How Do Vision Transformers Work?

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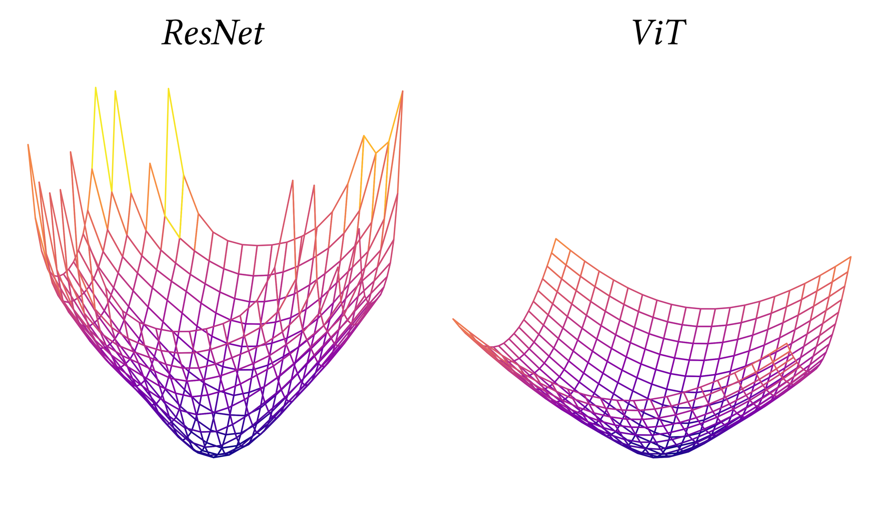
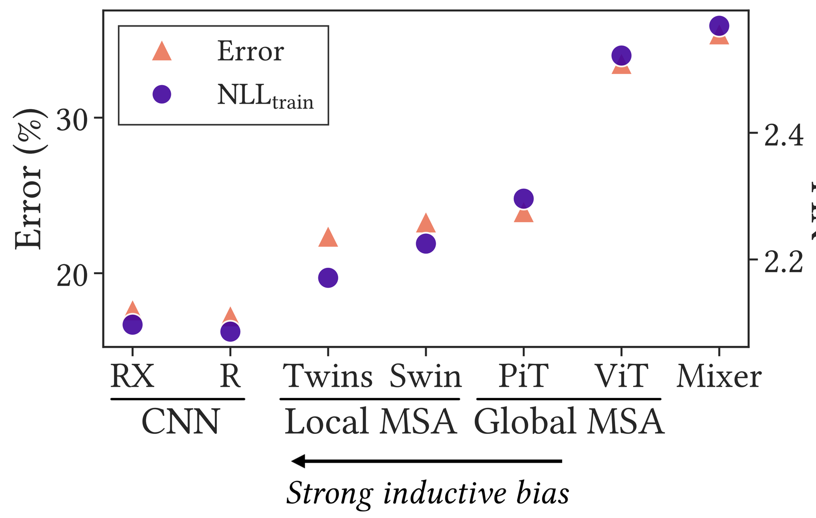
Paper: https://arxiv.org/abs/2202.06709
Code: https://github.com/xxxnell/how-do-vits-work

What Properties of Self-Attentions Do We Need?

MSAs (multi-head self-attention) have flat but non-convex losses. In contrast, Convs have convex but sharp losses.

