Self-supervised learning

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ECMWF

Introduction

"Self-supervised learning: The dark matter of intelligence"

https://ai.meta.com/blog/self-supervised-learning-the-dark-matter-of-intelligence/

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Motivation--two sides of the same coin:

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- Well-trained networks with 100s of millions or billions of parameters behave qualitatively differently and provide robust generalization
  - LLMs can answer a wide range of questions not seen during training
  - AIFS, Pangu-Weather, GraphCast provide skillful predictions multiple years past their training data set

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1. Feature spaces:

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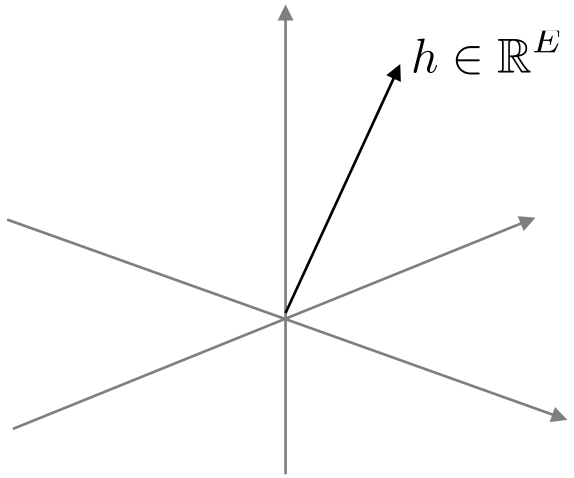

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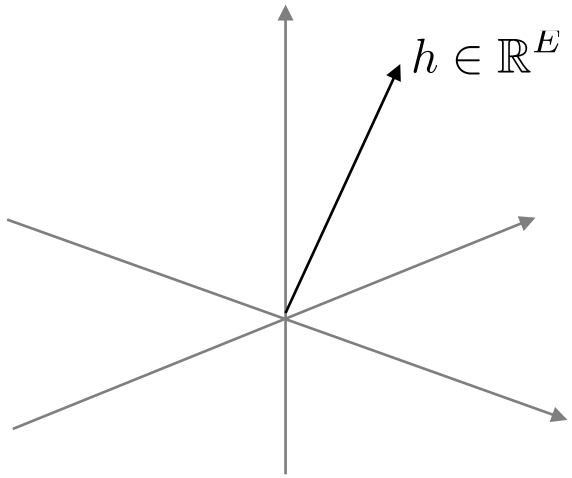

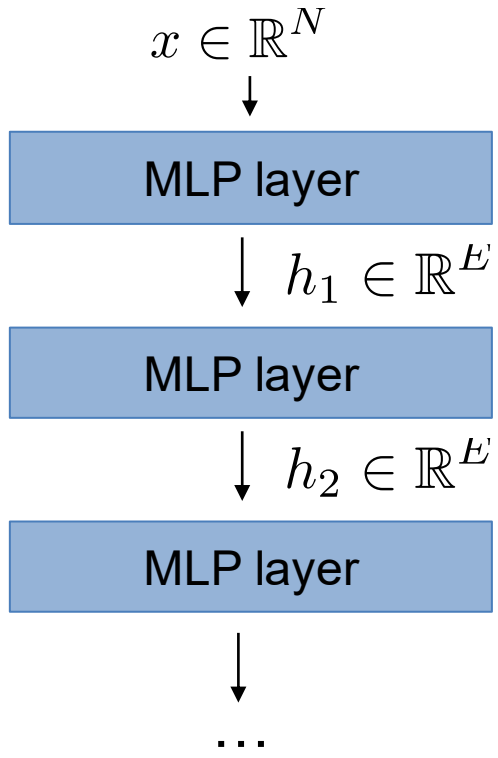

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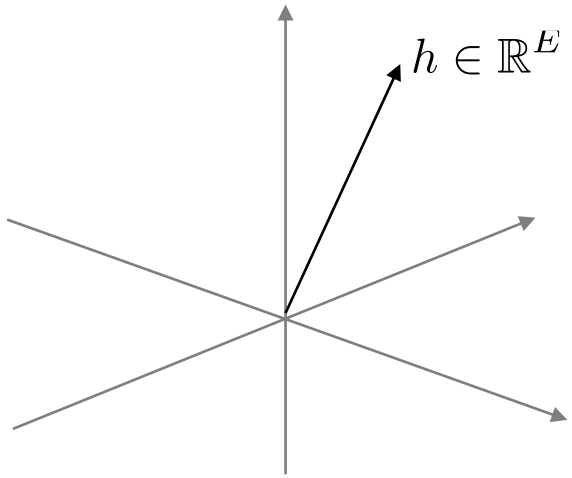

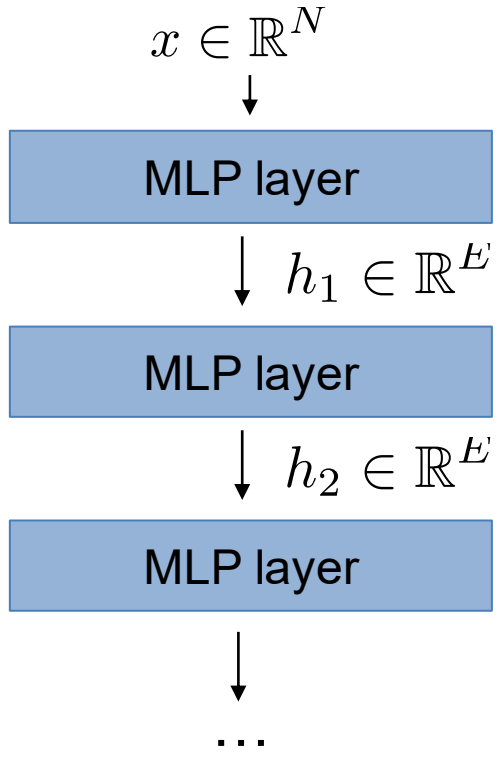

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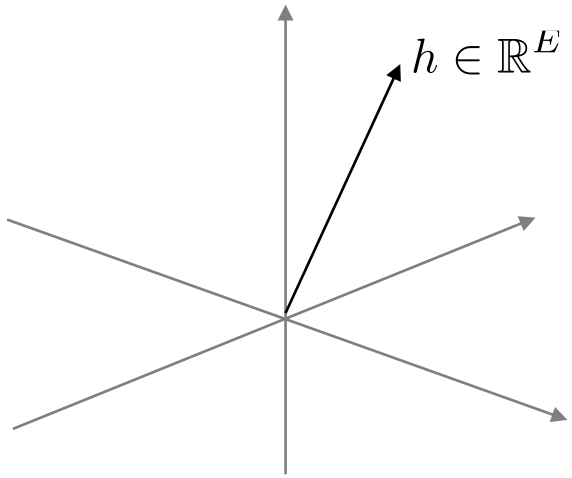

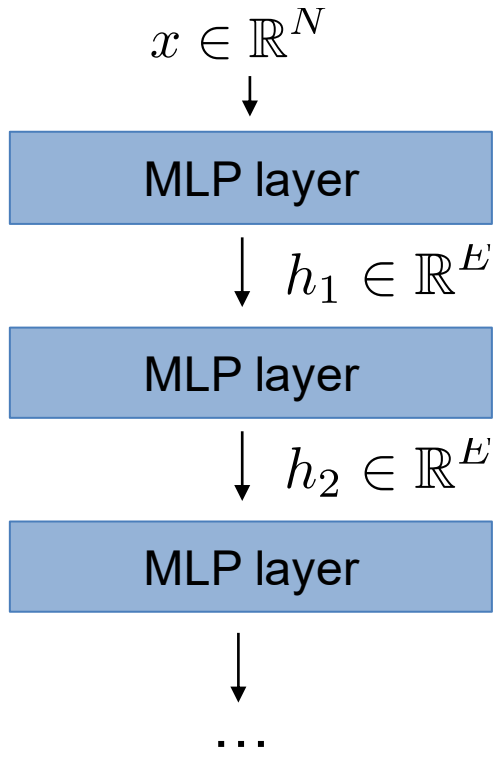

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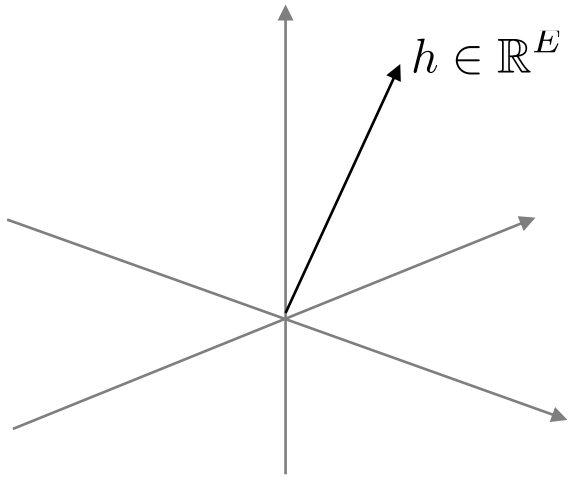

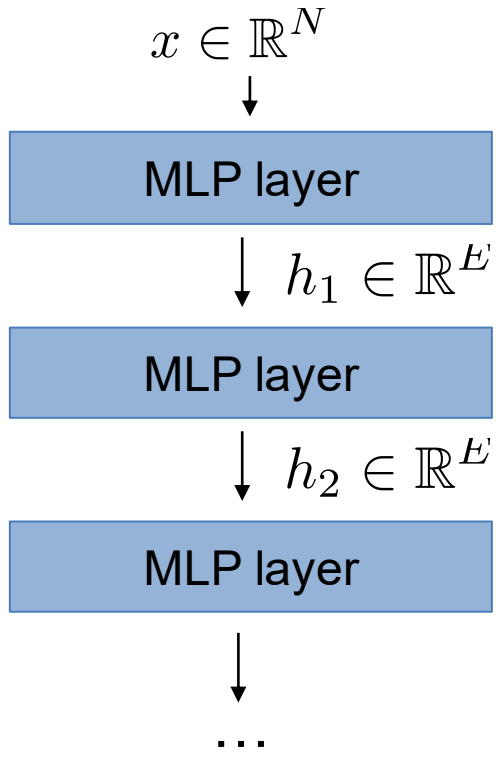

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1. Feature spaces: convolutional features

https://arxiv.org/pdf/1506.06579

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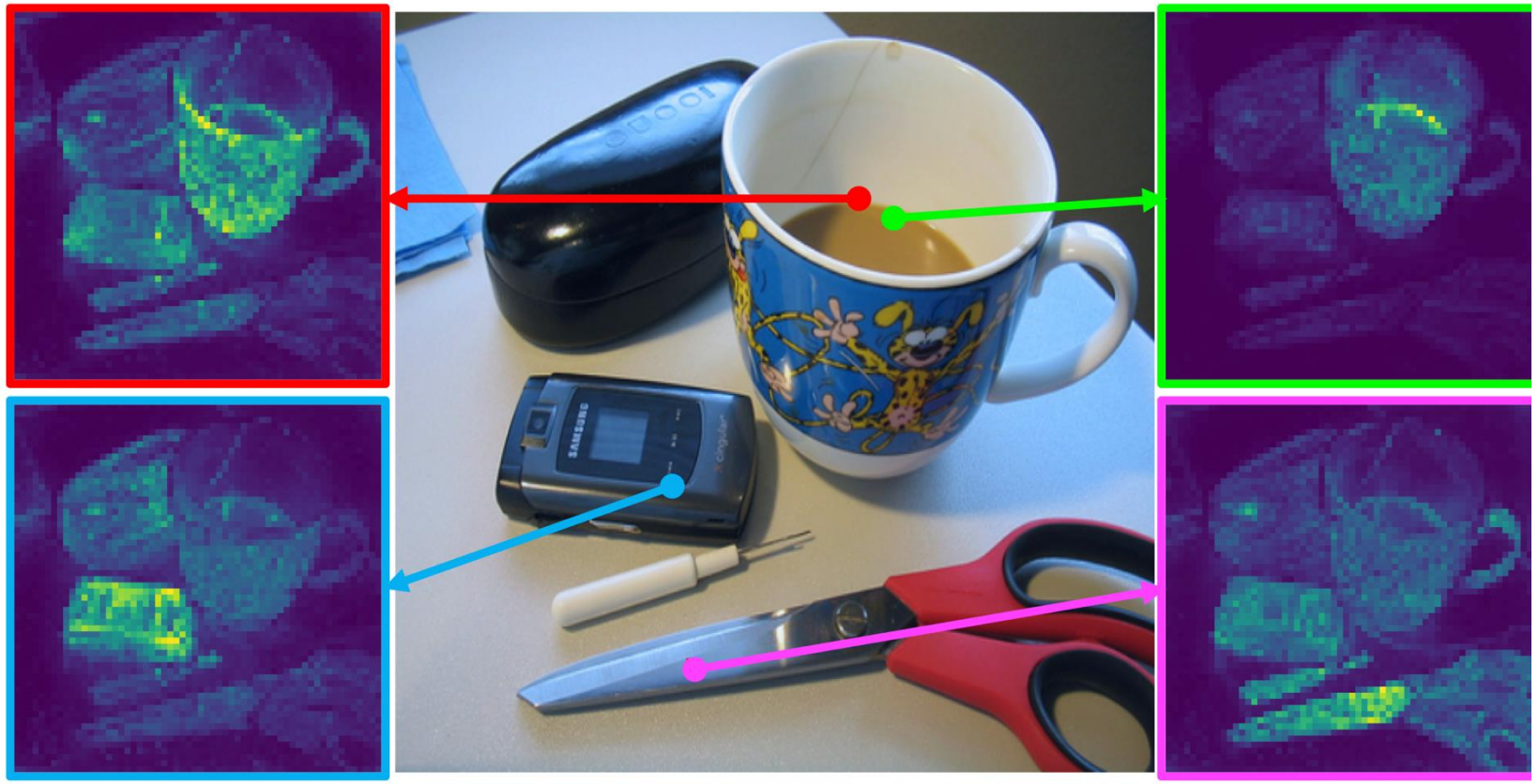
1. Feature spaces: attention maps



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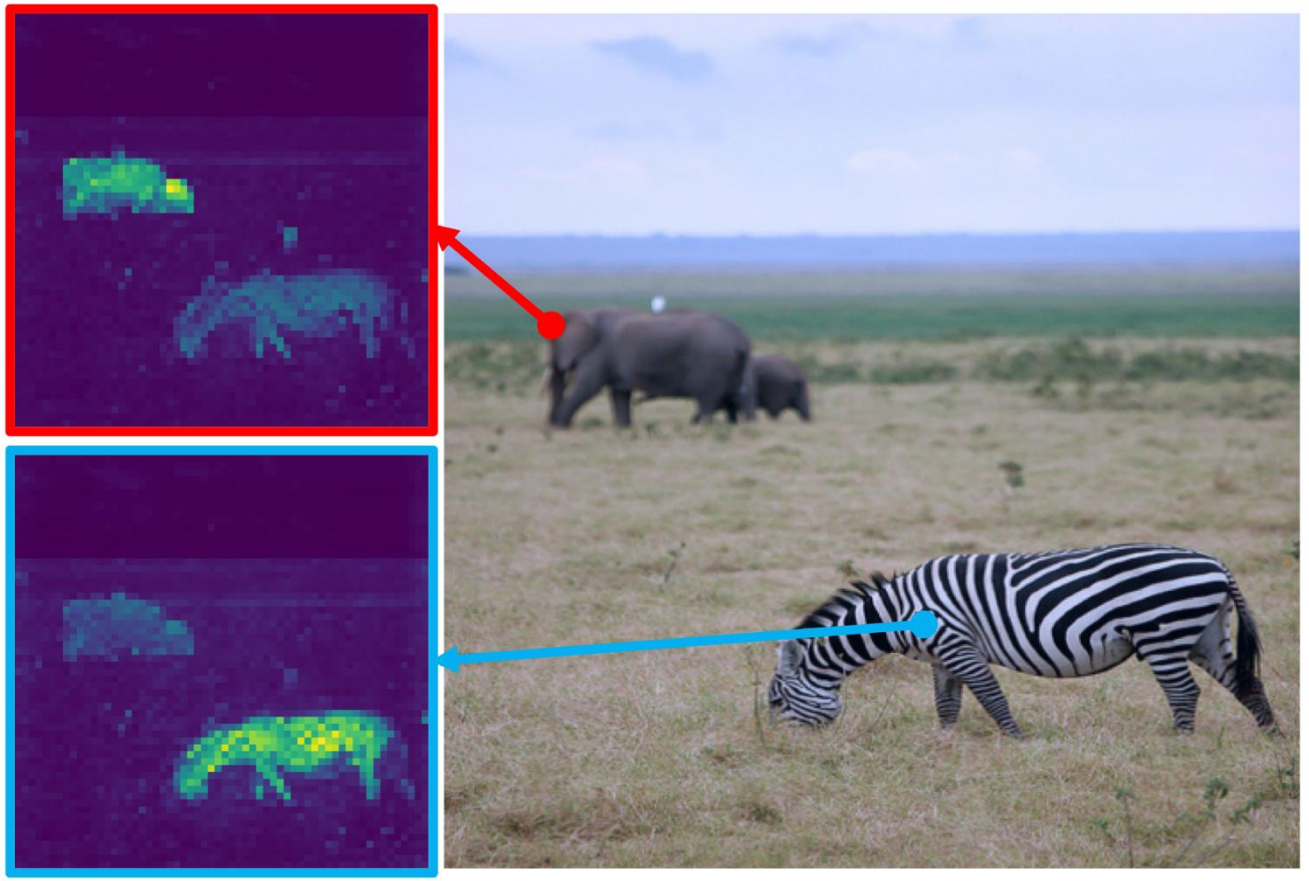

