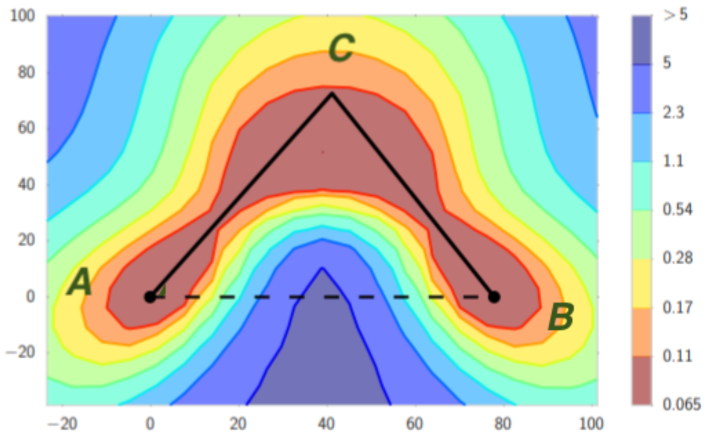
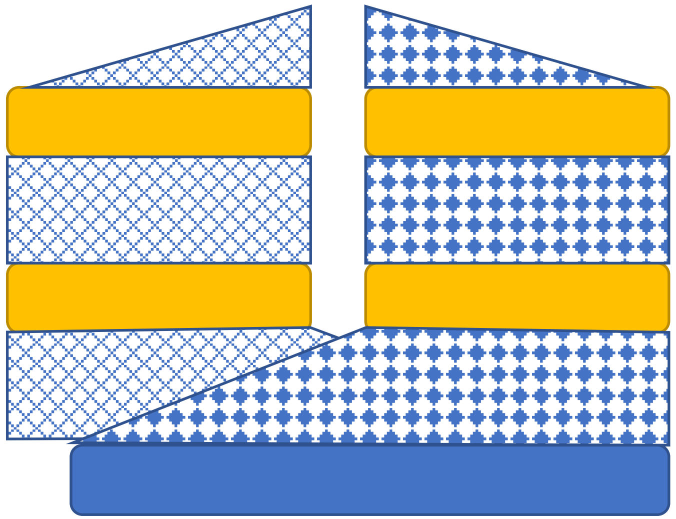


Explaining Landscape Connectivity of Low-cost Solutions for Multilayer Nets

Rong Ge, Duke University

Joint work with Rohith Kuditipudi, Xiang Wang (Duke)
Holden Lee, Yi Zhang, Zhiyuan Li, Wei Hu, Sanjeev Arora (Princeton)



Mode Connectivity[Freeman and Bruna 16, Garipov et al. 18, Draxler et al. 18]

- For neural networks, local minima found via gradient descent are connected by simple paths in the parameter space
- Every point on the path is another solution of almost the same cost.

