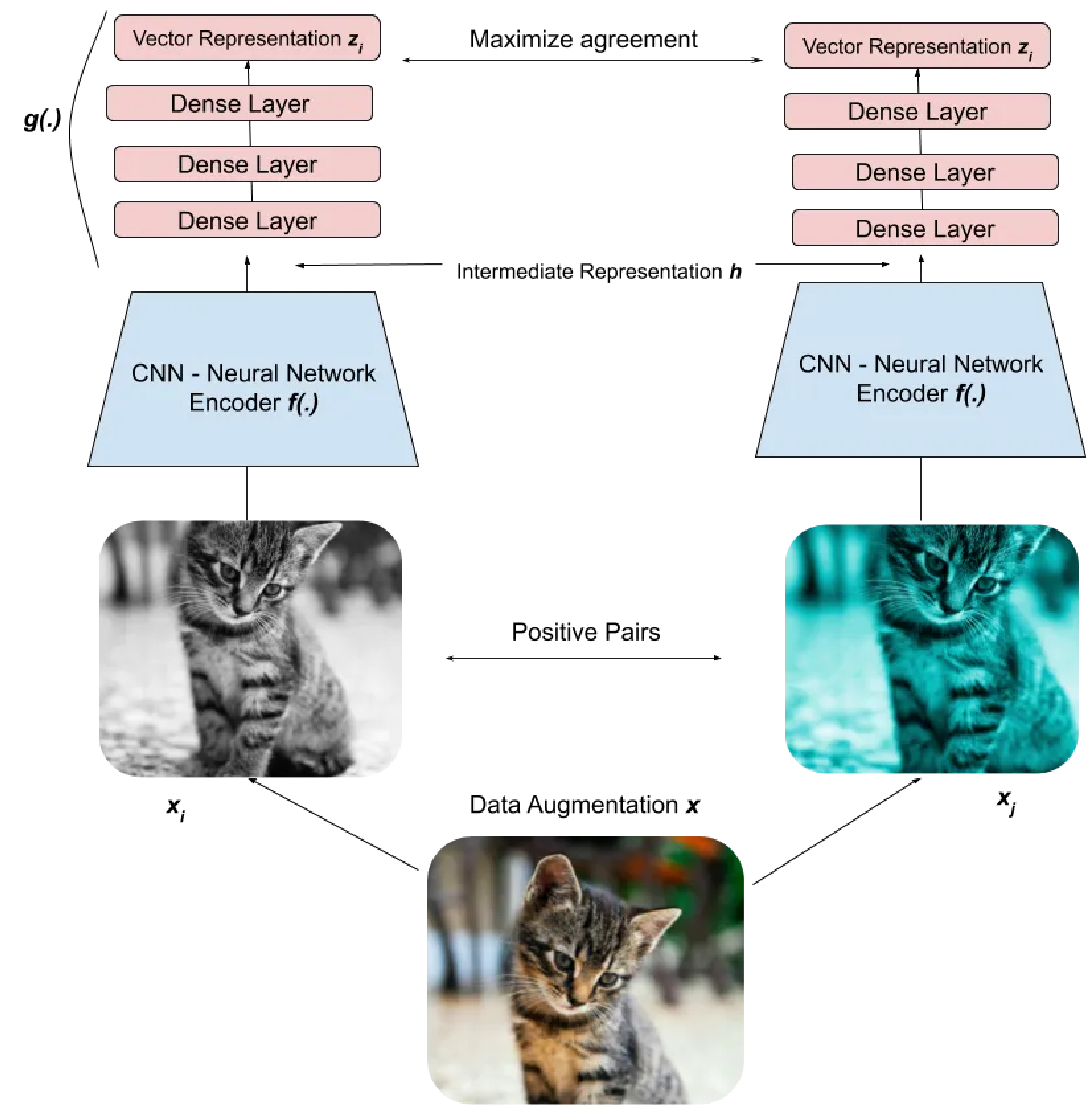
(a) Original (b) Crop and resize (c) Crop, resize (and flip) (d) Color distort. (drop) (e) Color distort. (jitter)

(f) Rotate $\{90°, 180°, 270°\}$ (g) Cutout (h) Gaussian noise (i) Gaussian blur (j) Sobel filtering

Source: Chen et al. (2020)

SimCLR

- SimCLR (**Sim**ple framework for **C**ontrastive **L**earning of visual **R**epresentations) generates a **positive pair** of augmented images.
- Both images $\mathbf{x}_i$ and $\mathbf{x}_j$ go through the same CNN encoder f (e.g. a ResNet-50) to produce high-level representations $\mathbf{h}_i$ and $\mathbf{h}_j$.
- The representations are passed through a FCN g to produce embeddings $\mathbf{z}_i$ and $\mathbf{z}_j$.
- The goal is to **maximize the similarity** or agreement between the embeddings $\mathbf{z}_i$ and $\mathbf{z}_j$, i.e. have the vectors as close as possible from each other..