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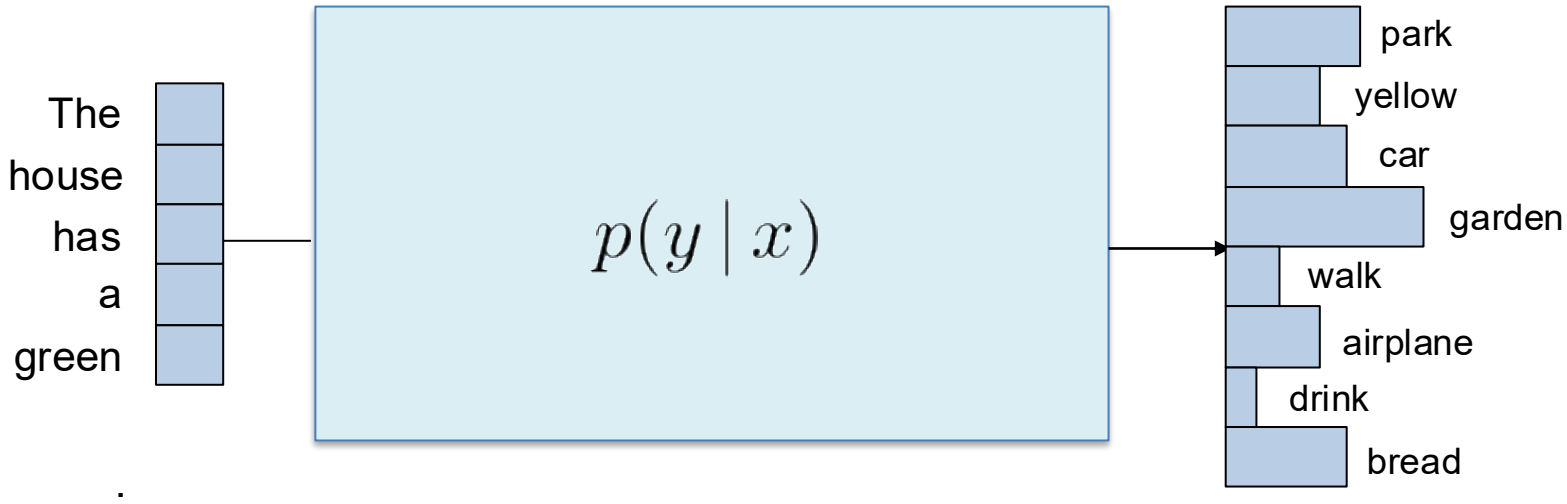

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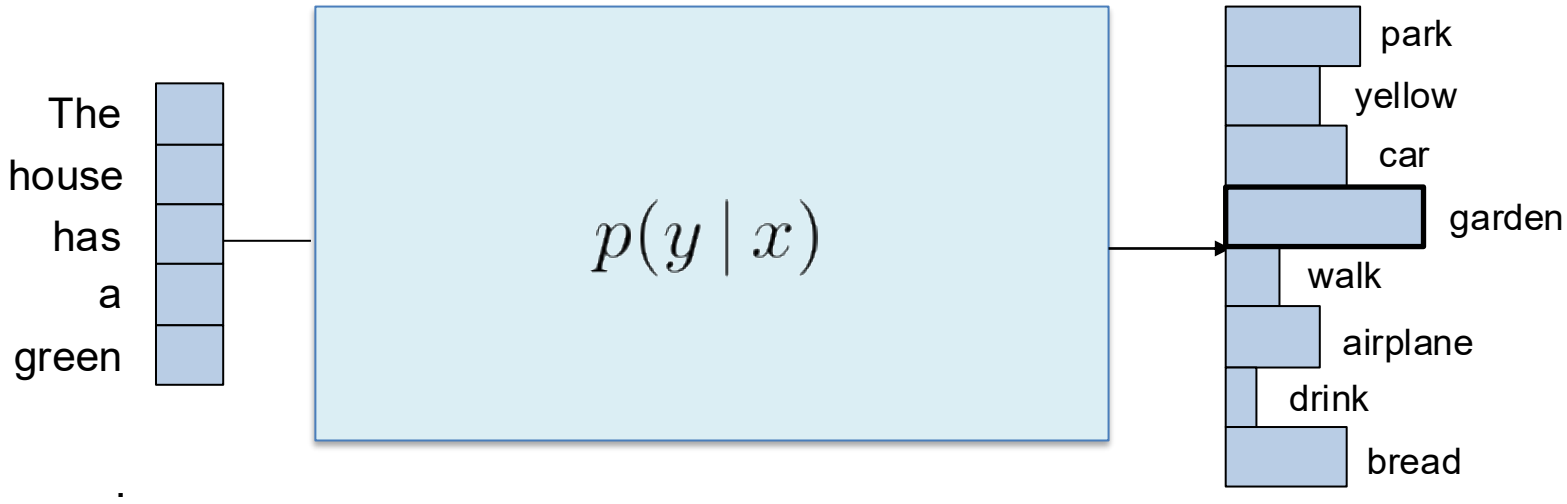

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     - Creative writing: x = content outline, y = long text form
     - …

How can large neural networks generalize?

Zero-shot

The model predicts the answer given only a natural language description of the task. No gradient updates are performed.

```
1  Translate English to French:        ← task description
2  cheese =>                           ← prompt
```

Brown et al., Language Models are Few-Shot Learners, 2020, https://arxiv.org/pdf/2005.14165.pdf

How can large neural networks generalize?

