

Understanding Masked Autoencoders via Hierarchical Latent Variable Models

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Masked Autoencoders: SOTA Self-supervised Learning Paradigm



Mask sampling: random masks are determined by *masking ratio* and *patch size*.

Encoding: the encoder maps the unmasked input to a representation.

Decoding: the decoder reconstructs the masked input from the representation and the positional information.

MAE attains state-of-the-art fine-tuning performance on various vision tasks, including classification, detection, segmentation, and more.

Great! But in principle,

- a. Why can MAE learn meaningful representation?
- b. How do key hyperparameters determine the representation properties?

We offer insights from a latent-variable identification perspective!



A hierarchical data-generating process for vision data

"Hierarchical" to represent various levels of dependence among pixels:

- Low-level dependence within a single object.
- High-level dependence between distinct objects.



- No directed edge among observed variables (i.e., pixels).
- Generating processes are invertible.



MAE works by identifying latent variables in the generating process!

Each specific mask corresponds to a specific set of latent variables (Theorem 2).

MAE can provably recover the true latent variables specified by masking (Theorem 1, 2).



How do hyperparameters determine representation quality?

- Masking ratios and sizes induce the model to capture low- or high-level information.
- Learning high-level representations is generally hard with random masking.



Experiments: appropriate masking ratios capture high-level information



Higher masking ratios and sizes are structurally more similar to the original image and capture more high-level semantic information, but extreme masking induces model to capture low-level information.

Conclusion

- Why MAE can learn meaningful representation: MAE provably recovers high-level representations by identifying latent variables.
- Higher masking ratios and patch sizes induce the model to learn higher-level image representations.
- Learning high-level representations is generally hard with random masking.



Formulation of Masking

- Mask samples: random masks are sampled from a distribution determined by masking ratio and patch size
- MAE encoder maps the unmasked input to a representation
- MAE decoder reconstructs the masked input from the representation and the positional information

Contribution: Understanding with latent variable models

- In this work, we establish a framework to understand MAE via identifiability guarantees.
- We first formulate the underlying data-generating process as a hierarchical latent variable model; and
- Then, under reasonable assumptions, MAE can recover a subset of true latent variables in the generating process
- The level of latent variables in the hierarchical model depends on how masking performs (masking ratio and patch size)
- We show that a moderate-to-aggressive masking ratio captures high-level information, while extremely aggressive or conservative masking captures low-level information

Assumption: latent variable

Latent variable c: a minimal set of variables to satisfy the following:

- s_m
- TODO
- c is minimal



Results: Identifiability

Interpretations



- Conservative masking: undesirable, as the recovered latent variables are still at a low level
- (Too) aggressive masking: undesirable, as the recovered latent variables are also at a low level
- Ideal masking: moderate masking recovered latent variables at a high level

Assumption:

- There is no direct edge between any two observables Xs; and
- Each variable is generated by their parents from a higher layer in a directed acyclic graph (DAG), combined with the exogenous variable in each layer.



Identifiability assumptions

- In a hierarchical latent variable structure, for any specific mask, there exists a minimal set of latent variables such that the generating process can be expressed using the figure.
- Essentially, we want to locate a subset of true latent variables that fully captures the statistical dependency between the masked and visible parts.
- The transformations from a higher layer to a lower layer in the data-generating process are invertible.
- , where or refers to the information specific to the masked or unmasked part.
- The content variable is minimal in terms of dimensions.



Identifiability results

- Result 1: for each mask m, there exists a unique that contains sufficient high-level information to reconstruct the masked and the unmasked.
- Result 2: For any mask, the MAE encoder can recover all the information of the minimal set .