Source: https://towardsdatascience.com/understanding-contrastive-learning-d5b19fd96607

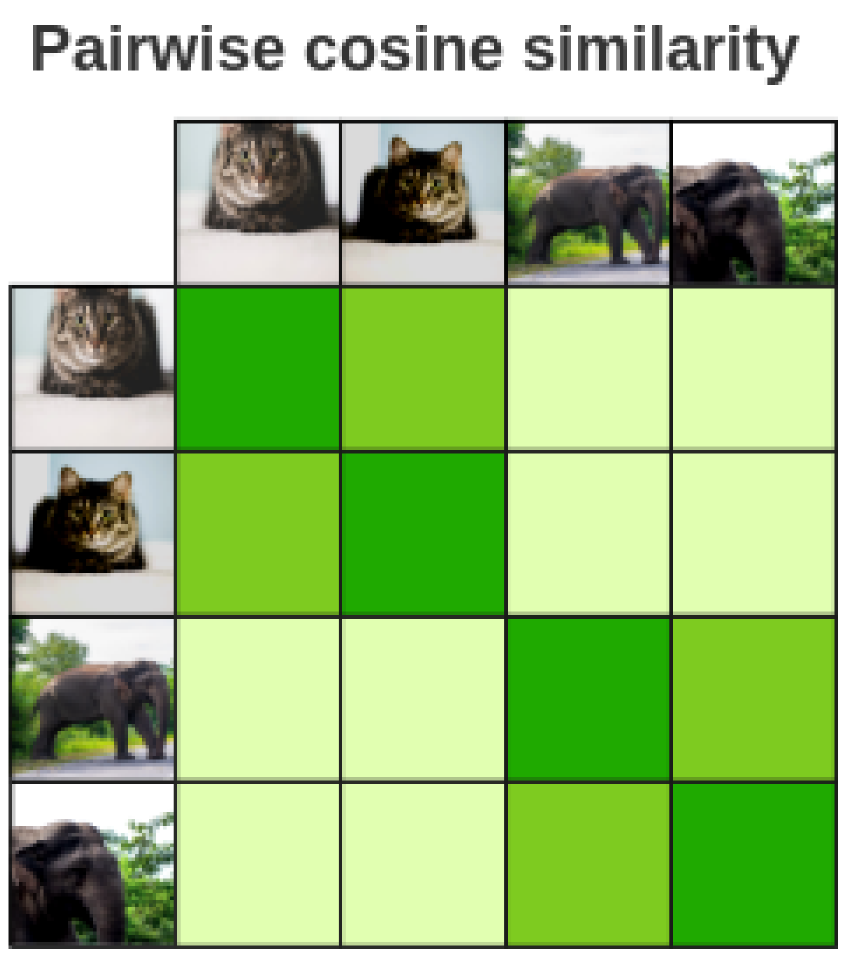
Chen et al. (2020) A Simple Framework for Contrastive Learning of Visual Representations. doi:10.48550/arXiv.2002.05709.