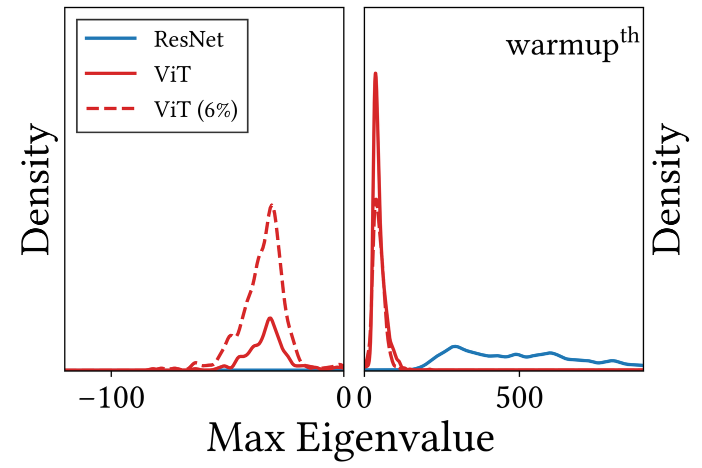


(a) Loss landscape visualization

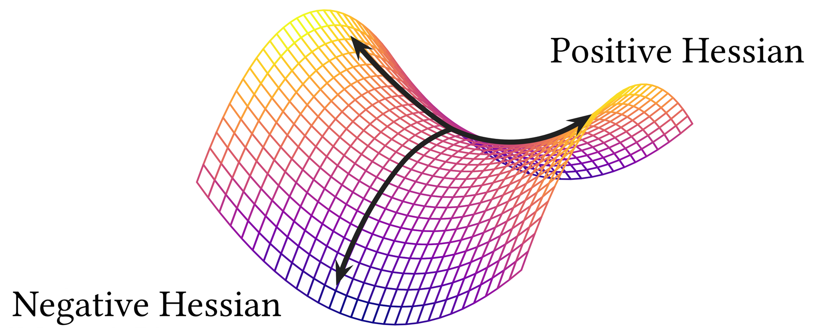


(b) Test error and training NLL for each model

Figure 1: *Left*: **Loss landscape visualization** show that ViT has a flatter loss than ResNet. *Right*: Weak inductive bias (e.g. long-range dependency) disturbs NN optimization.

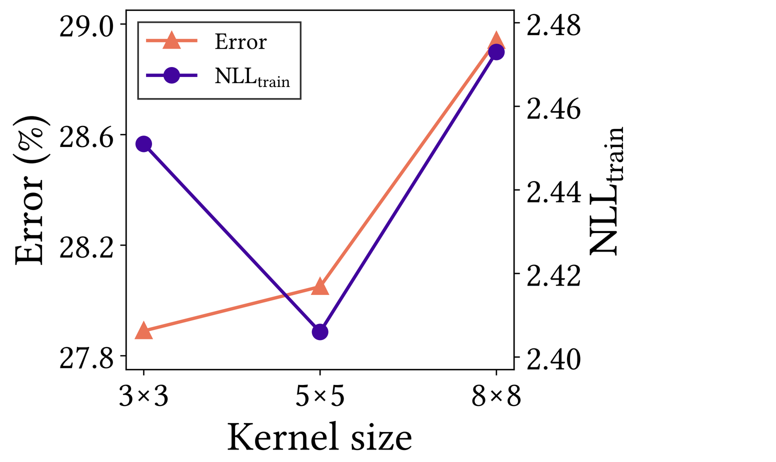


(a) Hessian max eigenvalue spectrum

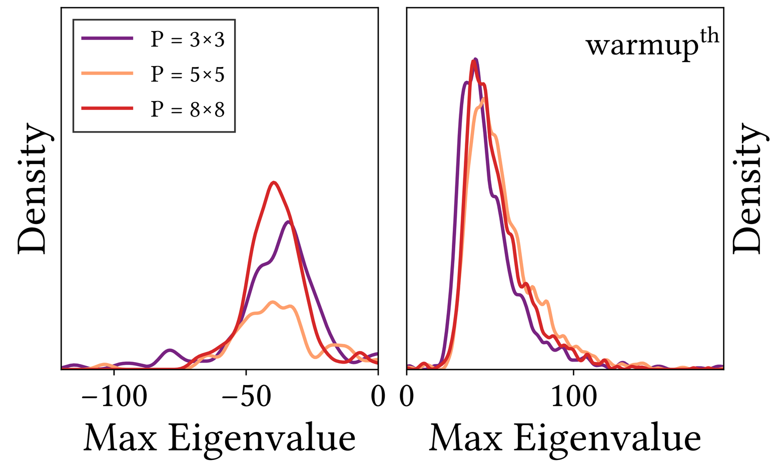


(b) Local geometry of non-convex (saddle) points

Figure 2: **Hessian max eigenvalue spectra** show that MSAs have their pros and cons. ViT has a number of negative Hessian eigenvalues, while ResNet only has a few. The magnitude of ViT's positive Hessian eigenvalues is small.



(a) Error and NLL of ViT with local MSA for kernel size



(b) Hessian max eigenvalue spectrum for kernel size

Figure 3: The key feature of MSA is data specificity, not long-range dependency. *Left*: Convolutional ViT demonstrates that locality constraint improves ViT. *Right*: Locality inductive bias suppresses the negative Hessian eigenvalues.

Do Self-Attentions Act Like Convs?

MSAs are low-pass filter, but Convs are high-pass filter. It suggests that MSAs are shape-biased, whereas Convs are texture-biased.