One-shot

In addition to the task description, the model sees a single example of the task. No gradient updates are performed.

```
1  Translate English to French:        ← task description
2  sea otter => loutre de mer          ← example
3  cheese =>                           ← prompt
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Few-shot

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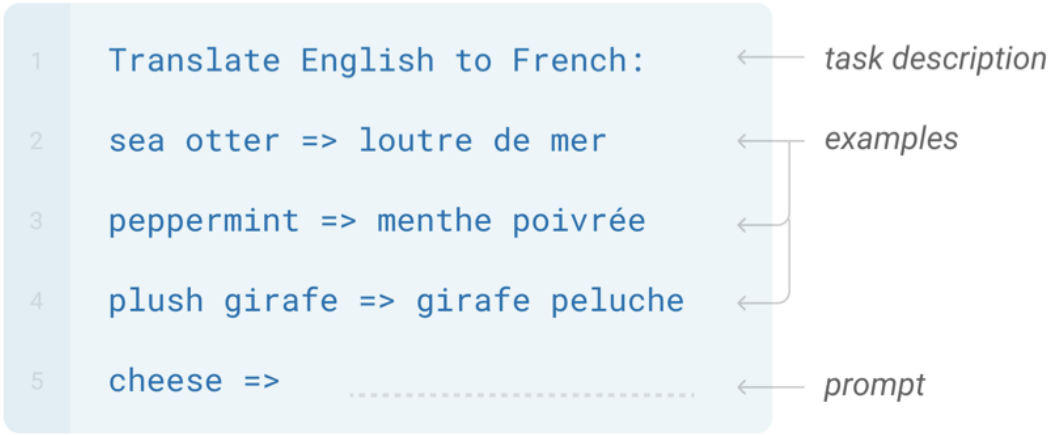

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     - Creative writing: x = content outline, y = long text form
   - Fine-tuning to calibrate the output distribution
     - E.g. make certain undesirable words/phrases less likely

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     - Spatial interpolation: x = incomplete state, y = completed state
     - …

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Two perspectives:

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   - Learning yields representation of data that reveals intrinsic structure
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=> Self-supervised learning to realize this

Self-supervised learning tasks

Self-supervised learning: define a training task from a dataset without an explicit set of labels

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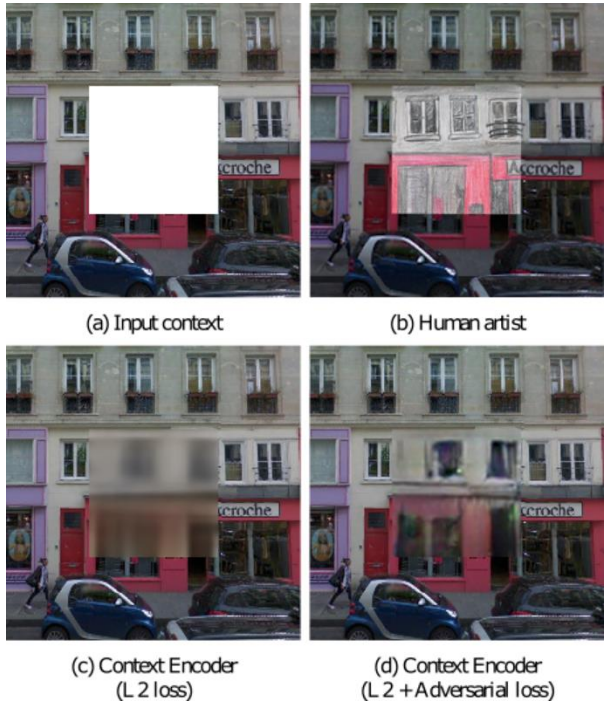

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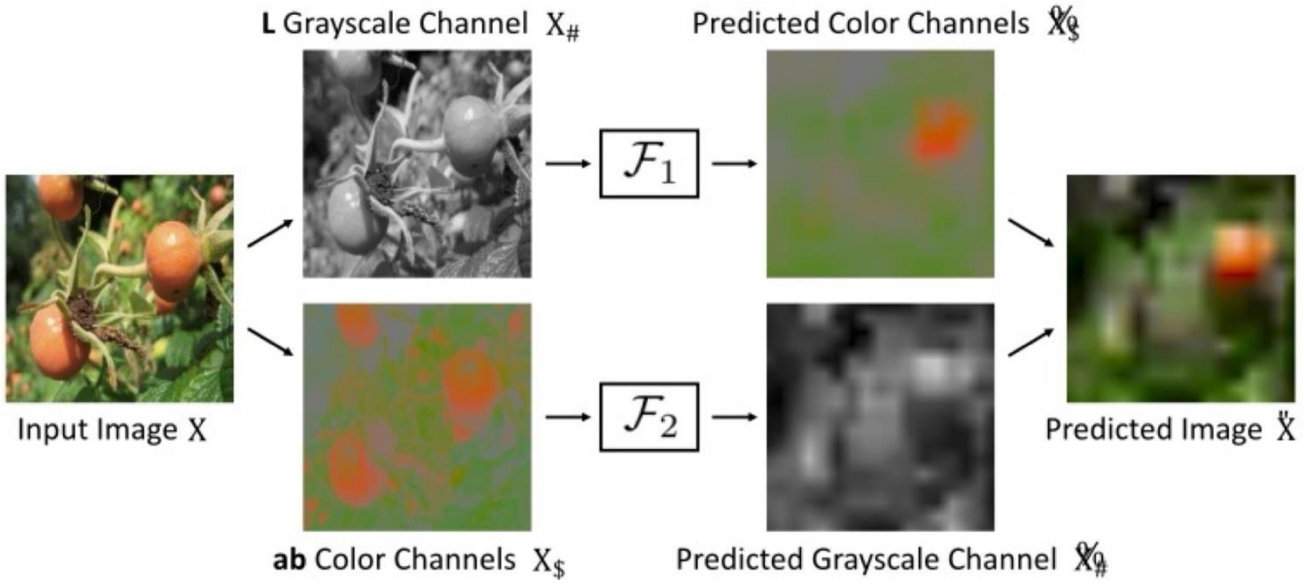

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Self-supervised learning tasks