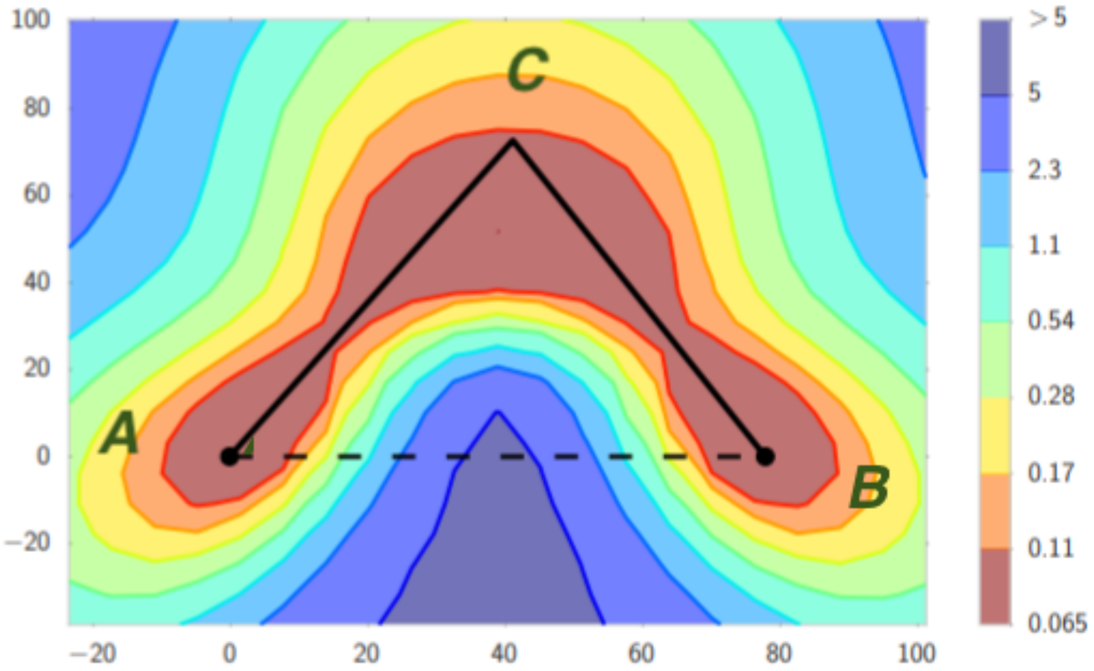
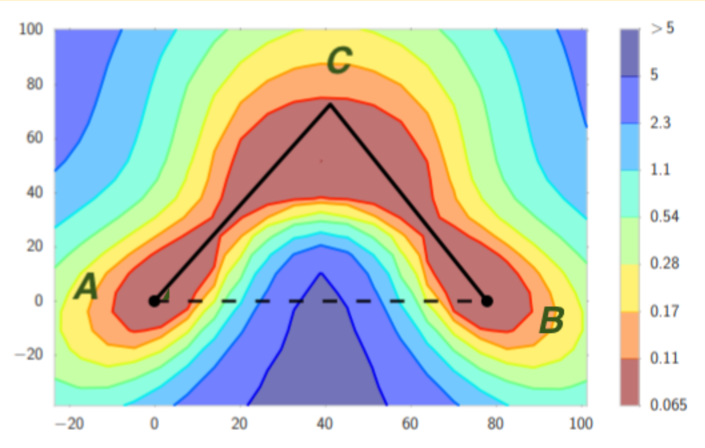
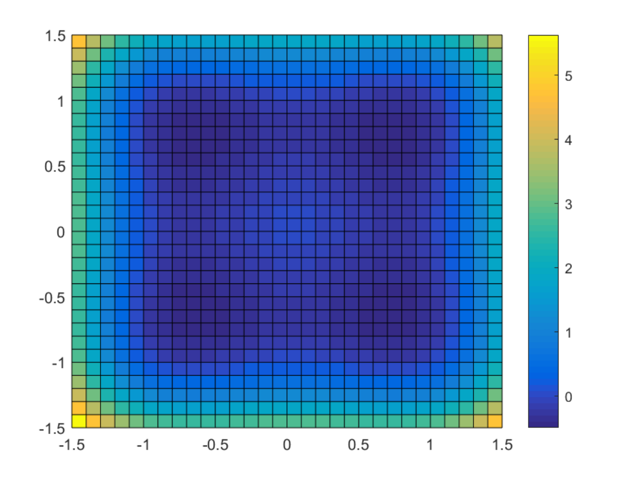


Image from [Garipov et al. 18]

Equivalent local minima and symmetry



(mostly) connected local min



Isolated local min

- Equivalent solutions:

$$X = X^* R, RR^\top = I$$

- Equivalent solutions:

$$X = X^* P, P\ permutation$$

Neural networks only have permutation symmetry,
why do they have connected local min?

(Partial) short answer: overparametrization

- Existing explanations of mode connectivity: [Freeman and Bruna, 2016, Venturi et al. 2018, Liang et al. 2018, Nguyen et al. 2018, Nguyen et al. 2019]
- If the network has special structure, and is highly overparametrized (#neurons > #training samples), then local mins are connected.

- Problem: Networks that are not as overparametrized were also found to have connected local min.
- Can we prove similar results in mildly overparametrized regime?

Our Results

- For neural networks, not all local/global min are connected, even in the overparametrized setting.
- Solutions that satisfy dropout stability are connected.
- Possible to switch dropout stability with noise stability (used for proving generalization bounds for neural nets)

Not all local min are connected

- Simple setting: 2-layer net, data (x_i, y_i) generated by ground truth neural network with 2 hidden neurons.
- Overparametrization: consider optimization of a 2 layer neural network with h ($h >> 2$) hidden neurons.