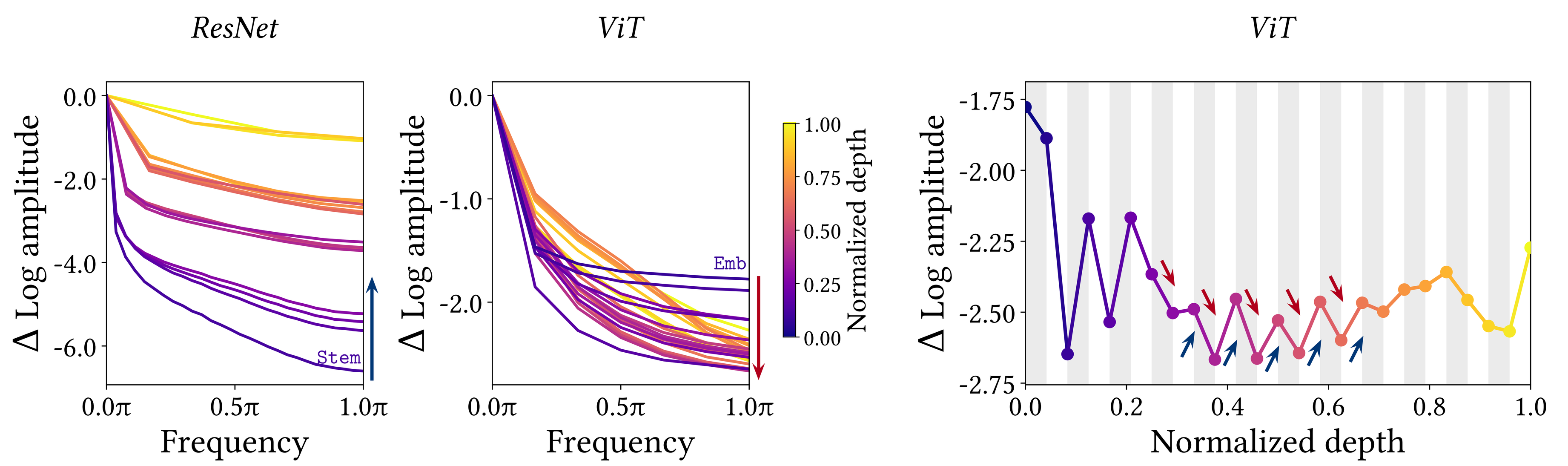
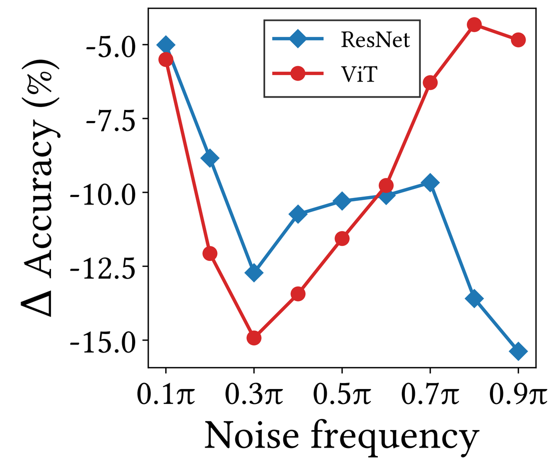
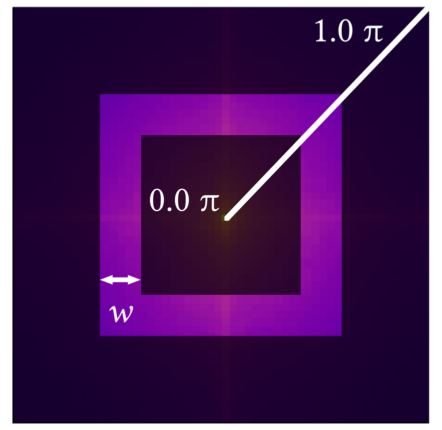


Figure 4: Relative log amplitudes of **Fourier transformed feature map** show that ViT tend to reduces high-frequency signals, while ResNet amplify them. ***Left***: In ViT, MSAs (gray area) generally reduce the high-frequency (1.0π) component of feature map, and Conv/MLPs (white area) amplify it.



(a) Robustness for noise frequency



(b) Frequency-based random noise

Figure 5: We measure the **decrease in accuracy against frequency-based random noise**. ViT is robust against high-frequency noise, while ResNet is vulnerable to them.