Self-supervised learning: define a training task from a dataset without an explicit set of labels

=> “hide” some information from the data when input to the network, and network predicts this information

Transformer takes sequence of data chunks (tokens) as input

- ((sub-)words, image patches, local atmospheric states, …)

=> mask some of the patches from the network during input (or remove them entirely) and network predicts these

Self-supervised learning tasks

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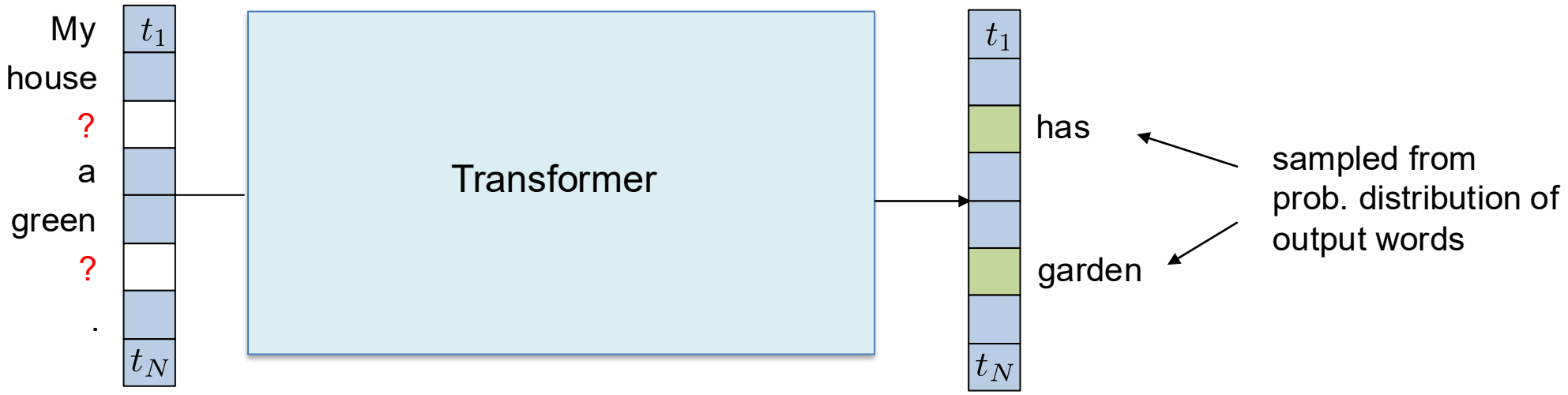
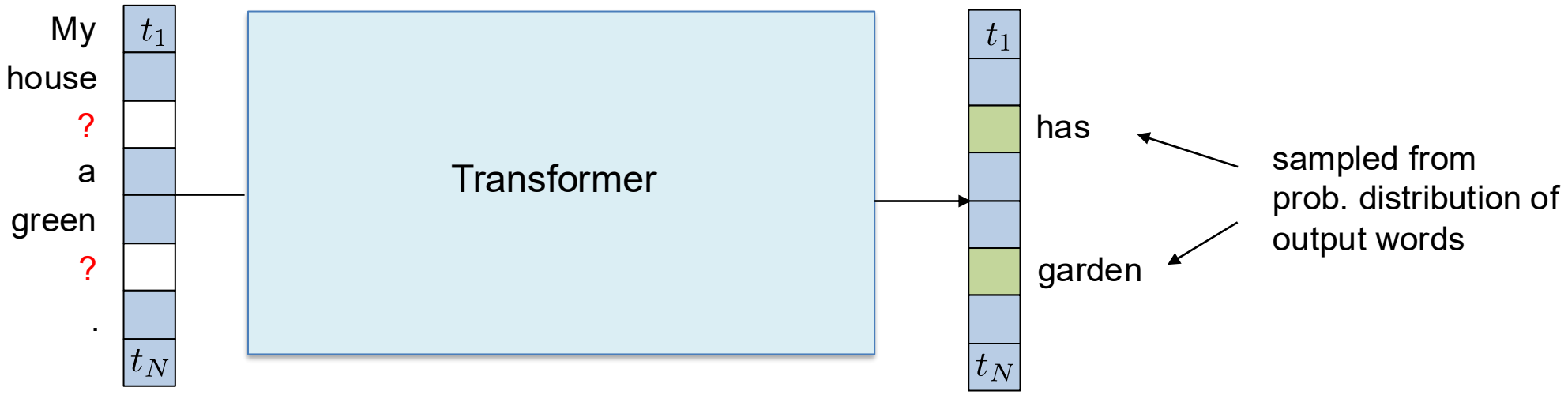


Self-supervised learning tasks

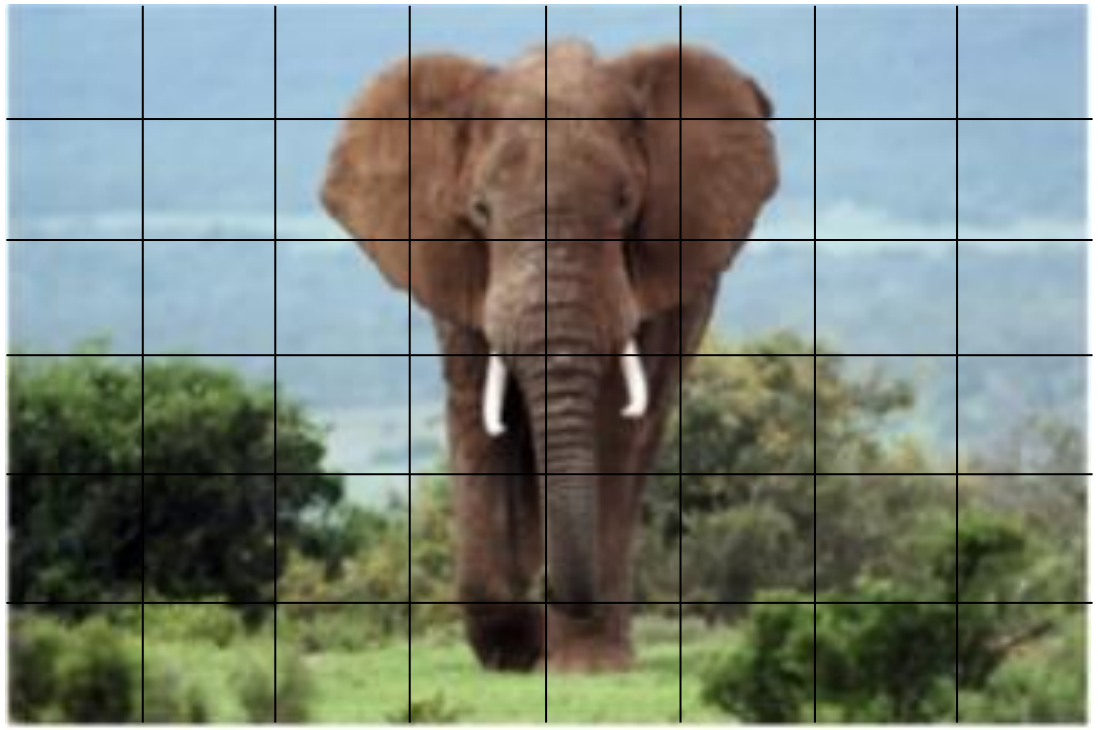
- BERT (Google):[1] randomly mask words from a sequence (and add some random distortions)
- Predictive masking (OpenAI):[2] always mask subsequent words



[1] Devlin et al., BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding, https://arxiv.org/abs/1810.04805
[2] Radford et al. Improving Language Understanding by Generative Pre-Training, https://cdn.openai.com/research-covers/language-unsupervised/language_understanding_paper.pdf

Self-supervised learning tasks

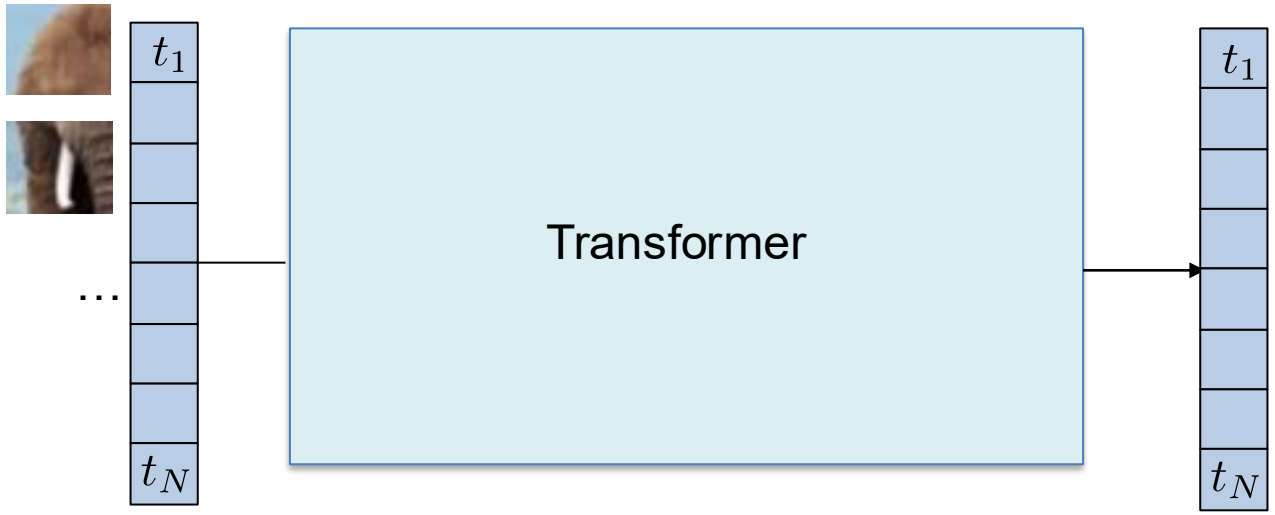
Vision transformer: image is a small patch



Dosovitskiy et al., An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale, 2021, https://arxiv.org/abs/2010.11929

Self-supervised learning tasks

Masked token modeling for images



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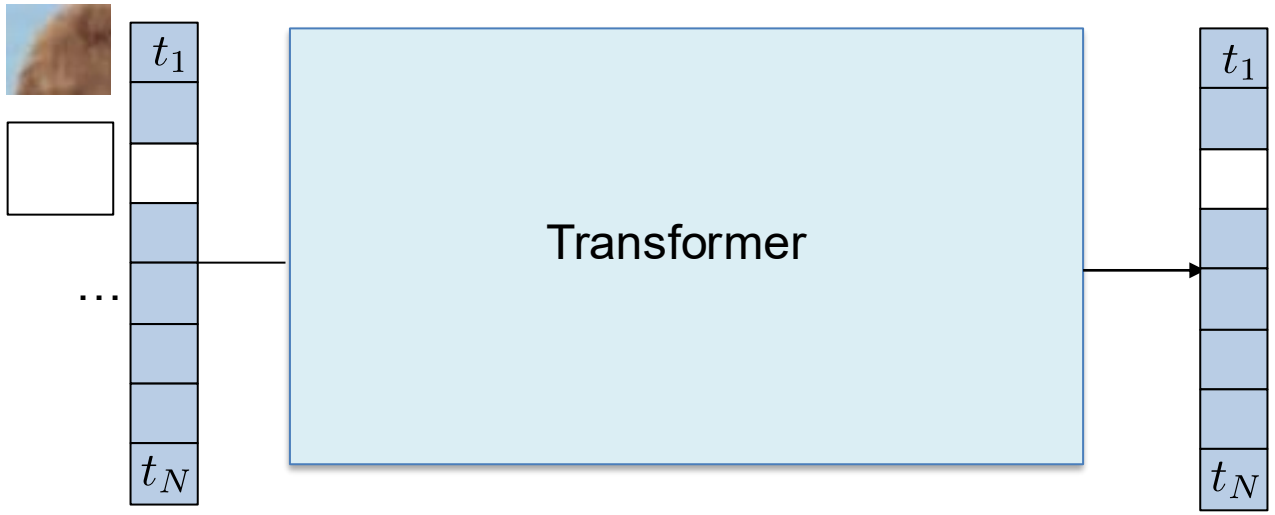