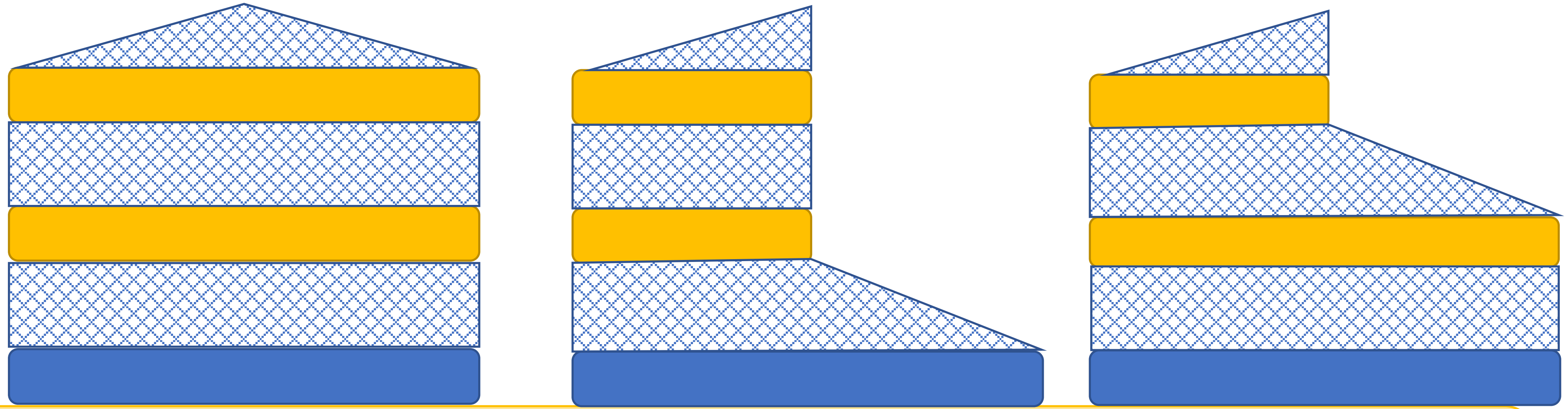
- Theorem: For any $h > 2$, there exists a data-set with $h+2$ samples, such that the set of global minimizers are not connected.

What kind of local min are connected?

- Only local min found by standard optimization algorithms are known to be connected.
- Properties of such local min?
  - Closely connected to the question of generalization/implicit regularization.
  - Many conjectures: “flat” local min, margin, etc.
- This talk: Dropout stability

Dropout stability

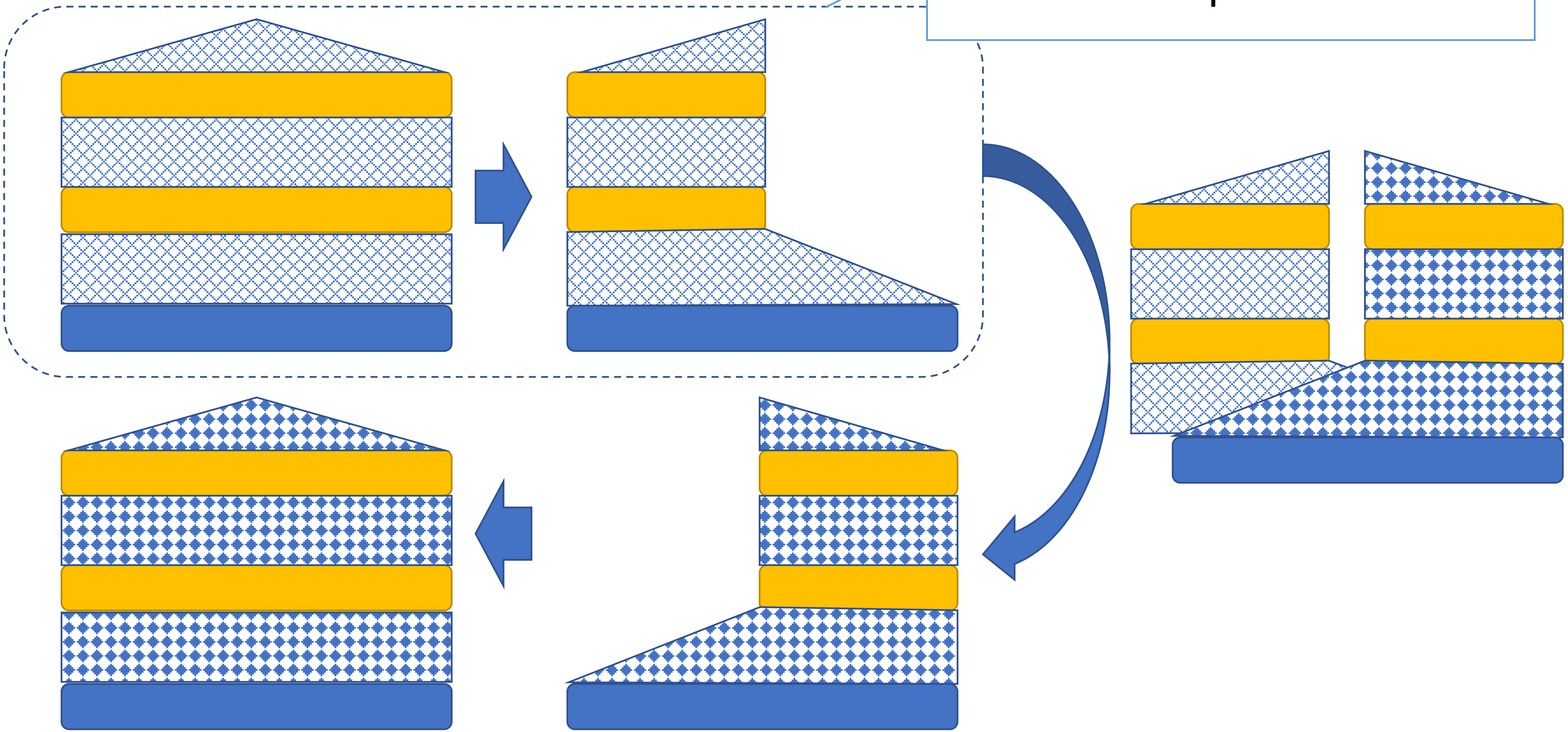
- A network is ε-dropout stable, if zeroing out 50% nodes at every layer (and rescale others appropriately) increases its loss by at most ε.