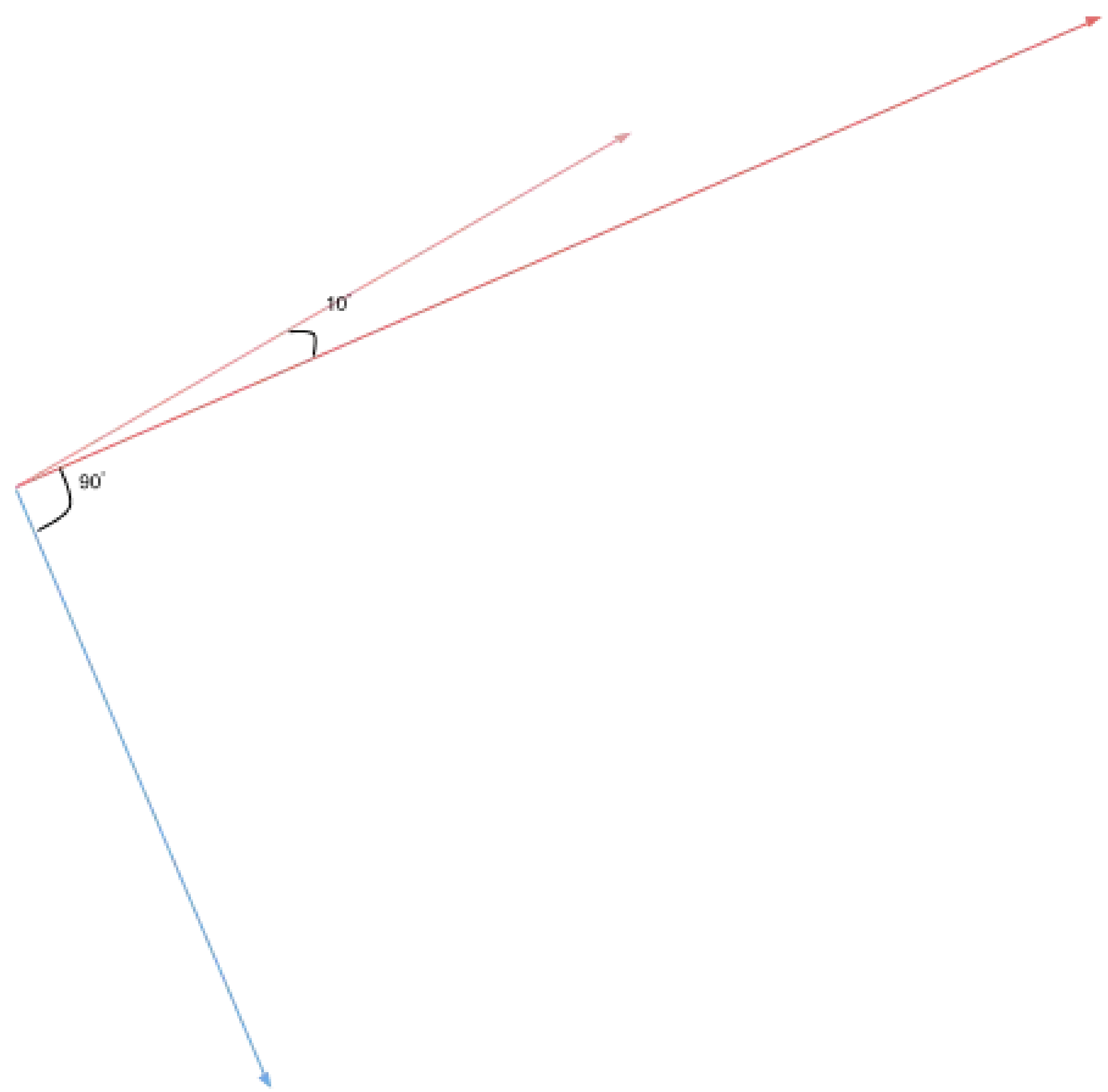
SimCLR

- The similarity between the embeddings $\mathbf{z}_i$ and $\mathbf{z}_j$ is calculated using the **cosine similarity**:

$$\cos(\mathbf{z}_i, \mathbf{z}_j) = \frac{\mathbf{z}_i^T \, \mathbf{z}_j}{||\mathbf{z}_i|| \, ||\mathbf{z}_j||}$$

- Colinear vectors have a cosine similarity of 1 (or -1), orthogonal vector have a cosine similarity of 0.
- Note: One could use the L2-norm, but it would force the vectors to have the same norm.





Source: https://towardsdatascience.com/understanding-contrastive-learning-d5b19fd96607

SimCLR

- SimCLR actually selects a minibatch of K images and generates two augmented images for each of them.
- For an image k, the goal is to:
  - **maximize** the similarity between the embeddings $\mathbf{z}_{2k}$ and $\mathbf{z}_{2k+1}$ of the positive pair,
  - **minimize** their similarity with the other augmented images ($(K-1)$ negative pairs).
- There could be another instance of the same class in the minibatch, but in practice it will not matter much.
- The batch size should be quite big ($K = 8192$) to allow for many relevant negative pairs.

Source: https://ai.googleblog.com/2020/04/advancing-self-supervised-and-semi.html

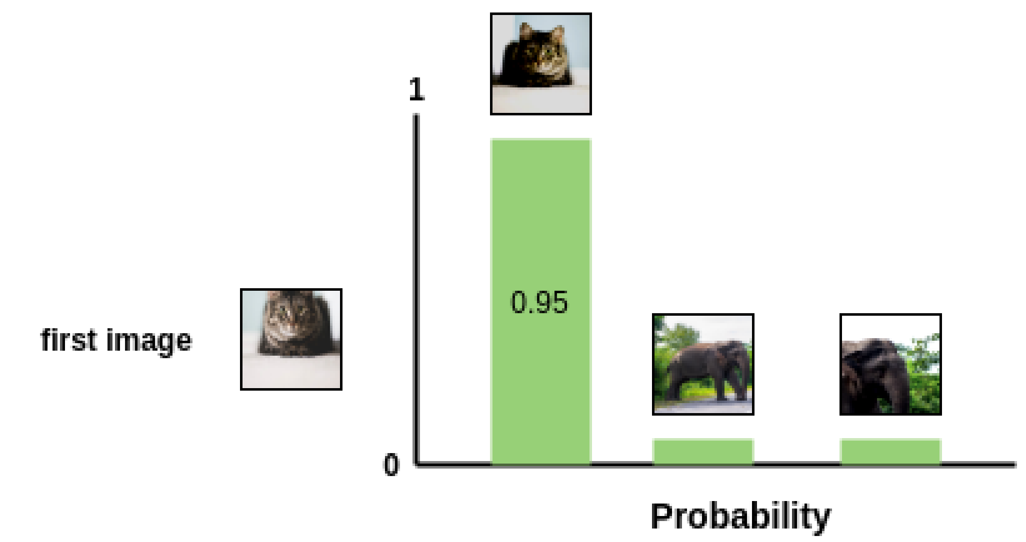
Chen et al. (2020) A Simple Framework for Contrastive Learning of Visual Representations. doi:10.48550/arXiv.2002.05709.