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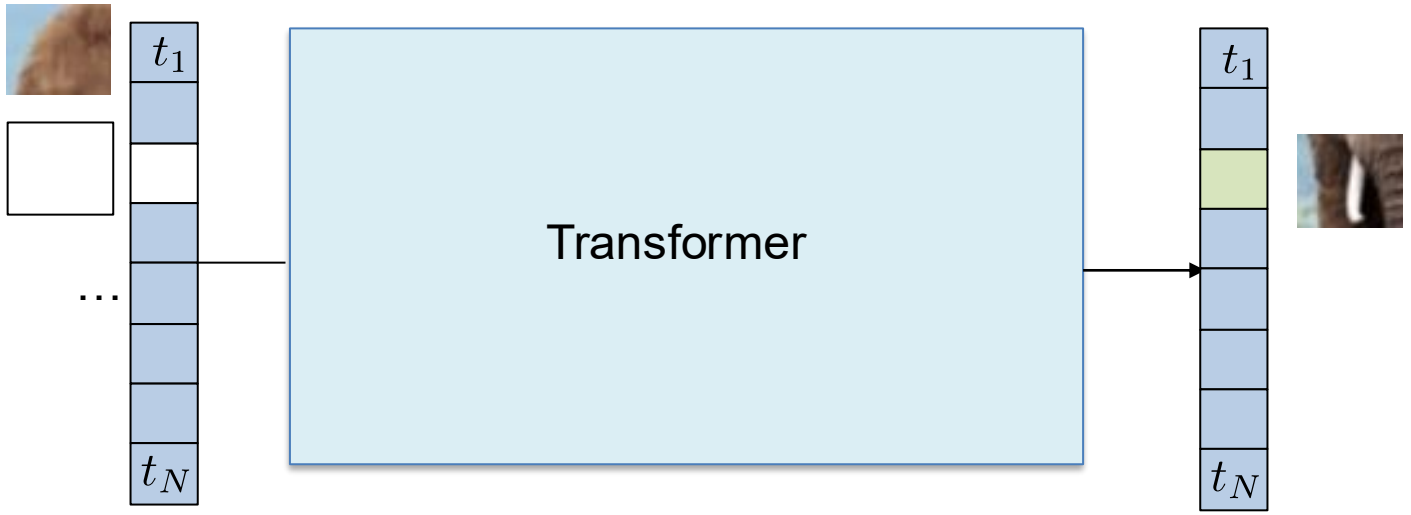

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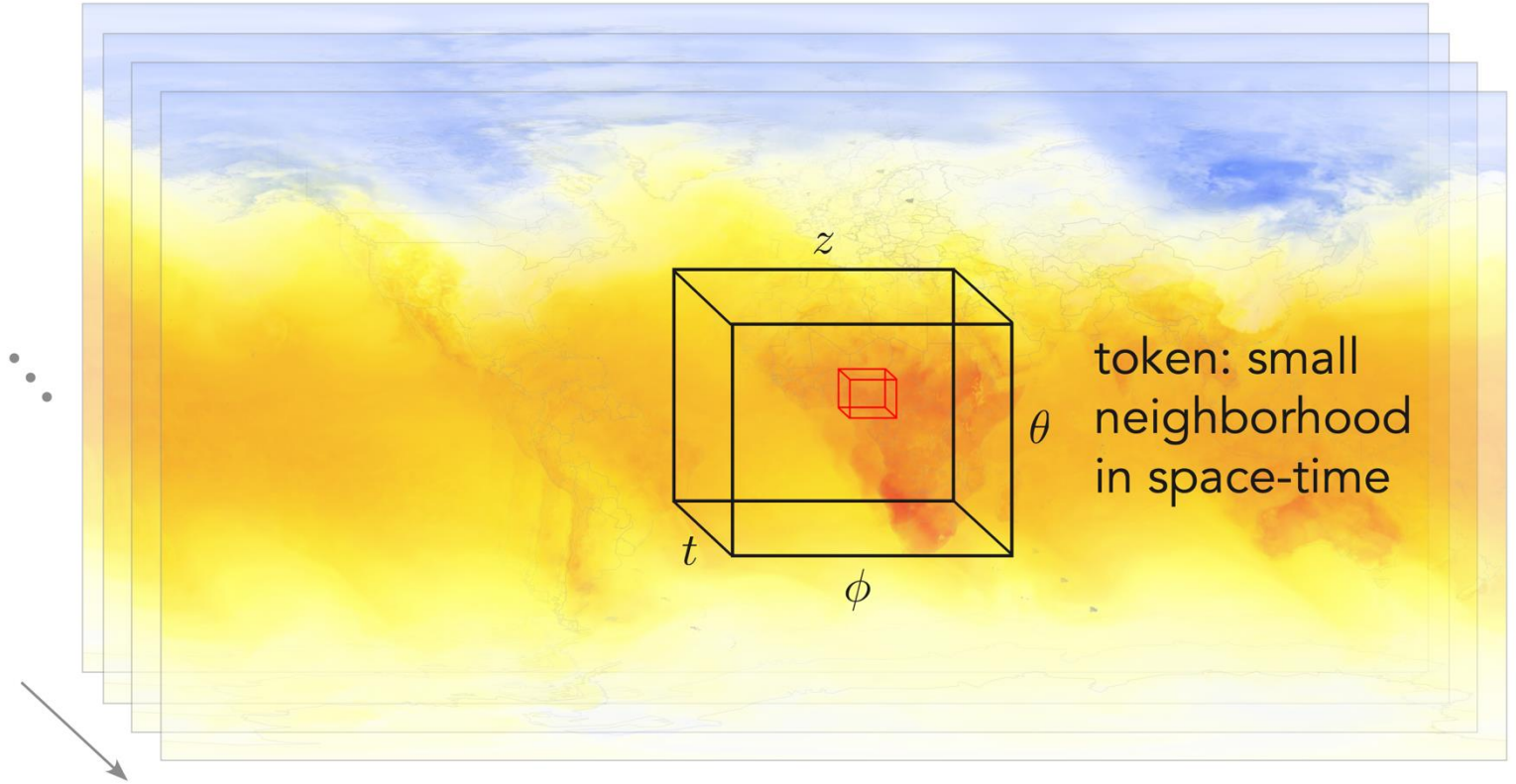
Self-supervised learning tasks

AtmoRep: masked token modeling for atmospheric dynamics



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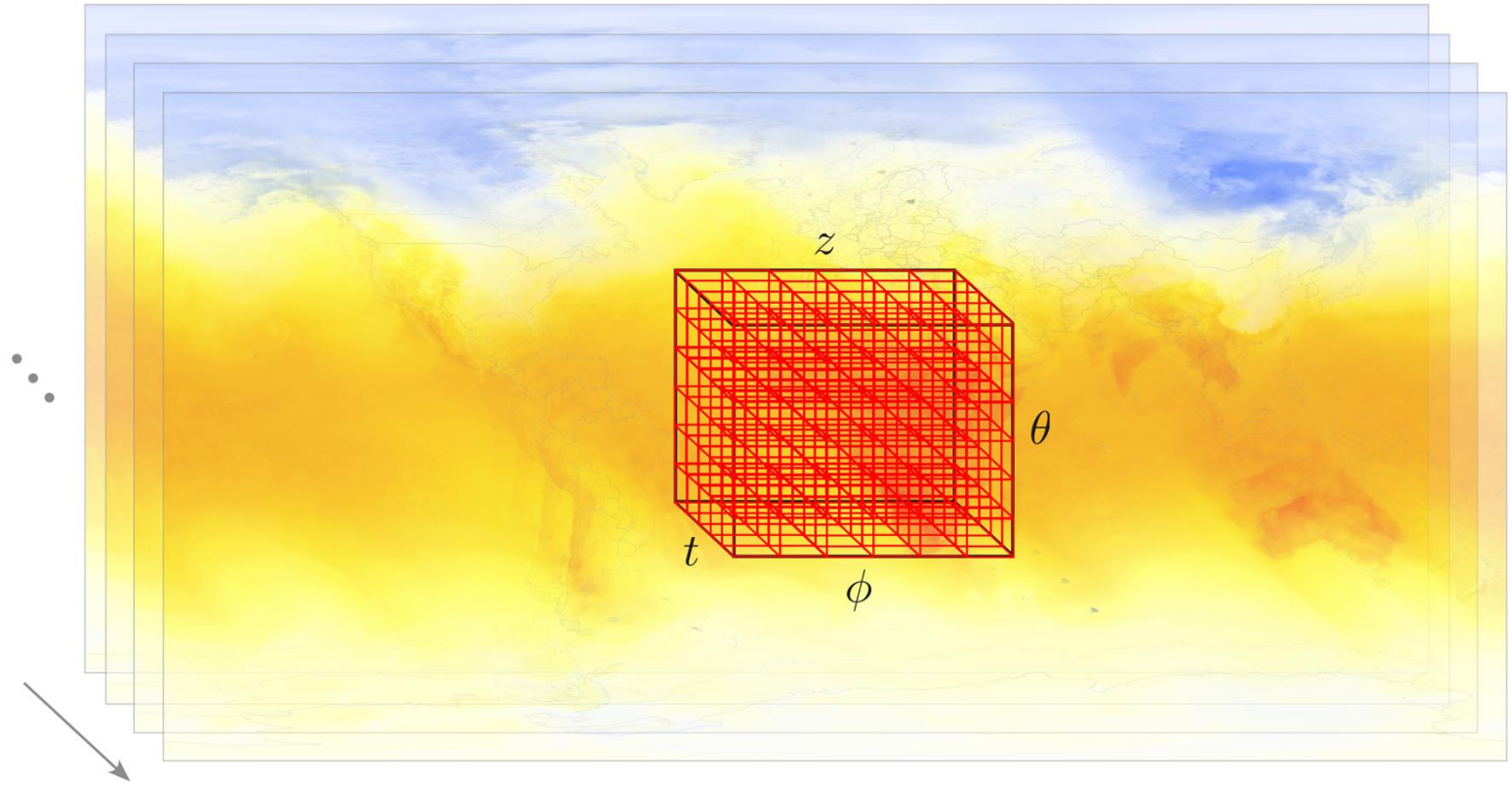

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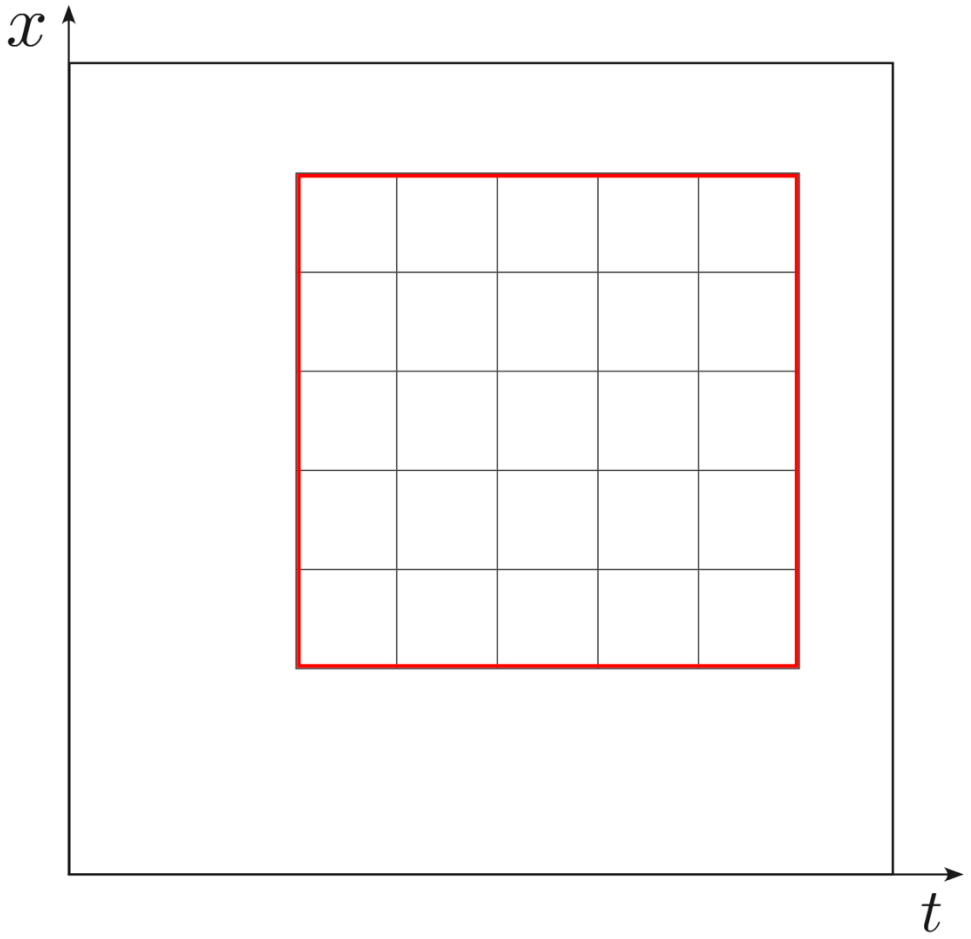
Self-supervised learning tasks

Flatland view



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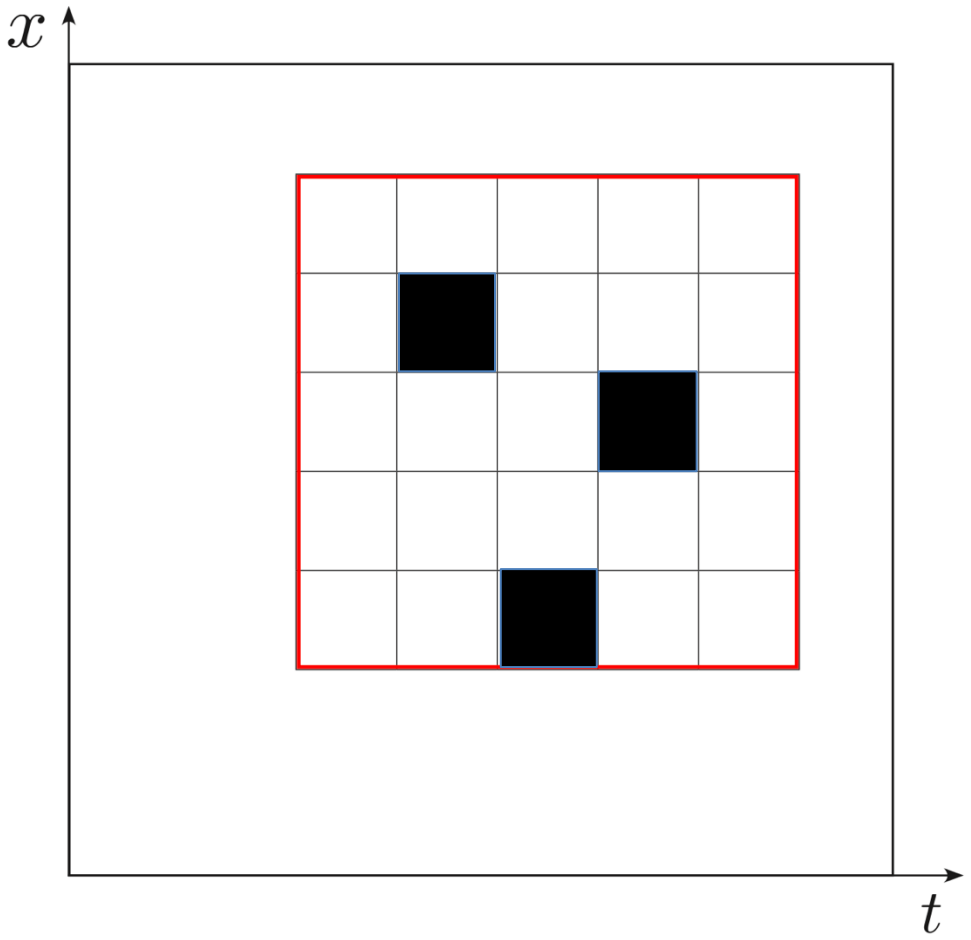

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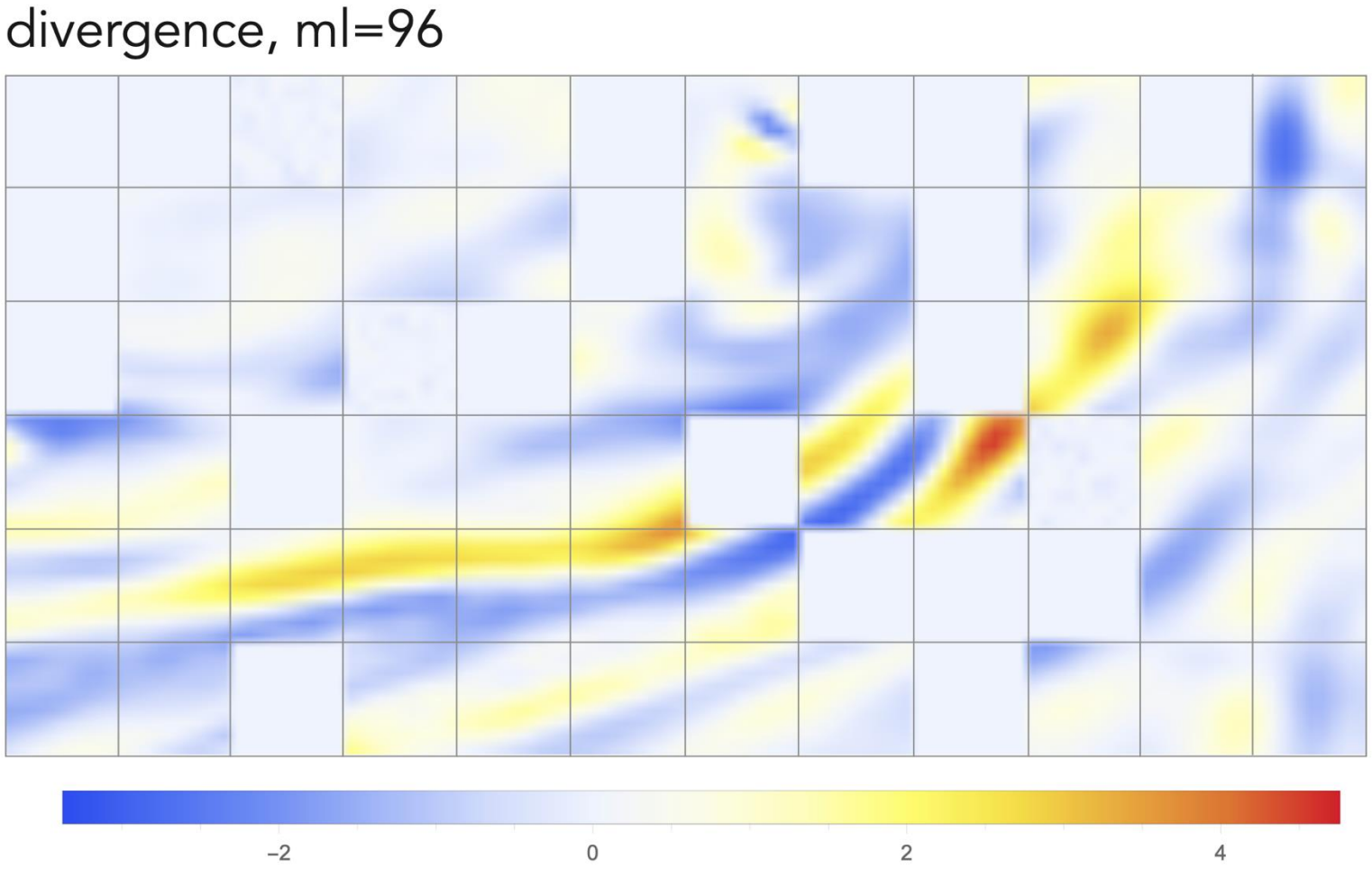

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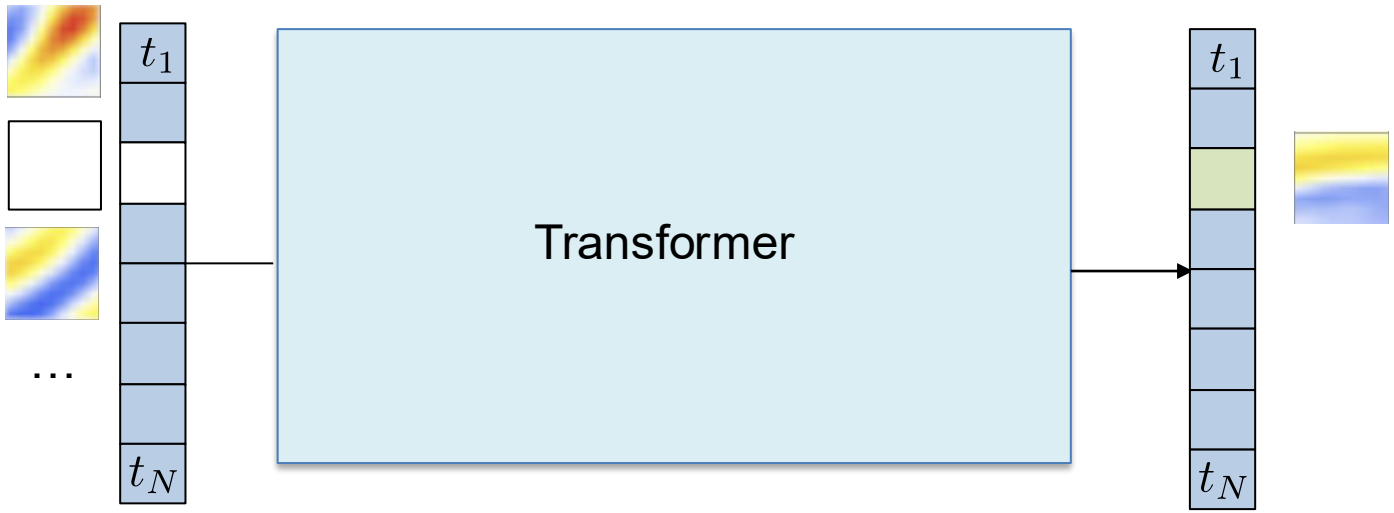

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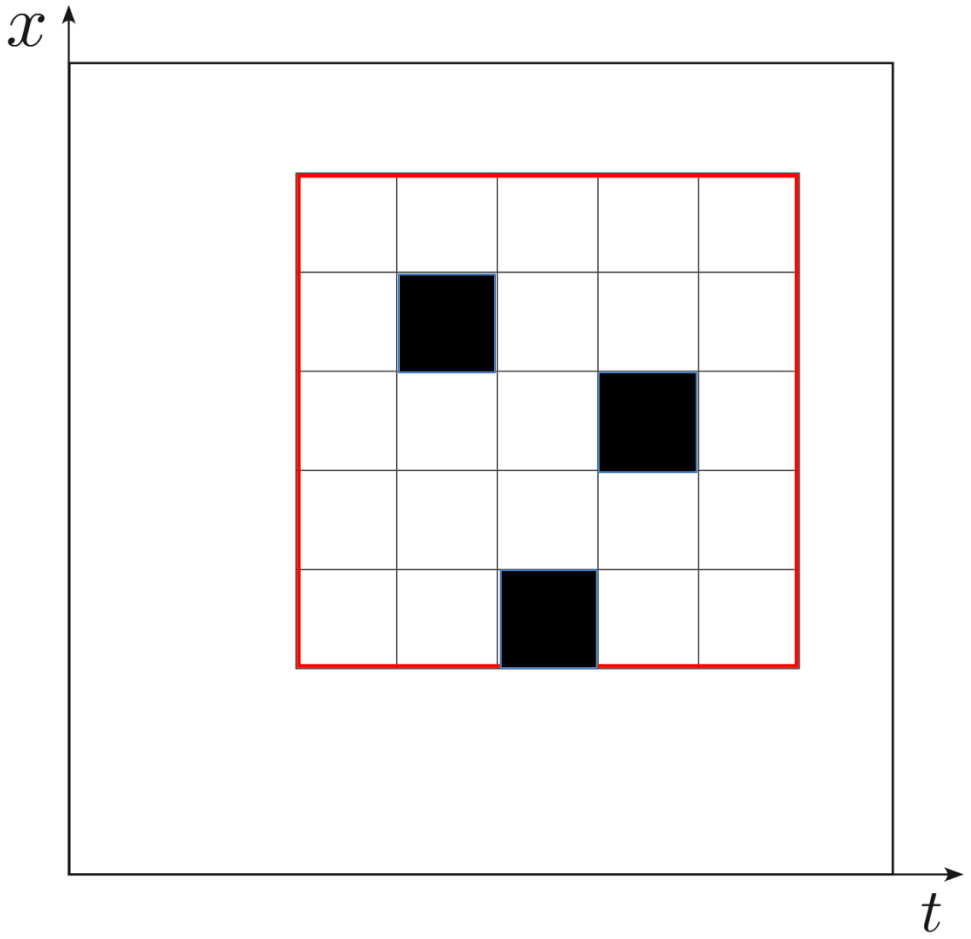
Self-supervised learning tasks

Zero-shot capabilities



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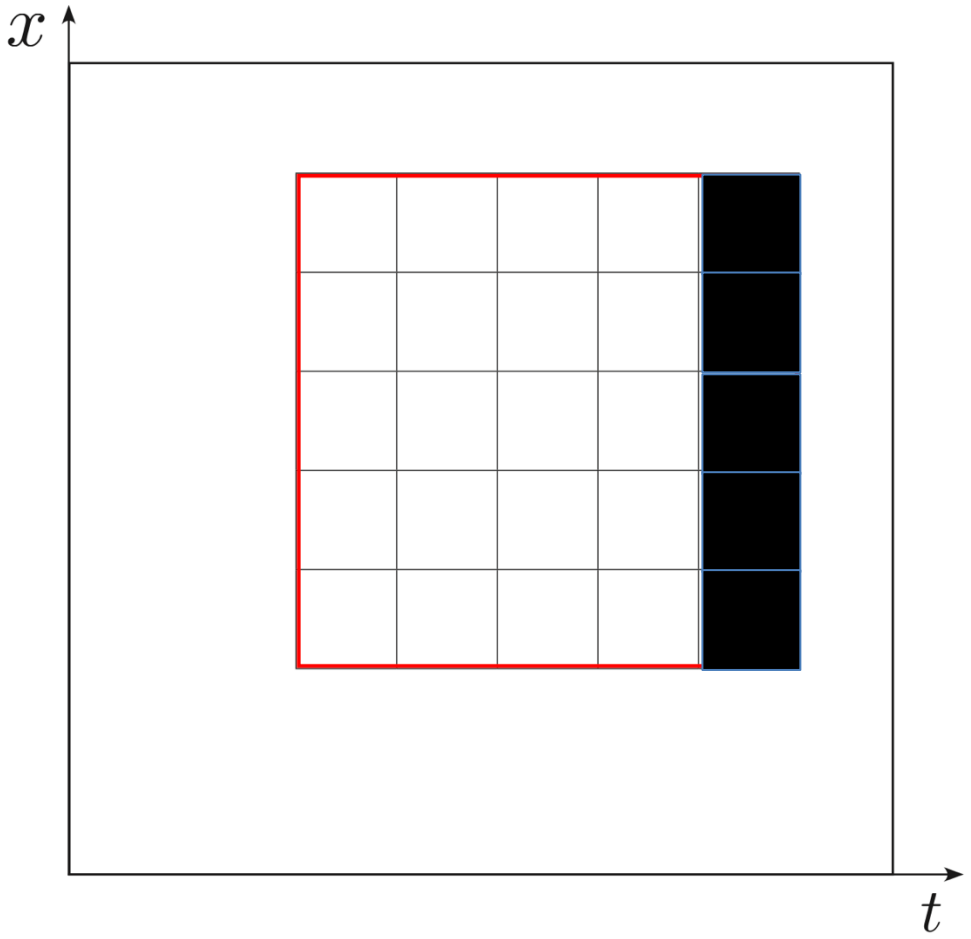

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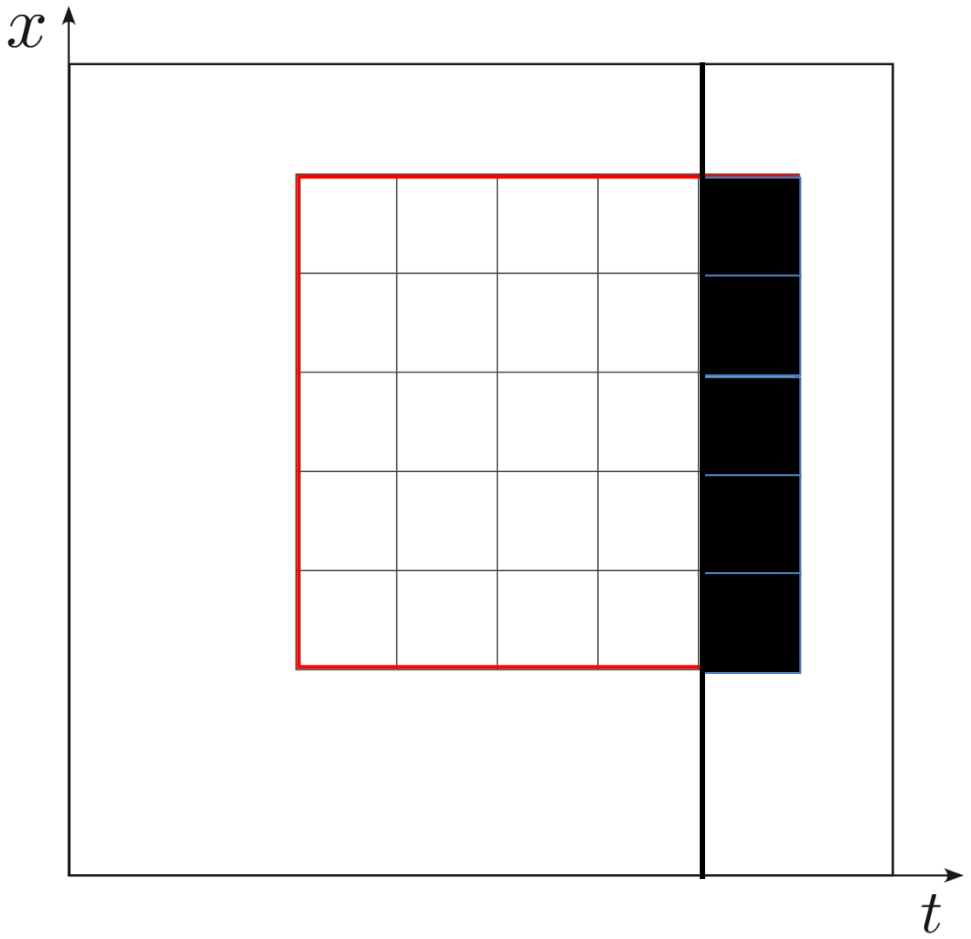

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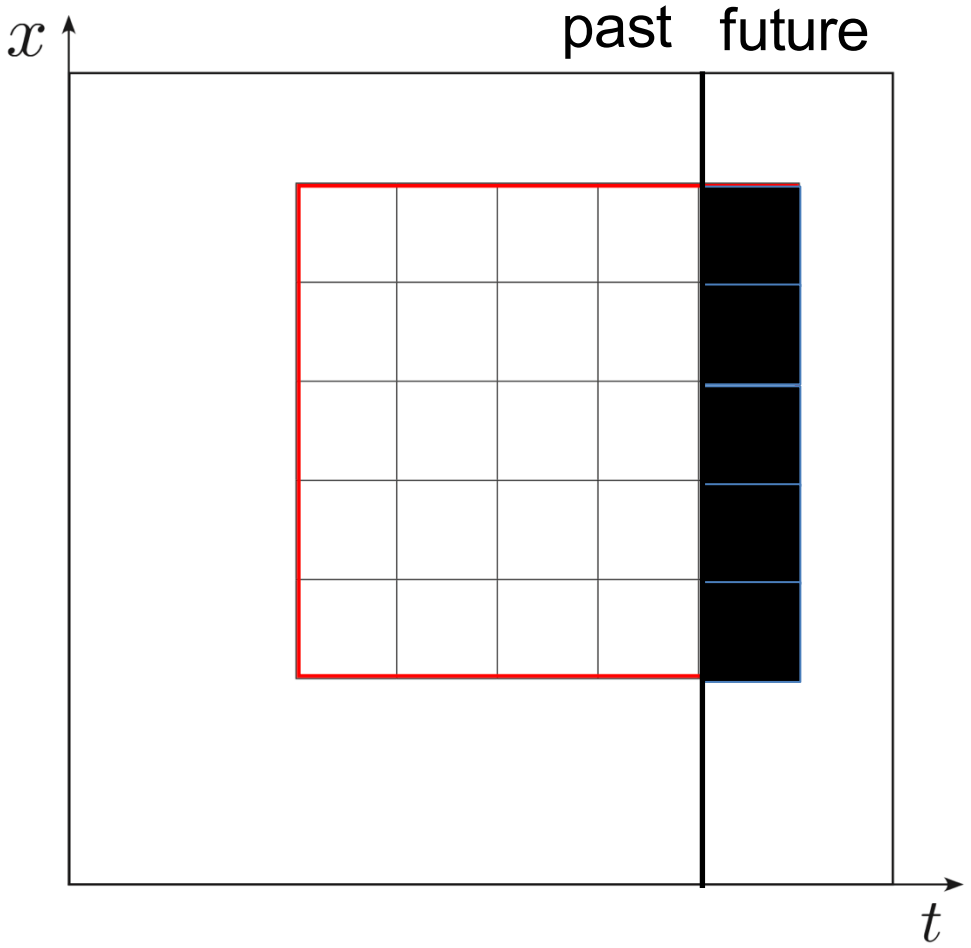
Self-supervised learning tasks

Zero-shot capabilities



Lessig et al., AtmoRep: A Stochastic Model of Atmospheric Dynamics, 2023, https://arxiv.org/abs/2308.13280

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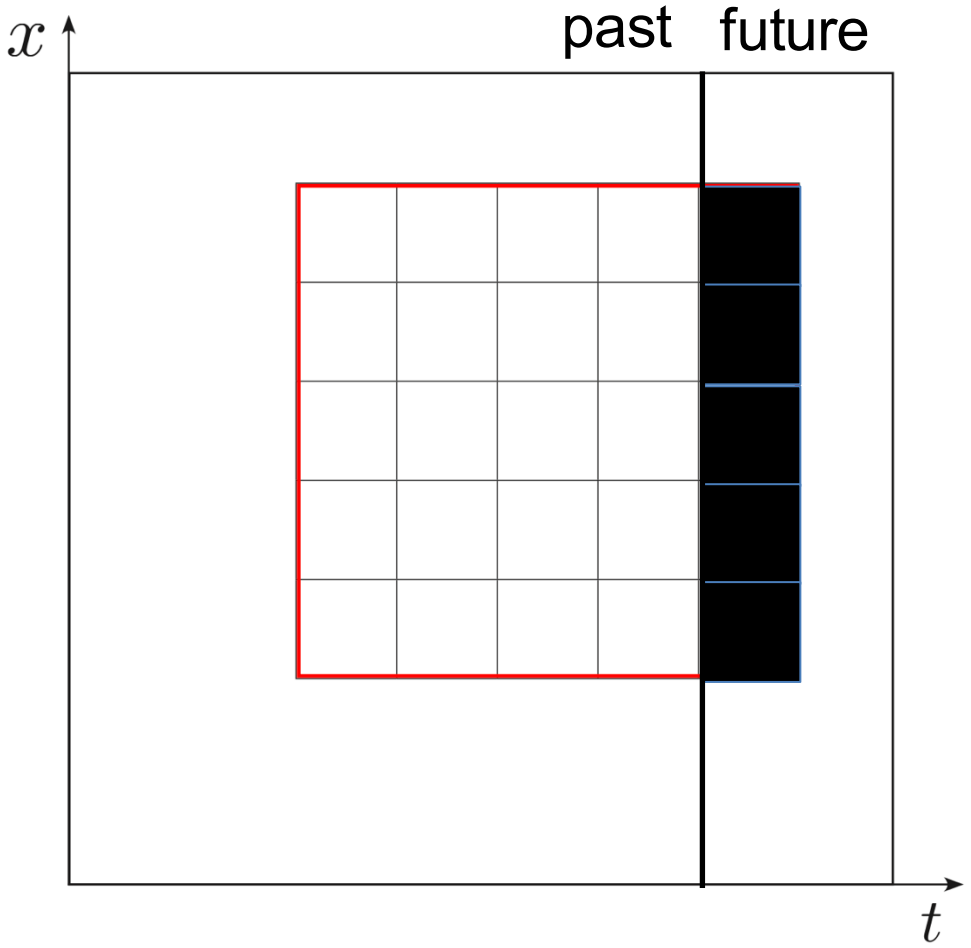