It suggests that low-frequency signals and high-frequency signals are informative to MSAs and Convs.

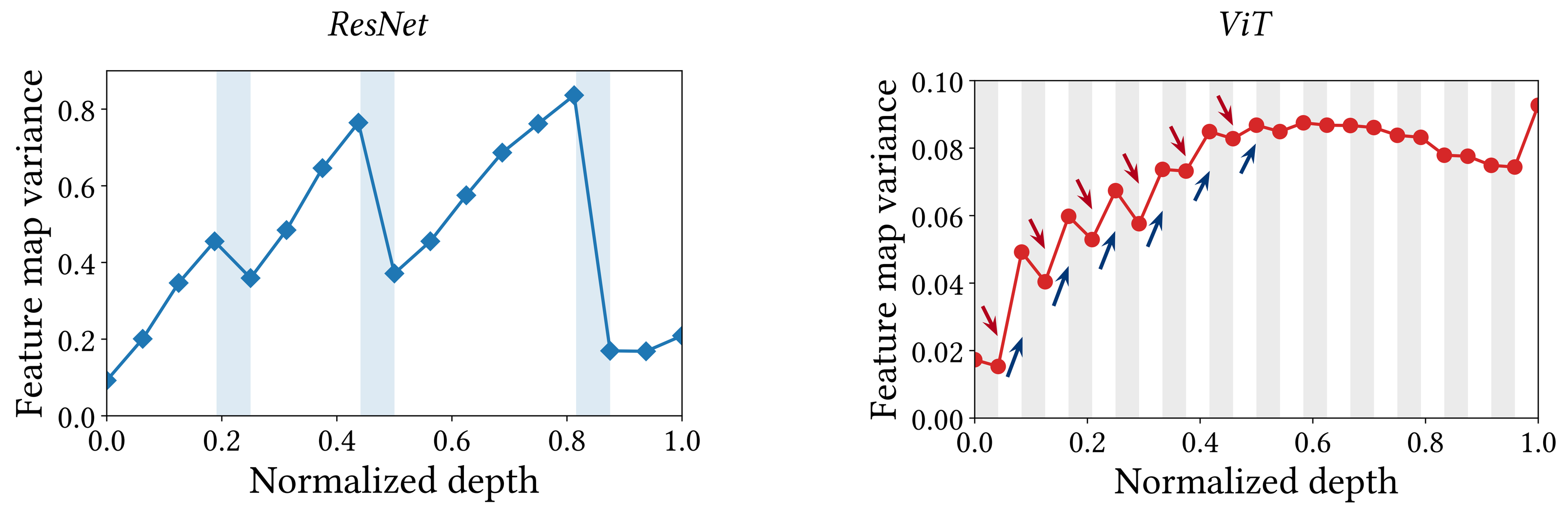


Figure 6: MSAs (gray area) reduce **the variance of feature map points**, but Convs/MLPs (white area) increase the variance. The blue area is subsampling layer. The results implies that MSAs aggregate feature maps, and Convs convert them.

How Can We Harmonize Self-Attentions with Convs?

MSAs closer to the end of a stage (not a model) and Convs at the beginning of a stage significantly improve the performance.