SimCLR

- The NT-Xent (Normalized Temperature-Scaled Cross-Entropy Loss) loss function allows to achieve this. It is a variant of the Noise Contrastive Estimator (NCE) loss.

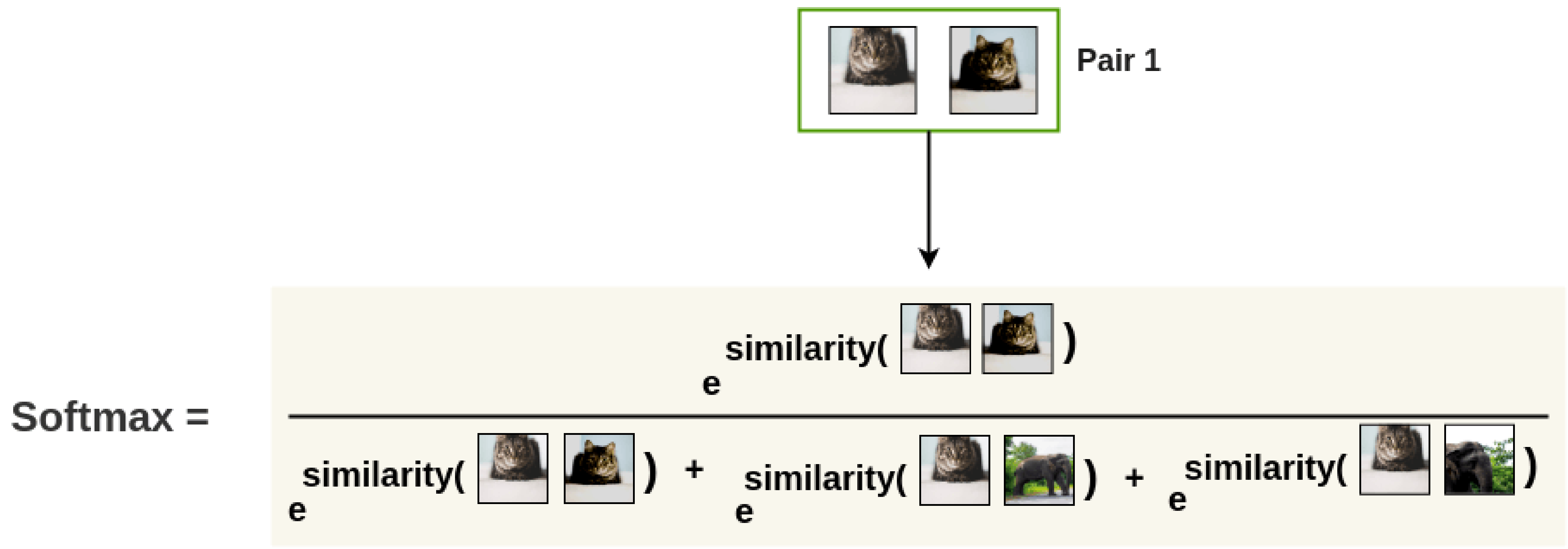
- Let's first transform the cosine similarity between two images i and j into a probability using a softmax:

$$s(i,j) = \frac{\exp \frac{\cos(\mathbf{z}_i, \mathbf{z}_j)}{\tau}}{\sum_{k \neq i} \exp \frac{\cos(\mathbf{z}_i, \mathbf{z}_k)}{\tau}}$$