forecasting

Lessig et al., AtmoRep: A Stochastic Model of Atmospheric Dynamics, 2023, https://arxiv.org/abs/2308.13280

Self-supervised learning tasks

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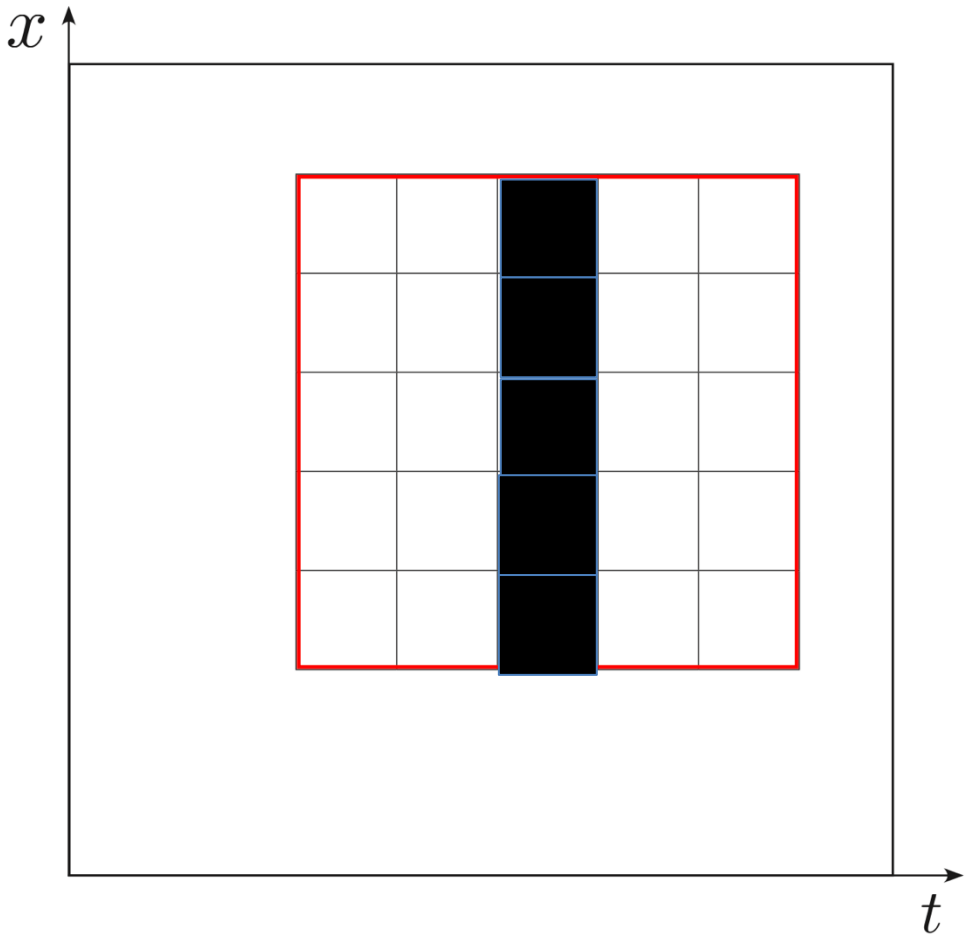

temporal interpolation

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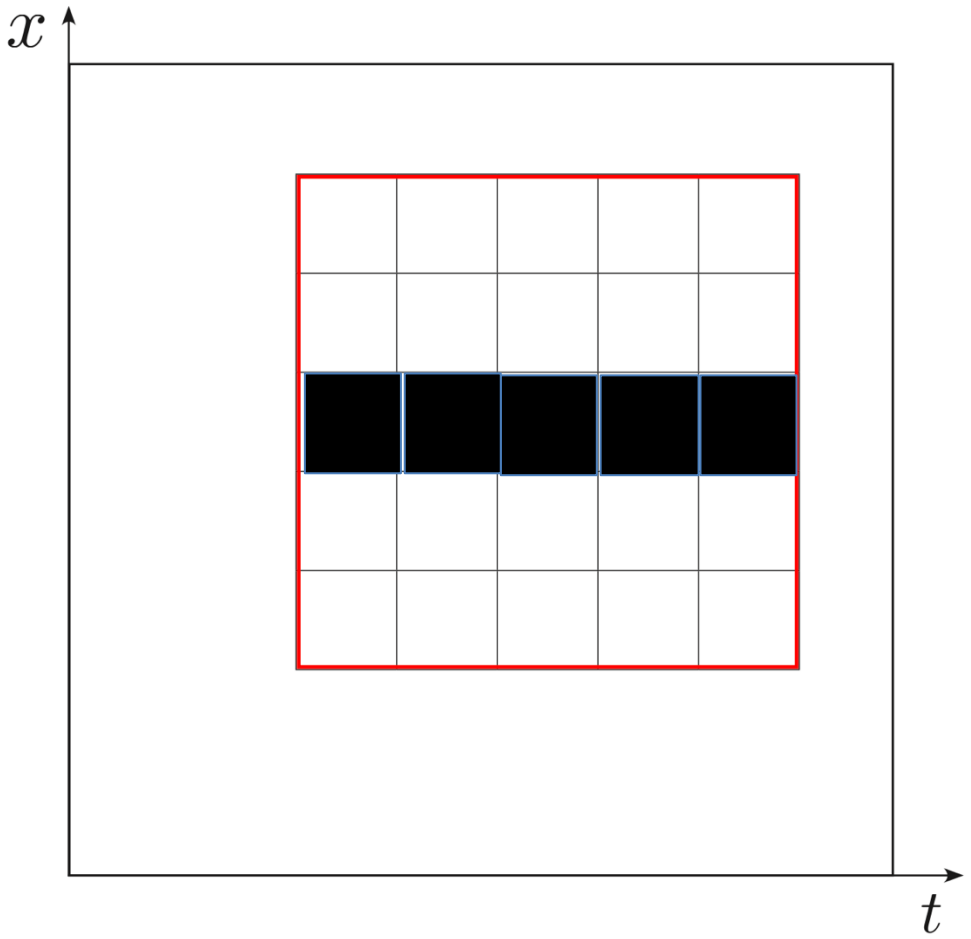

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Self-supervised learning tasks

- Contrastive learning: make sure latent representation is semantic

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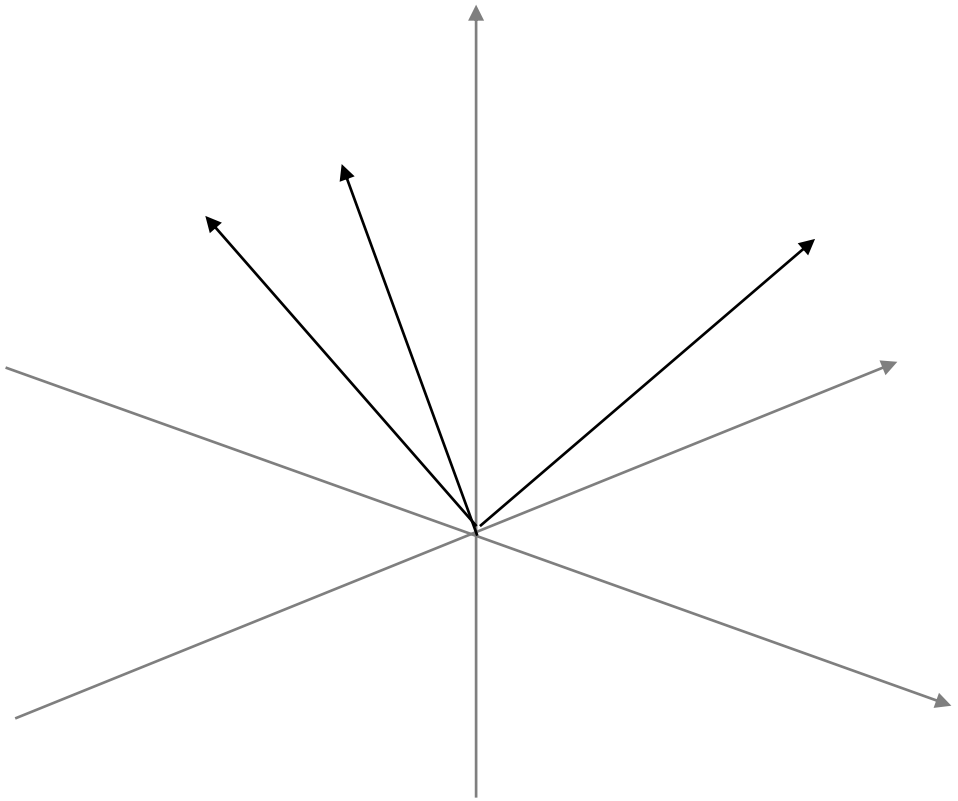

From imagenet dataset

Self-supervised learning tasks

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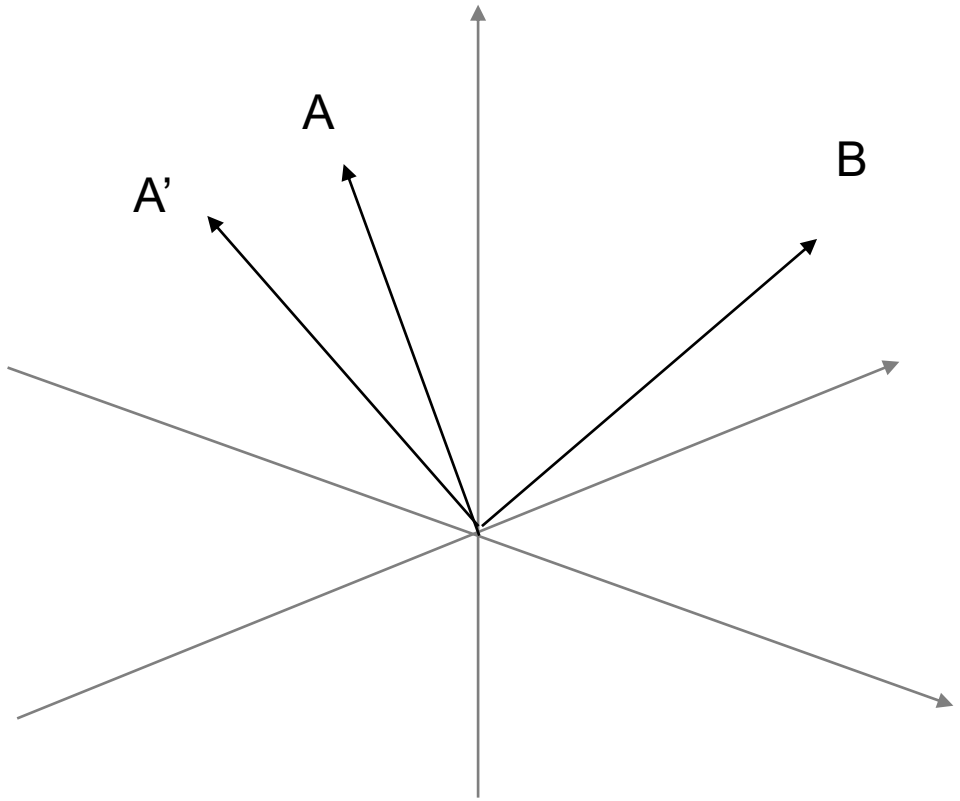

From imagenet dataset

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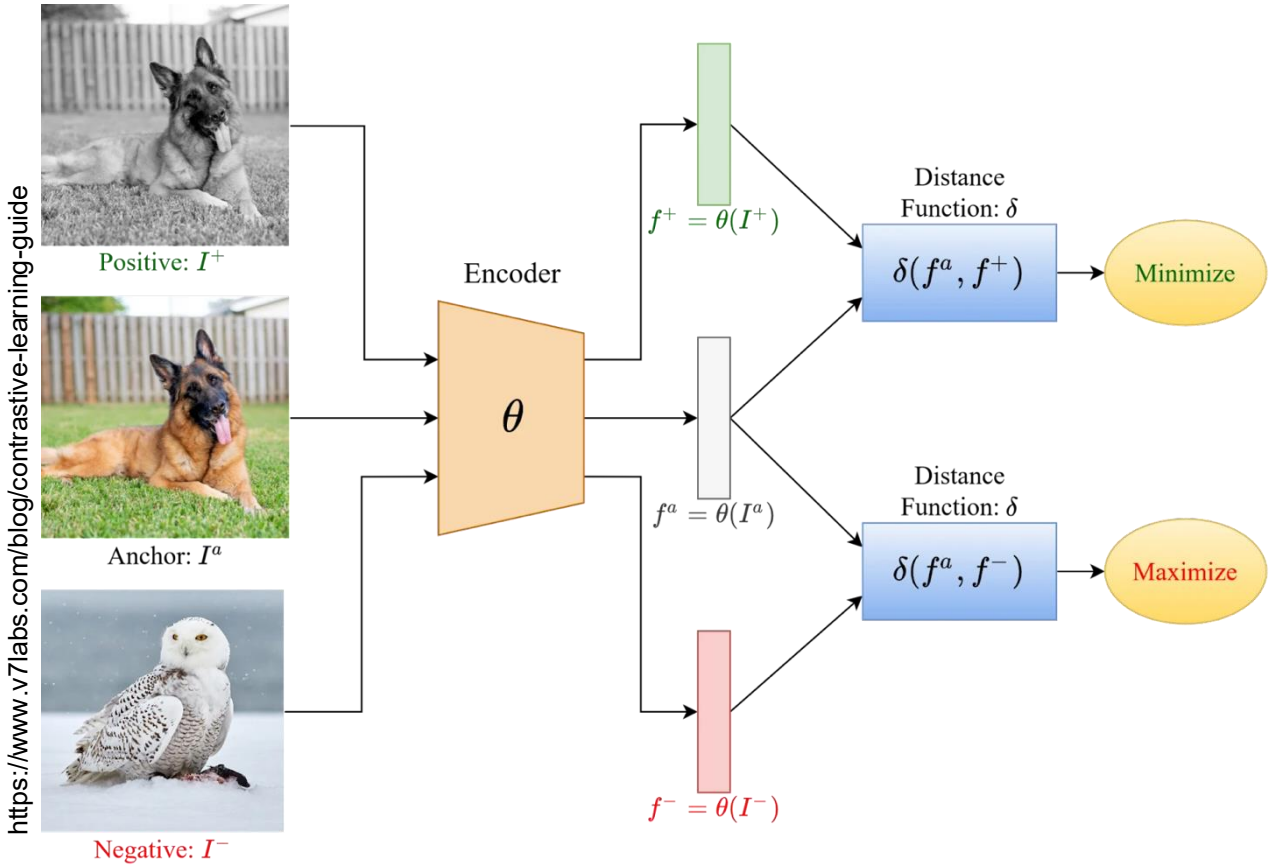
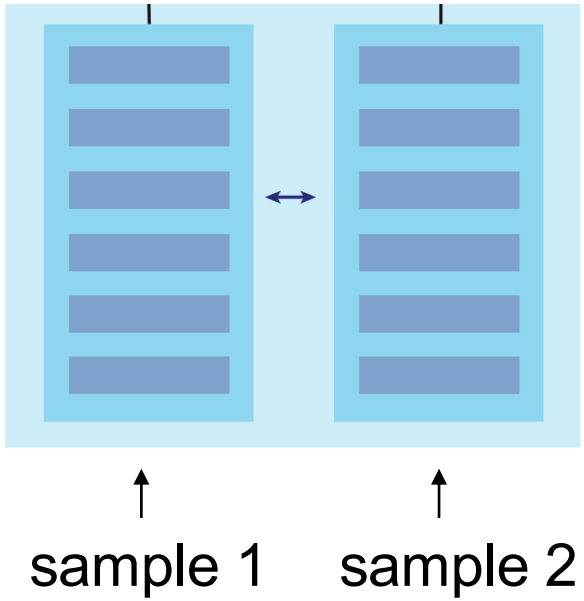


Self-supervised learning tasks

- Siamese networks



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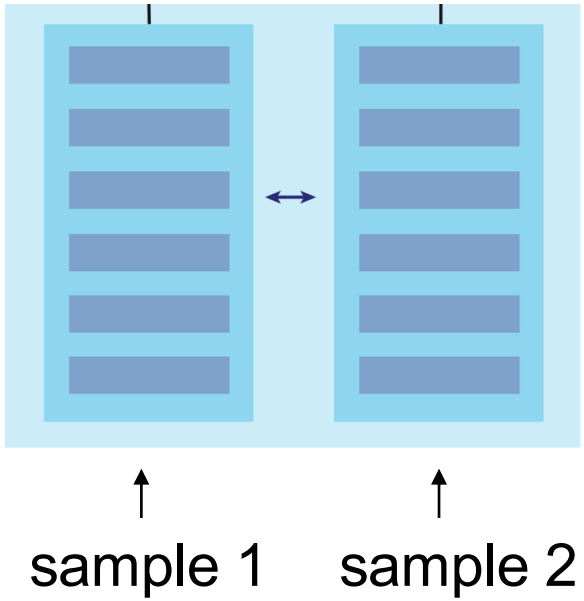

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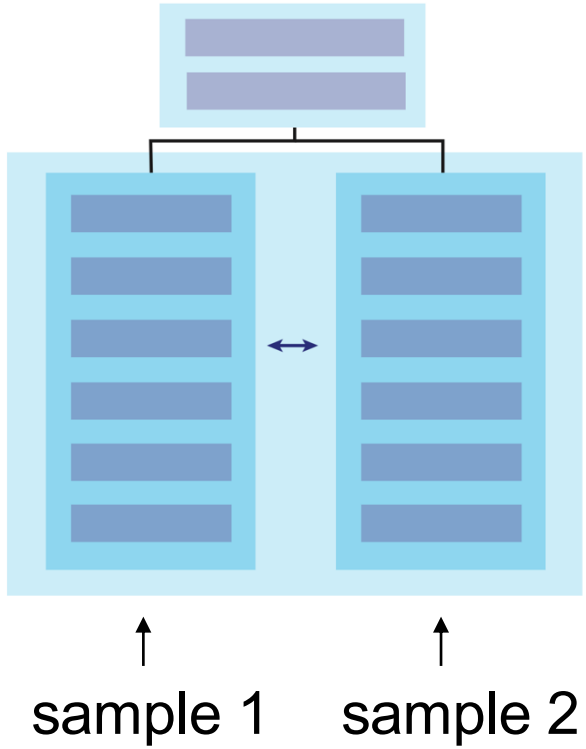

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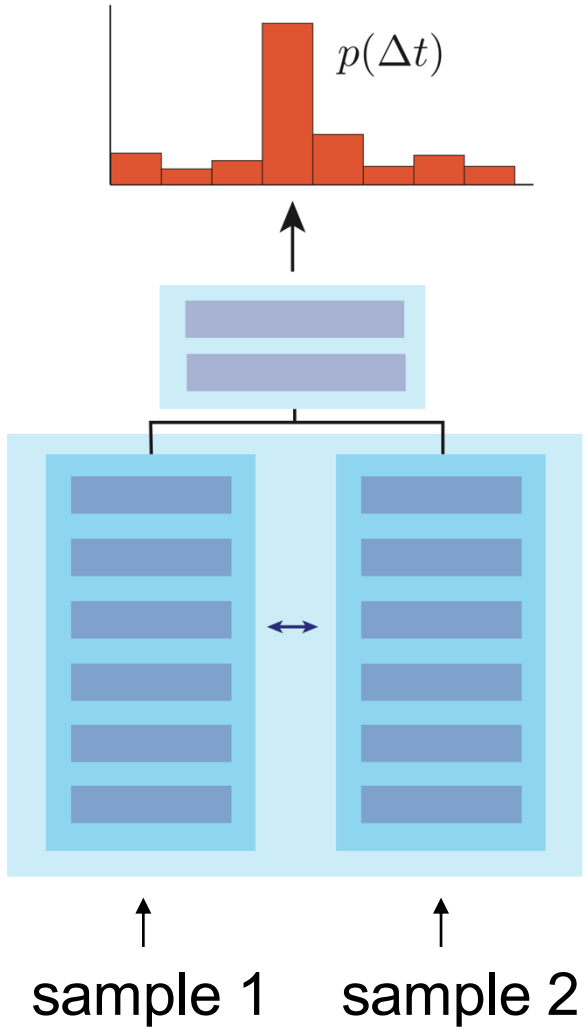


predict (known) similarity between samples

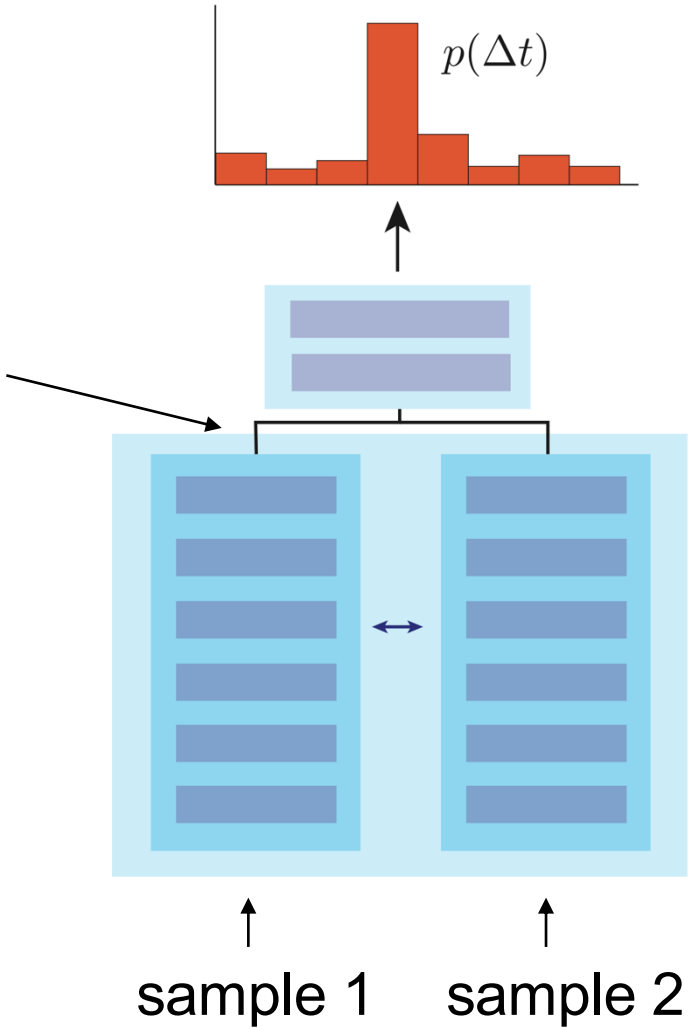
classification head

same network for both samples

Self-supervised learning tasks

- Siamese networks

Learn similar latent representation for similar samples



