# A Theoretical Understanding of Shallow Vision Transformers: Learning, Generalization, and Sample complexity

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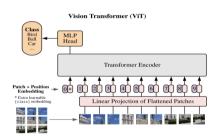
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# Transformers and Vision Transformers (ViTs)

- Transformers achieved great empirical success in numerous areas.
- Transformer-based models gradually become prevalent in vision tasks.



Transformer-based foundation models



Vision Transformer [Dosovitskiy et al.21]

Under what conditions does a Vision Transformer achieve satisfactory generalization?

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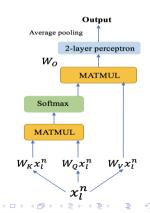
### Problem formulation and the ViT model

We study a binary classification problem with the dataset  $\{X^n, y^n\}_{n=1}^N$  with L patches, i.e, tokens in each  $X^n$ . Each token is a noisy version of a pattern. There are M patterns in total, where two are discriminative patterns that can determine the label.

- Labeling function: majority voting of discriminative tokens.
- Learner network: a shallow ViT with a single-head self-attention layer and a two-layer perceptron.

$$F(oldsymbol{X}^n) = rac{1}{|\mathcal{S}^n|} \sum_{l \in \mathcal{S}^n} oldsymbol{a}_{(l)}^ op \mathsf{Relu}(oldsymbol{W}_V oldsymbol{X}^n \mathsf{softmax}(oldsymbol{X}^{n op} oldsymbol{W}_K^ op oldsymbol{W}_Q oldsymbol{x}_l^n))$$

• Loss function: Hinge loss function. Training with SGD.



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#### Main theoretical results

Data model: We sample a set of tokens for each data. Define

- label-relevant tokens: tokens with the pattern that corresponds to the exact label of the data.
- confusion tokens: tokens with the pattern that corresponds to the other label of the data.

#### Theorem 1

Given a sufficient large model and  $\alpha_*$ ,  $\alpha_\#$  with

$$m \gtrsim M^2 \log N,$$
 (2)

$$\alpha_* \ge \alpha_\#/c$$
,  $\alpha_*$ ,  $\alpha_\#$ : average fraction of label-relevant, confusion tokens (3)

for some  $c \in (0, 1/(2e))$ , and large enough sizes of mini-batch and the set of sampled tokens for each data, zero generalization error is achieved with a sample complexity N and a number of iterations T:

$$N \ge \Omega(\alpha_*^{-2}), \quad T = \Theta(\alpha_*^{-1}\eta^{-1}), \quad \eta : \text{ step size}$$
 (4)

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# Main insights

- Requirements for the data: the fraction of label-relevant tokens is much more than that of confusion tokens in each data.
- Sample complexity N: linear in  $\alpha_*^{-2}$ .
- Required number of iterations T: linear in  $\alpha_*^{-1}$ .
- **Technical novelty**: A new theoretical framework to analyze the nonconvex interactions in shallow ViTs, which contain a trainable self-attention layer.

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## Comparison between ViT and CNN

#### Proposition 1

With an approximately the same size of the model, the sample complexity of using CNN to achieve zero generalization error is  $\Omega(\alpha_*^{-4})$ , which is an increase by a factor of  $\alpha_*^{-2}$  compared to ViT.

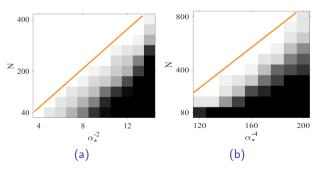


Figure 1: The impact of  $\alpha_*$  on the sample complexity for (a) ViT and (b) CNN.

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# Sparse attention map and token sparsification

#### Proposition 2

- The summation of attention weights correlated with label-relevant tokens converges to  $1 \eta^C$  at a sublinear rate of O(1/t) for C > 0 when t is large.
- Removing label-irrelevant tokens or tokens with large noise can improve the generalization.

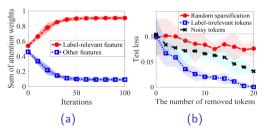


Figure 2: (a) Concentration of attention weights (b) Impact of token sparsification on testing loss.

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