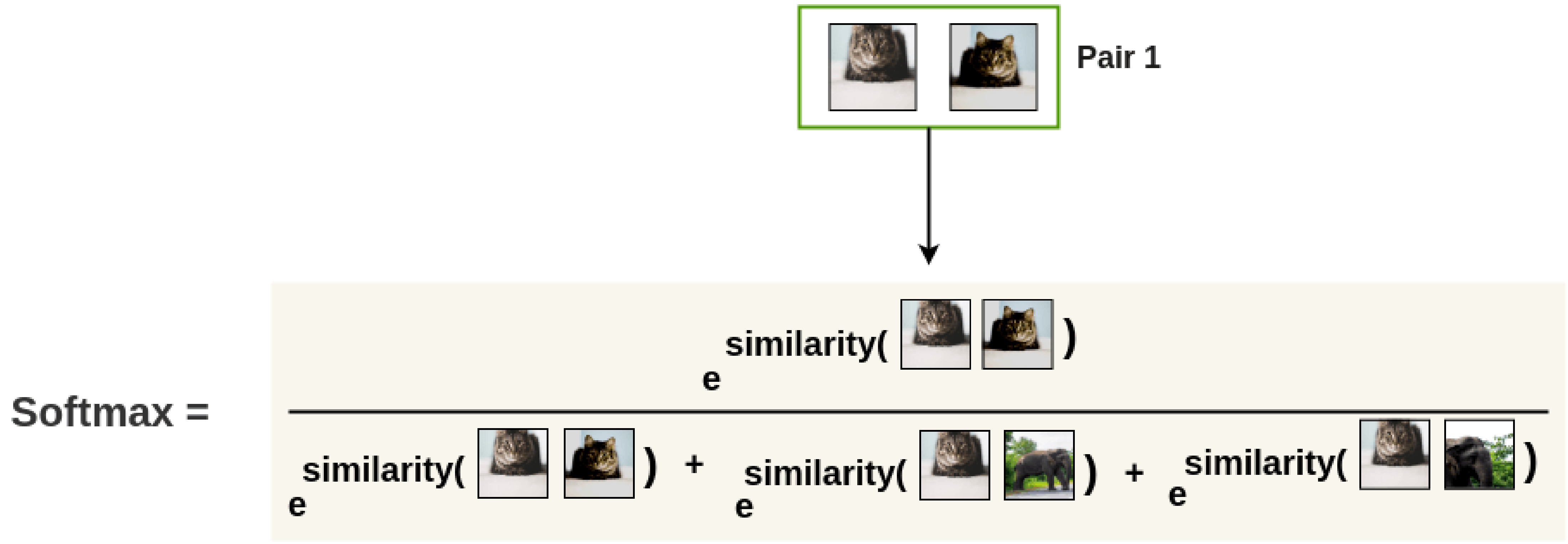
Source: https://amitness.com/2020/03/illustrated-simclr/

- For a positive pair, this softmax represents the probability that the second augmented cat is closer to the first one, compared to the other negative images in the minibatch:



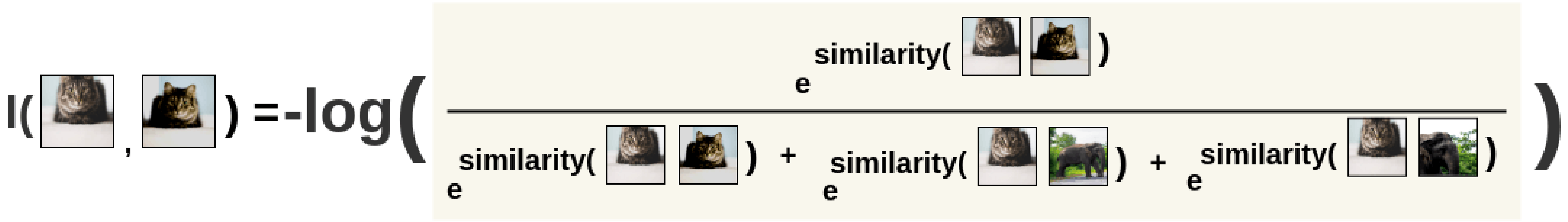
SimCLR

- By maximizing this probability for a positive pair, we not only maximize the similarity between them, but we also minimize the similarity with the negative pairs, as they appear at the denominator!



- In practice, we will minimize the **negative log-likelihood**:

$$l(i, j) = -\log s(i, j)$$



Source: https://amitness.com/2020/03/illustrated-simclr/

SimCLR

- Note that the loss function is not symmetric, as the denominator changes:

Source: https://amitness.com/2020/03/illustrated-simclr/

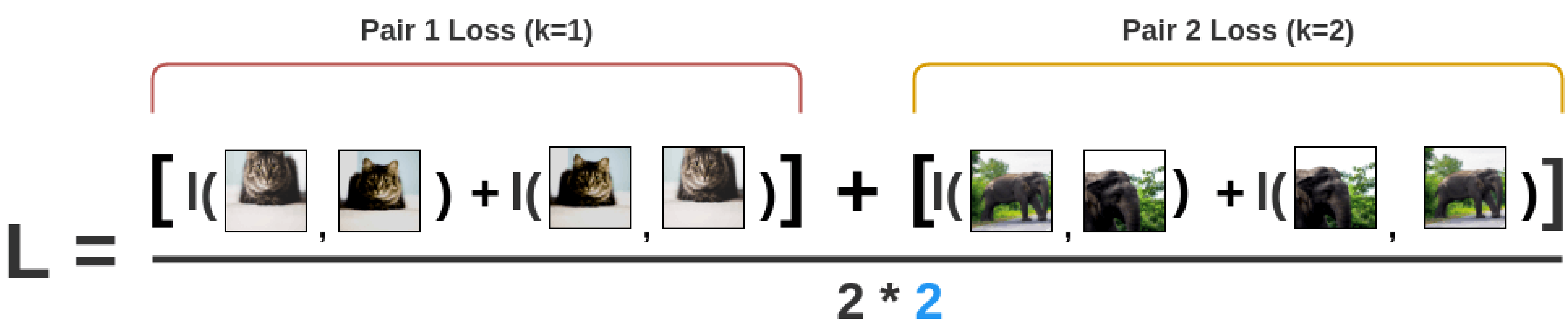
- For a positive pair $(2k, 2k+1)$, we will then average the two losses:

$$l(k) = \frac{- \log s(2k, 2k+1) - \log s(2k+1, 2k)}{2}$$

SimCLR

- Finally, we sum over all positive pairs in the minibatch to obtain the **NT-Xent** (Normalized Temperature-Scaled Cross-Entropy Loss) loss:

$$\mathcal{L}(\theta) = - \frac{1}{2\,K} \sum_{k=1}^{K} \log s(2k, 2k+1) + \log s(2k+1, 2k)$$