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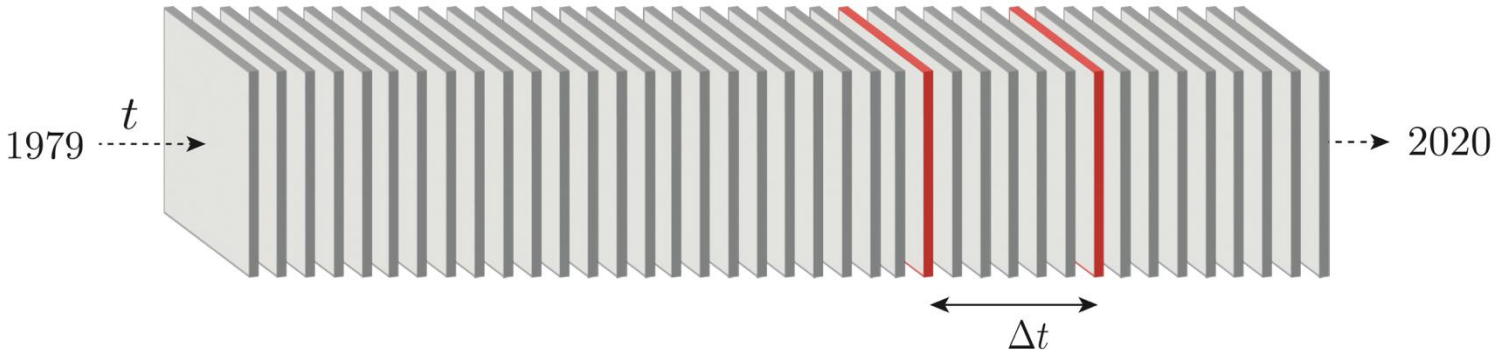
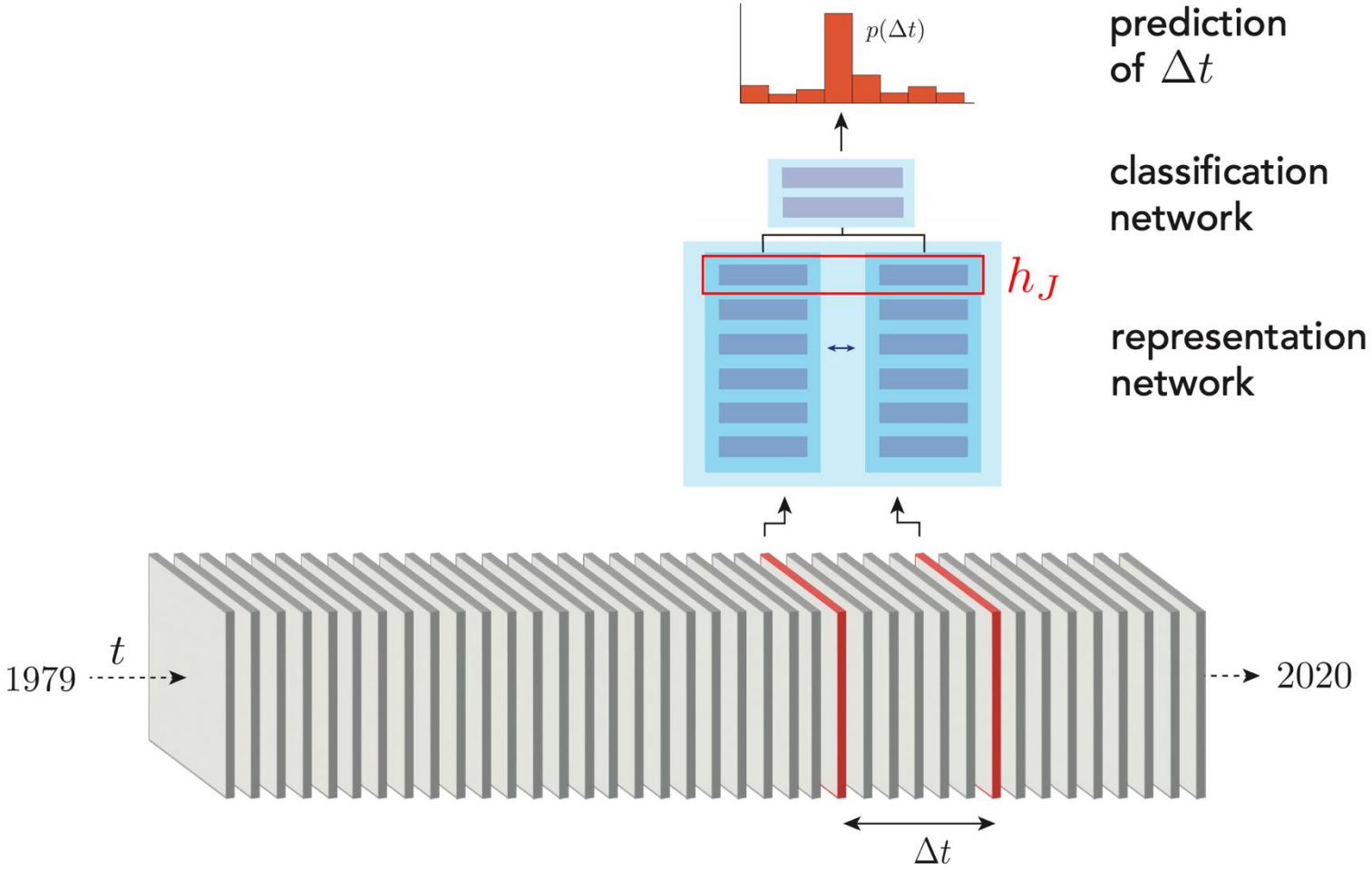
Self-supervised learning tasks



Hoffmann and Lessig, AtmoDist: Self-supervised Representation Learning for Atmospheric Dynamics, 2022, https://arxiv.org/abs/2202.01897

Self-supervised learning tasks



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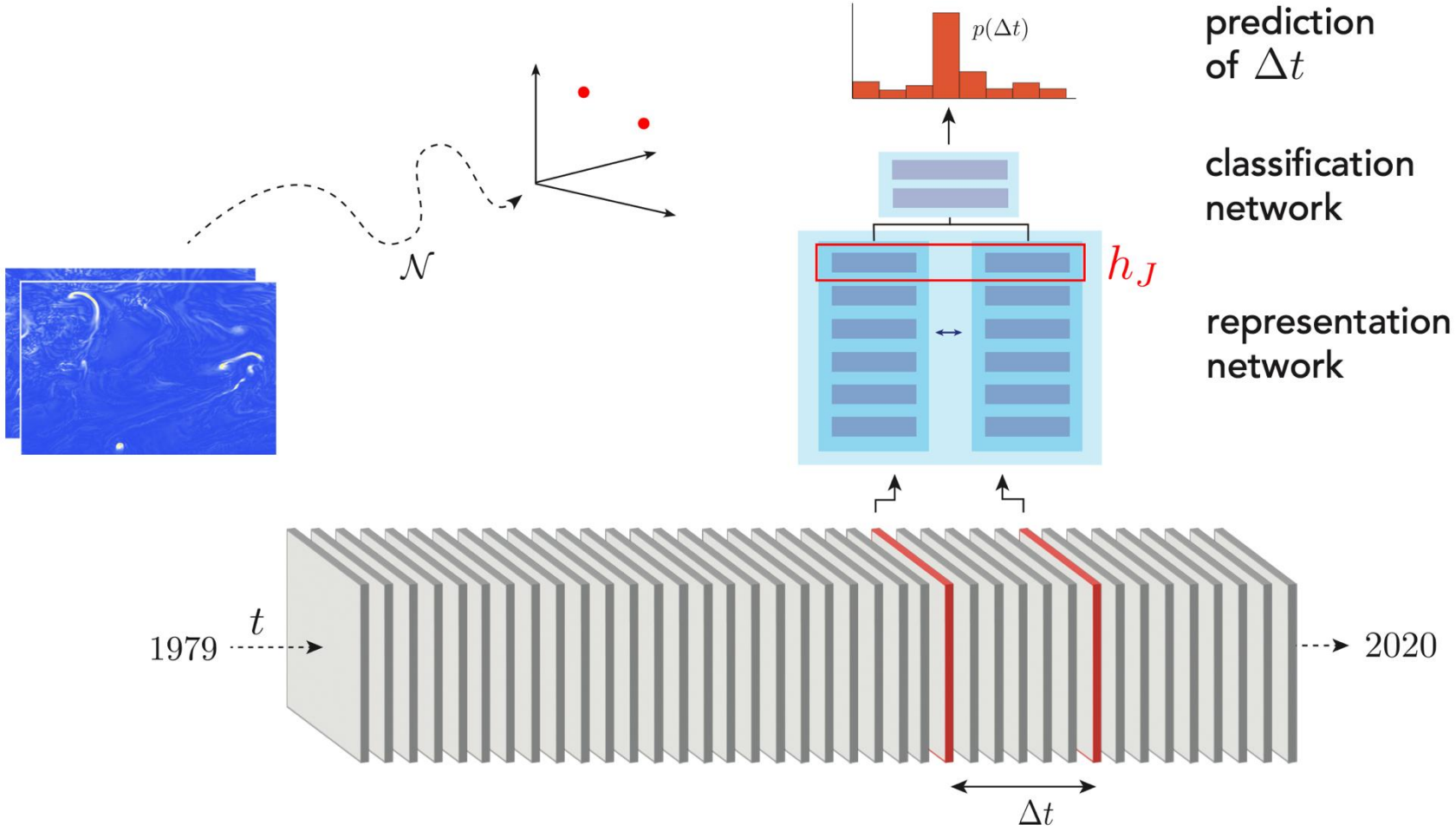

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Self-supervised learning tasks

- Joined Embedding Predictive Architecture (JEPA)
  - Mask but compute loss in hidden/latent space instead of by reconstructing
  - Learn more abstract and robust representations

Bardes et al., Revisiting Feature Prediction for Learning Visual Representations from Video, 2024, https://scontent-cdg4-2.xx.fbcdn.net/v/t39.2365-6/427986745_768441298640104_1604906292521363076_n.pdf?_nc_cat=103&ccb=1-7&_nc_sid=3c67a6&_nc_ohc=Lpq5IeF5ftUAX9EN6b7&_nc_ht=scontent-cdg4-2.xx&oh=00_AfCFIyd8GMJnqQsG90WY-ccXwWEooa0XgiWXZm06nd1-pw&oe=65D69EB1

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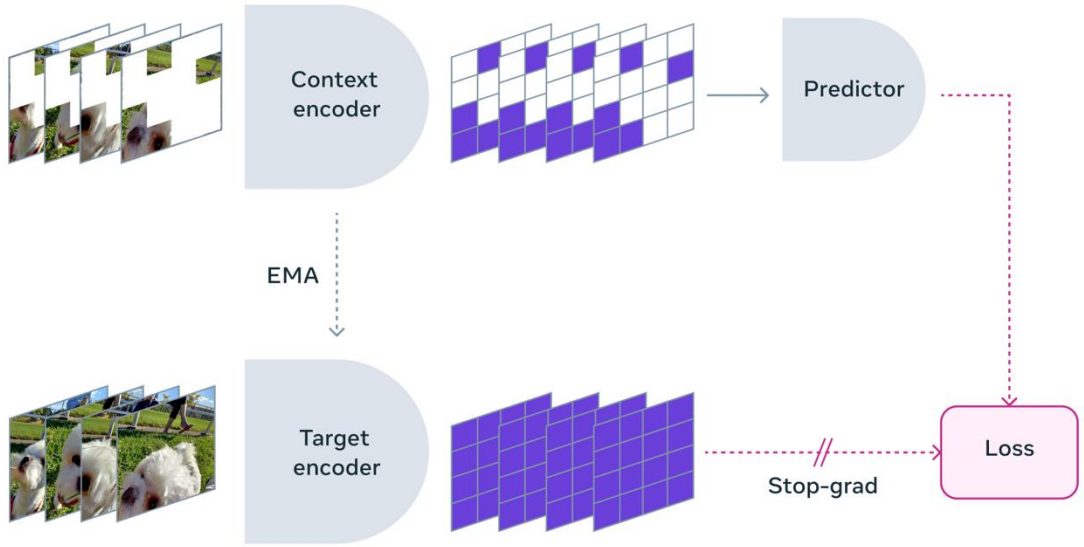

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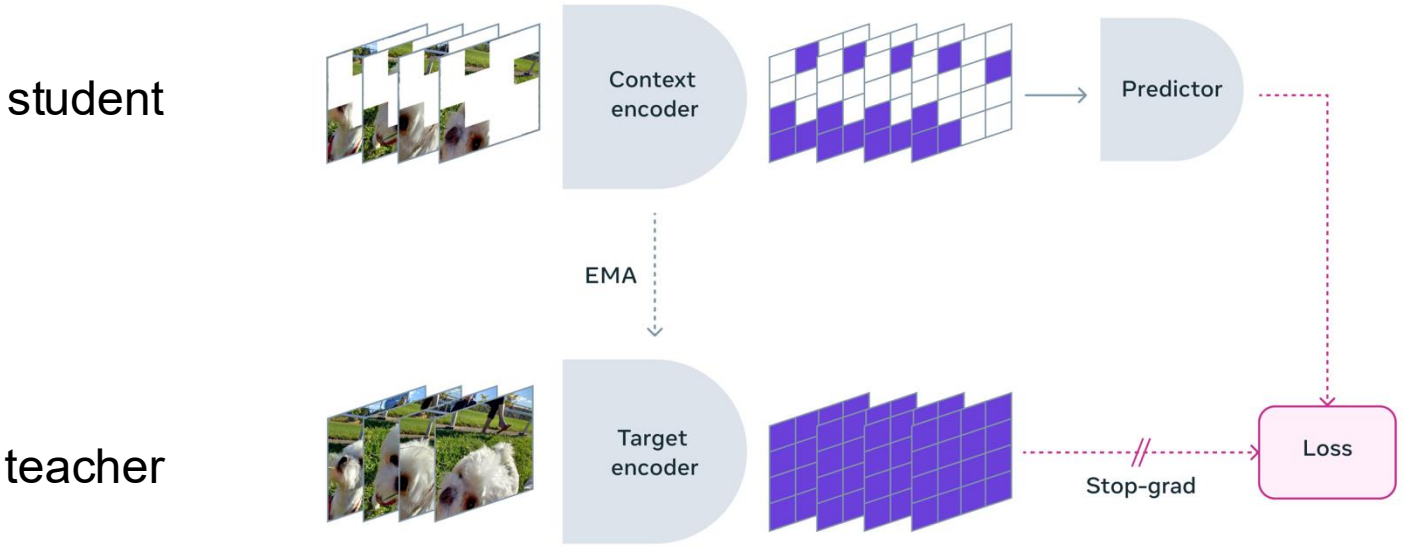

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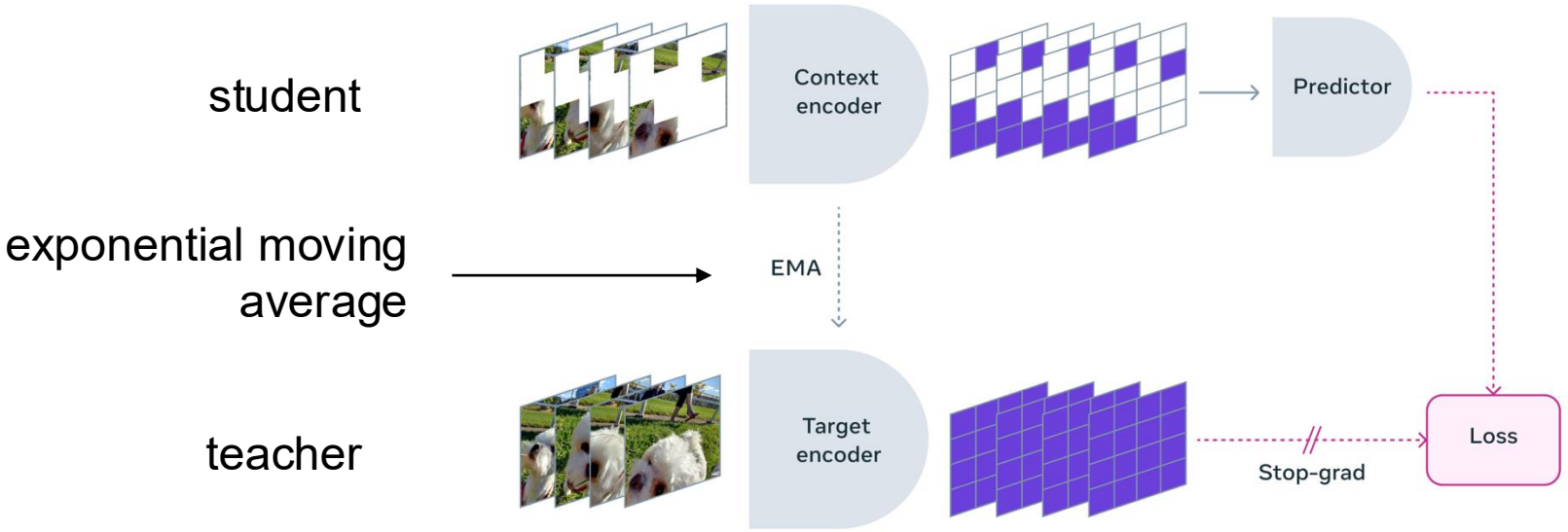

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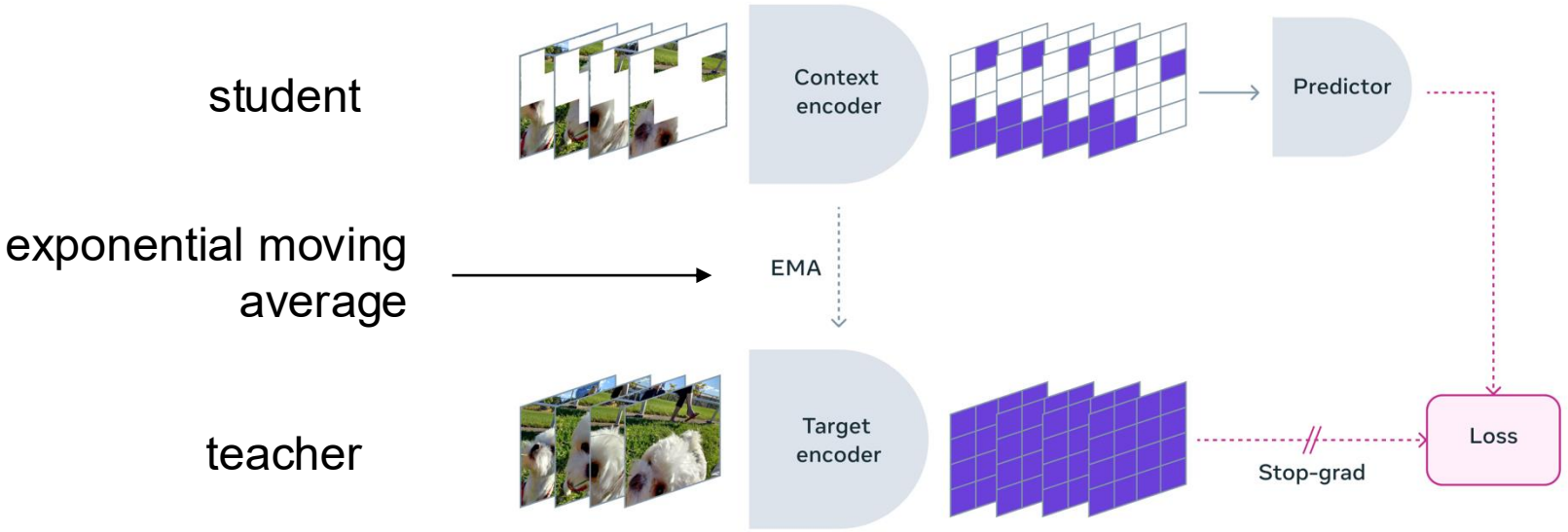

teacher is identical to student except that weights are averaged from last training steps