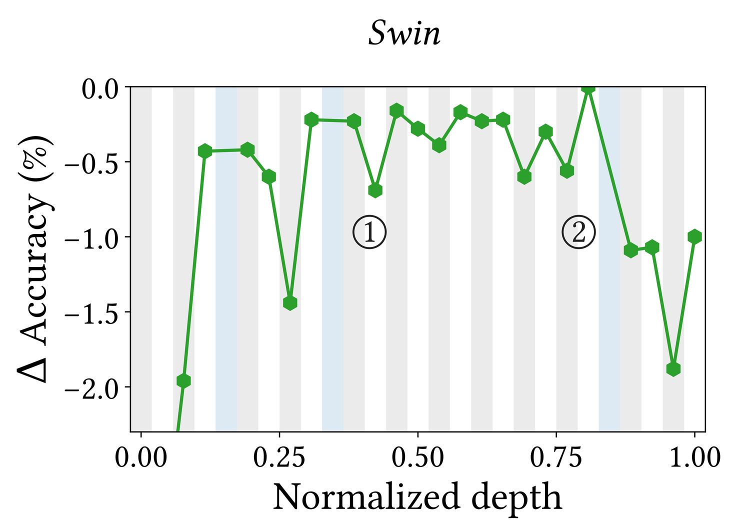
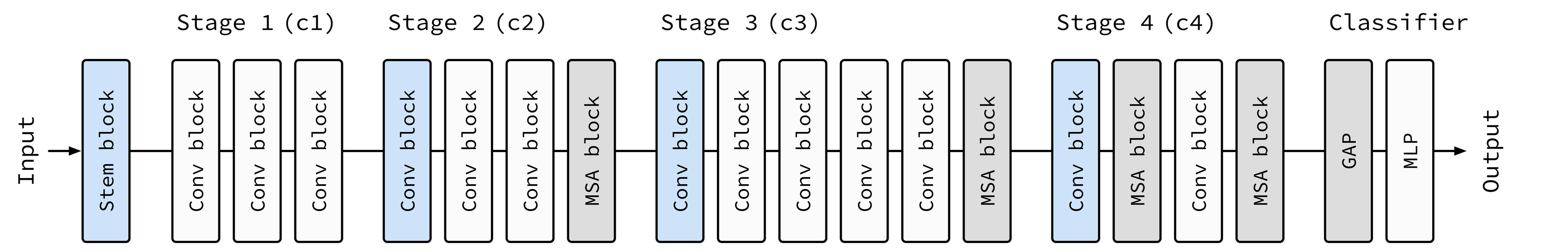
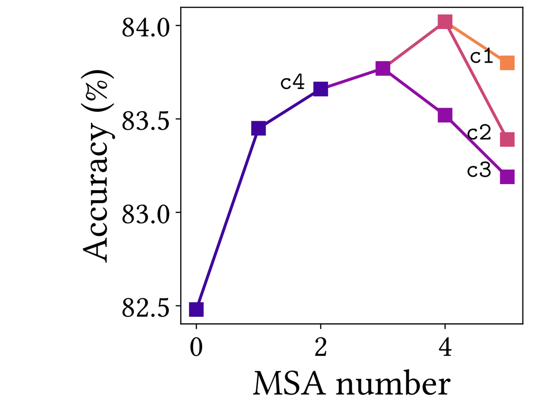


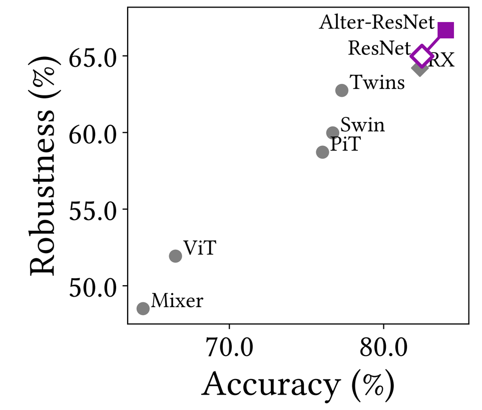
Figure 7: We measure **decrease in accuracy after removing one unit** from the trained model. Accuracy changes periodically, and this period is one stage. In Swin, ① Convs (white area) play an important role at the beginning of a stage, and ② MSAs (gray area) play an important role at the end of a stage.



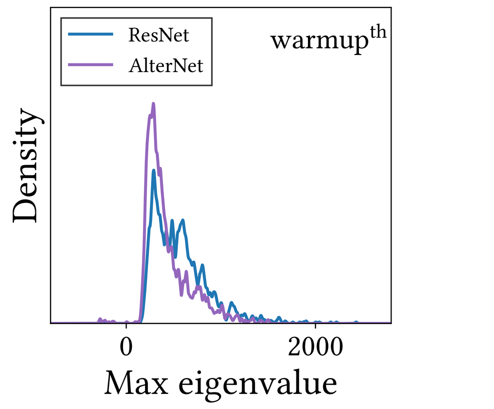
(a) Architecture of Alter-ResNet-50 for CIFAR-100



(b) Accuracy of AlterNet for MSA number



(c) Accuracy and robustness in a small data regime (CIFAR-100)



(d) Hessian max eigenvalue spectra

Figure 8: We propose ***AlterNet***, a model in which Conv blocks at the end of *a stage* are replaced with MSA blocks. AlterNet outperforms CNNs even in small data regimes.

In summary, appropriate inductive biases improves NN optimization, and self-attentions have a spatial smoothing inductive bias.

	Self-Attention	Convolution
Loss Landscape	Flat but non-convex	Convex but sharp
Fourier Analysis	Low-pass filter (shape-biased)	High-pass filter (texture-biased)
Best Practice	The end of a stage	The beginning of a stage