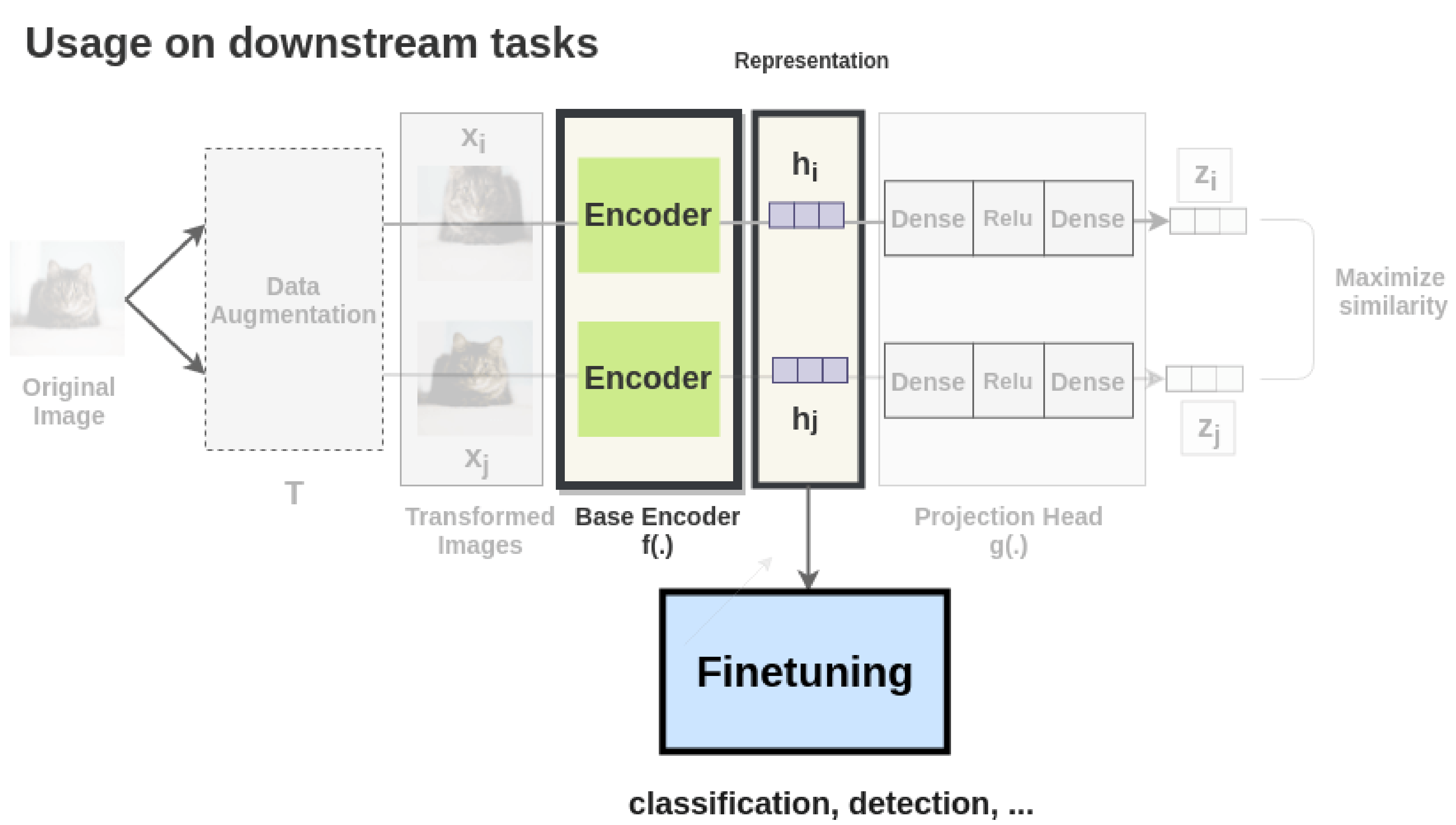
- The loss is defined only over positive pairs in the minibatch, but the negative pairs influence it through the softmax.
- The temperature plays an important role and should be adapted to the batch size and the number of epochs.