Bardes et al., Revisiting Feature Prediction for Learning Visual Representations from Video, 2024, https://scontent-cdg4-2.xx.fbcdn.net/v/t39.2365-6/427986745_768441298640104_1604906292521363076_n.pdf?_nc_cat=103&ccb=1-7&_nc_sid=3c67a6&_nc_ohc=Lpq5IeF5ftUAX9EN6b7&_nc_ht=scontent-cdg4-2.xx&oh=00_AfCFlyd8GMJnqQsG90WY-ccXwWEooa0XgiWXZm06nd1-pw&oe=65D69EB1

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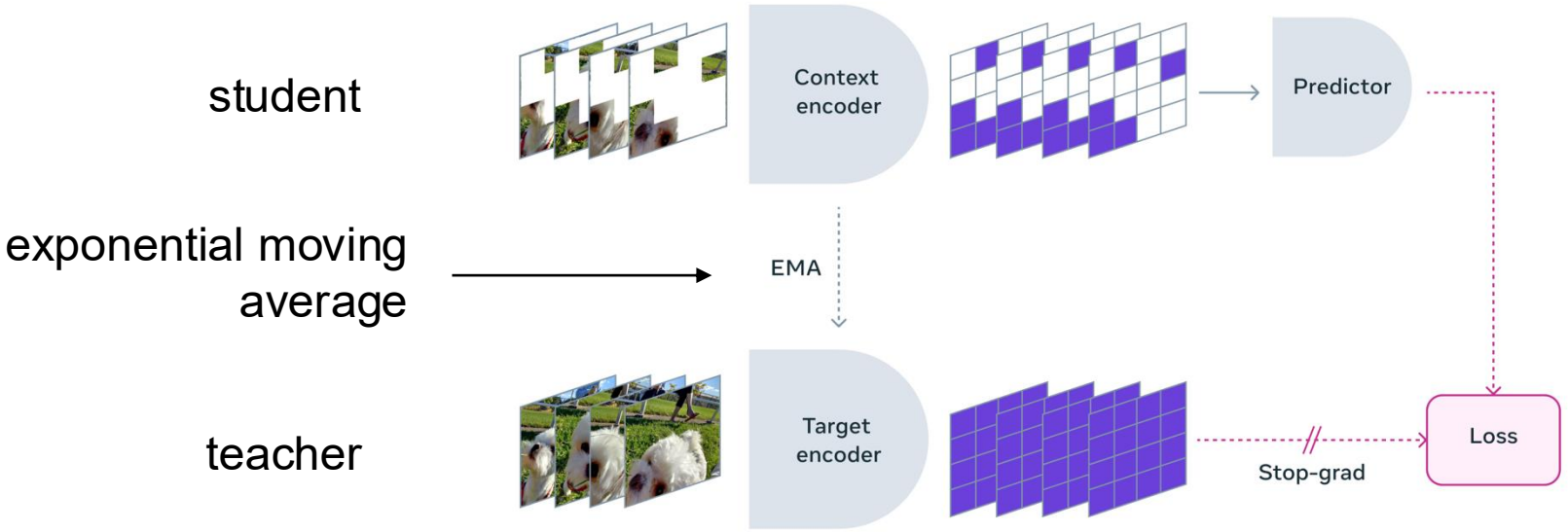

https://www.slideshare.net/slideshow/enact-carrot-stick/53622951

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Self-supervised learning tasks

- DINO
  - Mask but compute loss in hidden/latent space instead of by reconstructing
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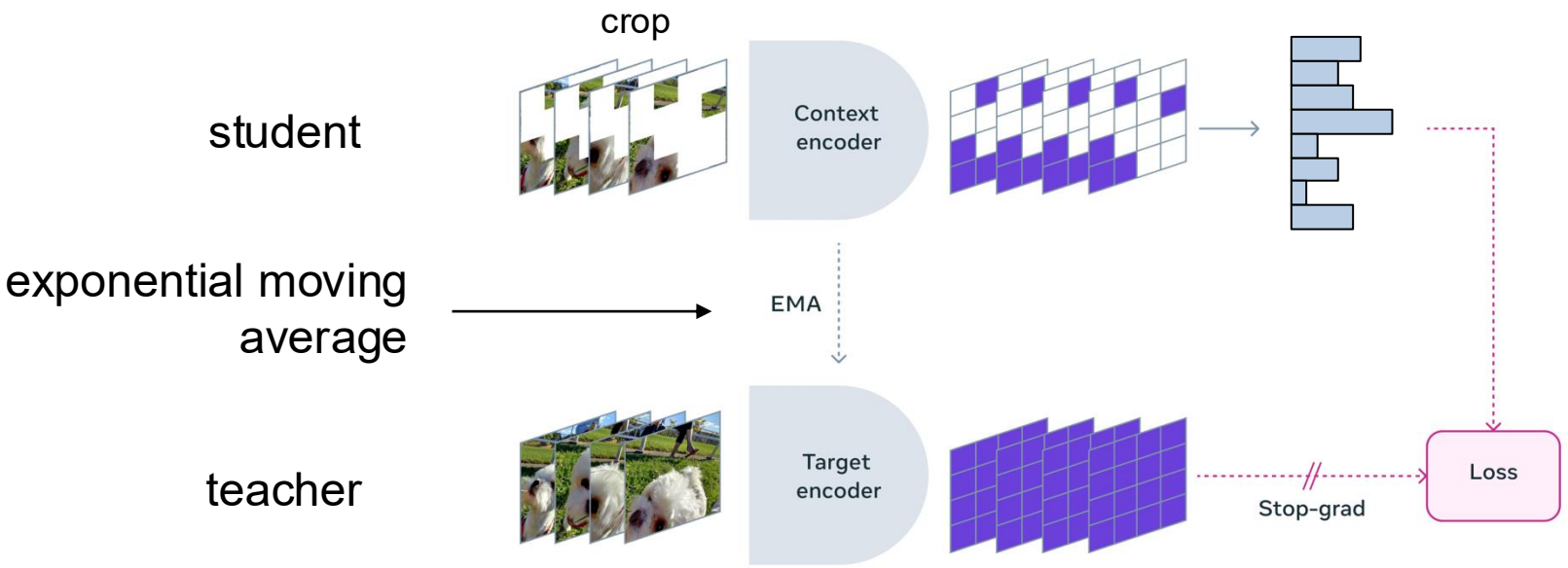

M. Caron, H. Touvron, I. Misra, H. Jegou, J. Mairal, P. Bojanowski, and A. Joulin, Emerging properties in self-supervised vision transformers, CoRR, abs/2104.14294, 2021, arXiv: 2104.14294

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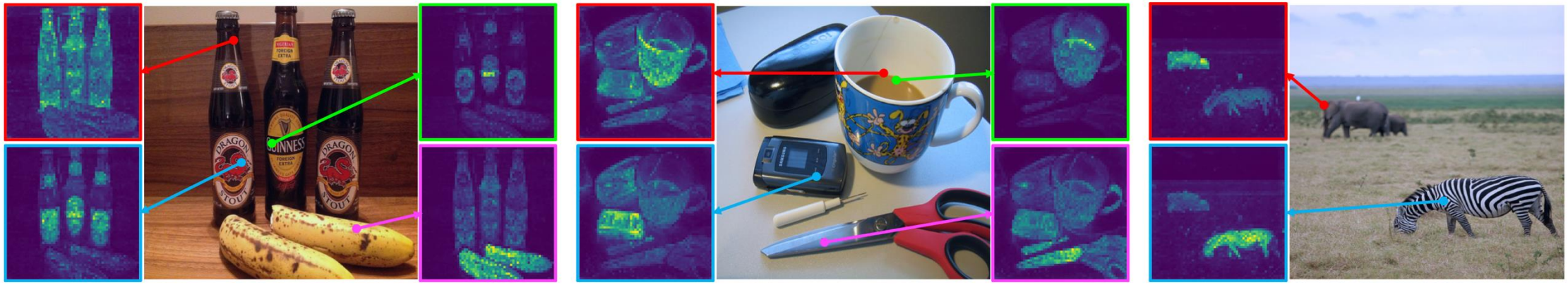

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Summary

- Self-supervised learning
  - Overcome the limits imposed by requiring labeling of data
  - Learn task-agnostic neural networks
- Essentially all of the most powerful vision and language models use self-supervised training
  - Fine-tuning for specific applications
  - Increased robustness and flexibility

Literature

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