SimCLR

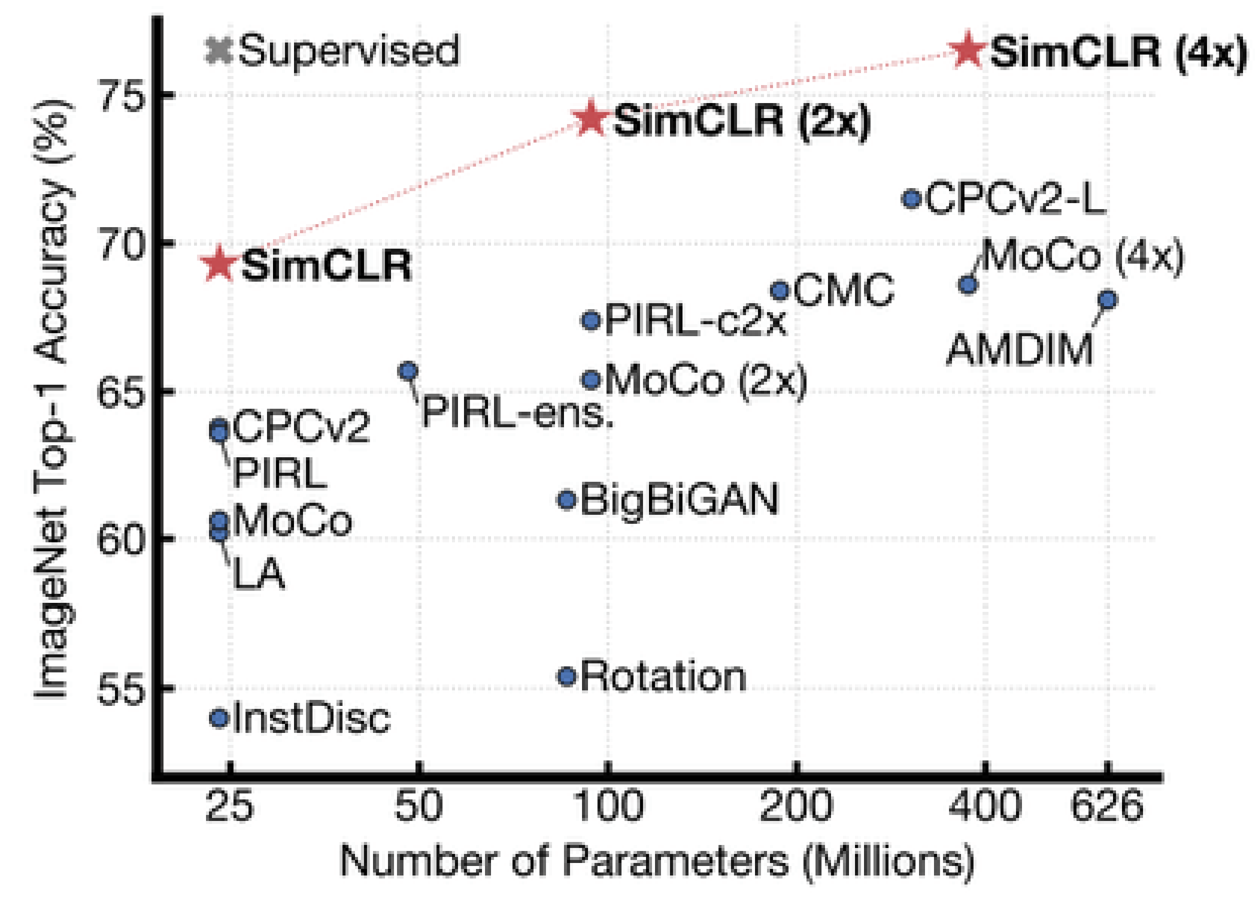
- After performing contrastive learning on the training set of ImageNet (or bigger), the Resnet-50 encoder can be used to:

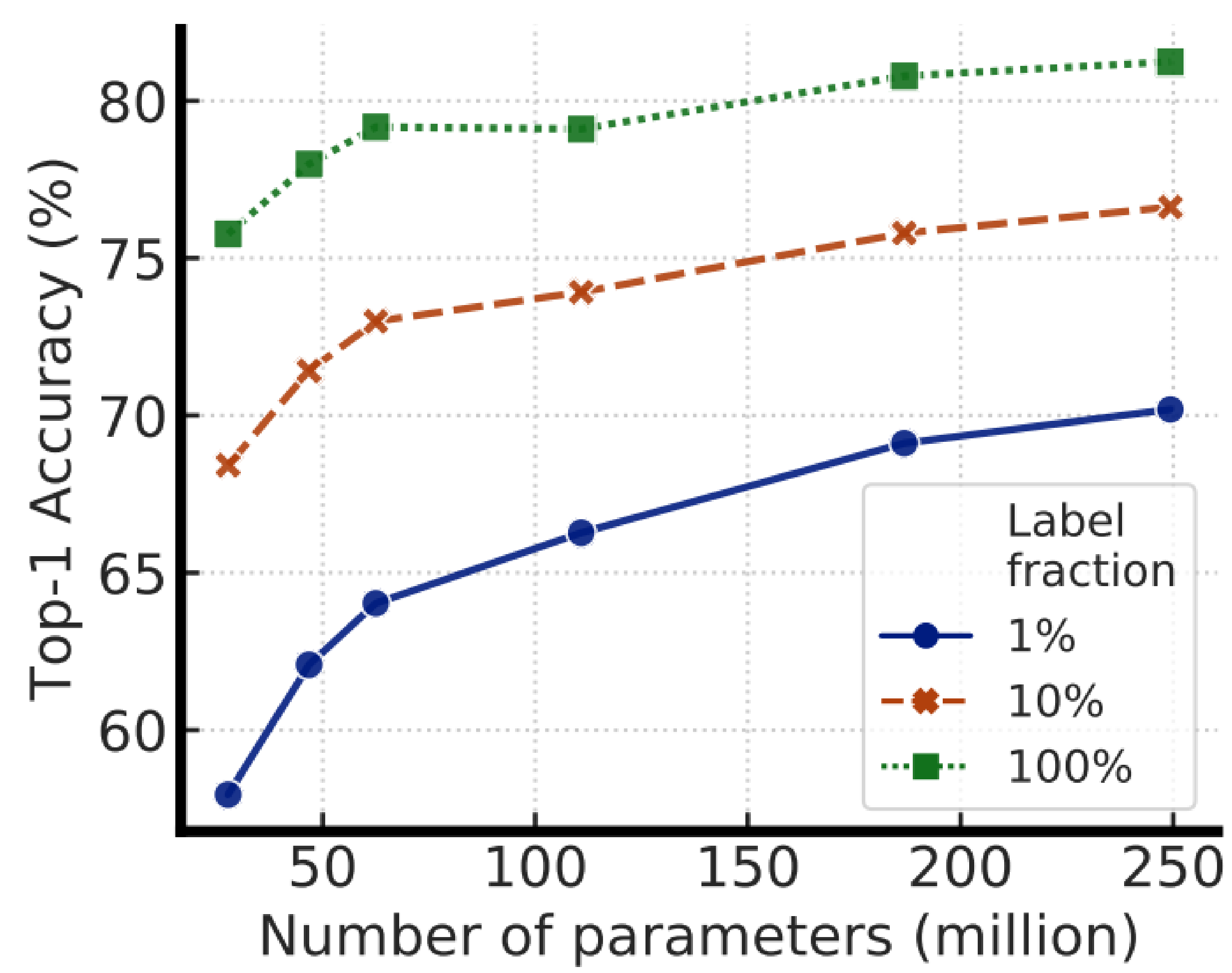
1. linearly predict the labels using logistic regression.
2. fine-tune on 1% of the training data.

- A simple logistic regression on the learned representations is already on-par with fully supervised models.



Source: https://amitness.com/2020/03/illustrated-simclr





(c) Semi-supervised (y-axis zoomed)

Additional resources

https://amitness.com/2020/03/illustrated-simclr/

https://towardsdatascience.com/understanding-contrastive-learning-d5b19fd96607

https://lilianweng.github.io/posts/2019-11-10-self-supervised/

https://lilianweng.github.io/posts/2021-05-31-contrastive

https://uvadlc-notebooks.readthedocs.io/en/latest/tutorial_notebooks/tutorial17/SimCLR.html

https://docs.google.com/presentation/d/1ccddJFD_j3p3h0TCqSV9ajSi2y1yOfh0-lJoK29ircs

https://sthalles.github.io/simple-self-supervised-learning/

References

Chen, T., Kornblith, S., Norouzi, M., and Hinton, G. (2020). A Simple Framework for Contrastive Learning of Visual Representations. doi:10.48550/arXiv.2002.05709.

Doersch, C., Gupta, A., and Efros, A. A. (2016). Unsupervised Visual Representation Learning by Context Prediction. doi:10.48550/arXiv.1505.05192.

Gidaris, S., Singh, P., and Komodakis, N. (2018). Unsupervised Representation Learning by Predicting Image Rotations. doi:10.48550/arXiv.1803.07728.

Mikolov, T., Chen, K., Corrado, G., and Dean, J. (2013). Efficient Estimation of Word Representations in Vector Space. http://arxiv.org/abs/1301.3781.

Misra, I., Zitnick, C. L., and Hebert, M. (2016). Shuffle and Learn: Unsupervised Learning using Temporal Order Verification. doi:10.48550/arXiv.1603.08561.

Noroozi, M., and Favaro, P. (2017). Unsupervised Learning of Visual Representations by Solving Jigsaw Puzzles. doi:10.48550/arXiv.1603.09246.

Pathak, D., Krahenbuhl, P., Donahue, J., Darrell, T., and Efros, A. A. (2016). Context Encoders: Feature Learning by Inpainting. doi:10.48550/arXiv.1604.07379.

Vincent, P., Larochelle, H., Lajoie, I., Bengio, Y., and Manzagol, P.-A. (2010). Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion. *J. Mach. Learn. Res.* 11, 3371–3408.