- Theorem: If both θ_A and θ_B are ε-dropout stable, then there exists a path between them with maximum loss $\leq \max\{L(\theta_A), L(\theta_B)\} + \varepsilon$

High level steps

How to connect a network with its dropout version?



Direct Interpolation

- Direct interpolation between the weights does not work.
- Even for a simple two layer linear network, if

$$f_A(x) = U_1^\top W_1 x, \qquad f_B(x) = U_2^\top W_2 x$$

- Interpolation between the parameters with coefficient $(\alpha, 1-\alpha)$

$$f_\alpha(x) = [\alpha^2 U_1^\top W_1 + \alpha(1-\alpha)(U_1^\top W_2 + U_2^\top W_1) + (1-\alpha)^2 U_2^\top W_2]x$$

θ_A

θ_B

- In general should have high cost.

Connecting a network with its dropout

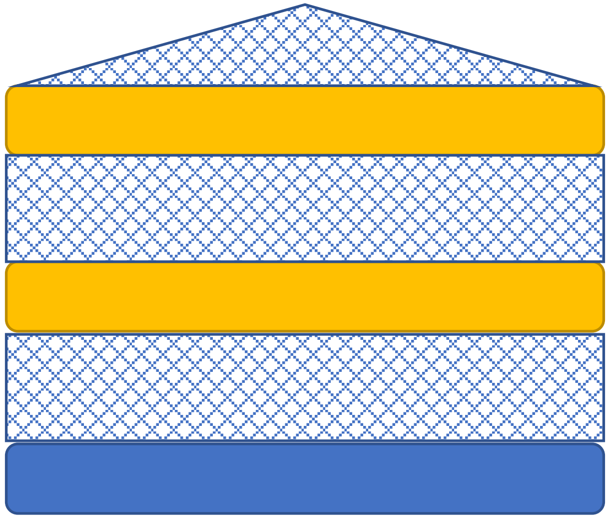
- Main observation: can use two types of line segments.

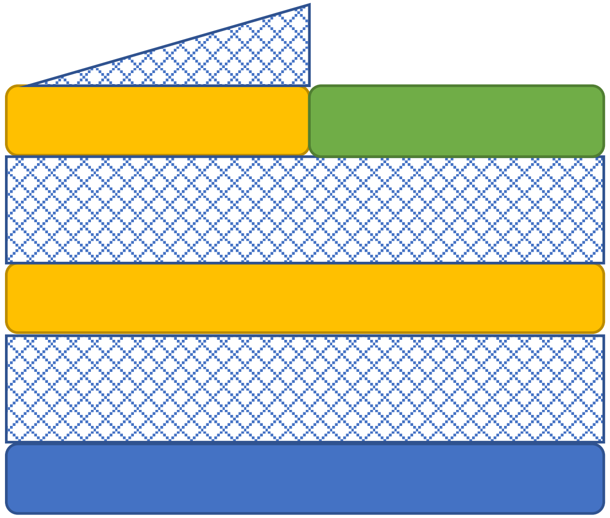
- Type (a): if θ_A and θ_B both have low loss, and they only differ in top layer weight, can linearly interpolate between them.

- Type (b): If a group of neurons do not have any outgoing edges, can change their incoming edges arbitrarily.

- Idea: Recurse from the top layer, use Type (b) moves to prepare for the next Type (a) move

Example 3-layer path (1) -> (2)

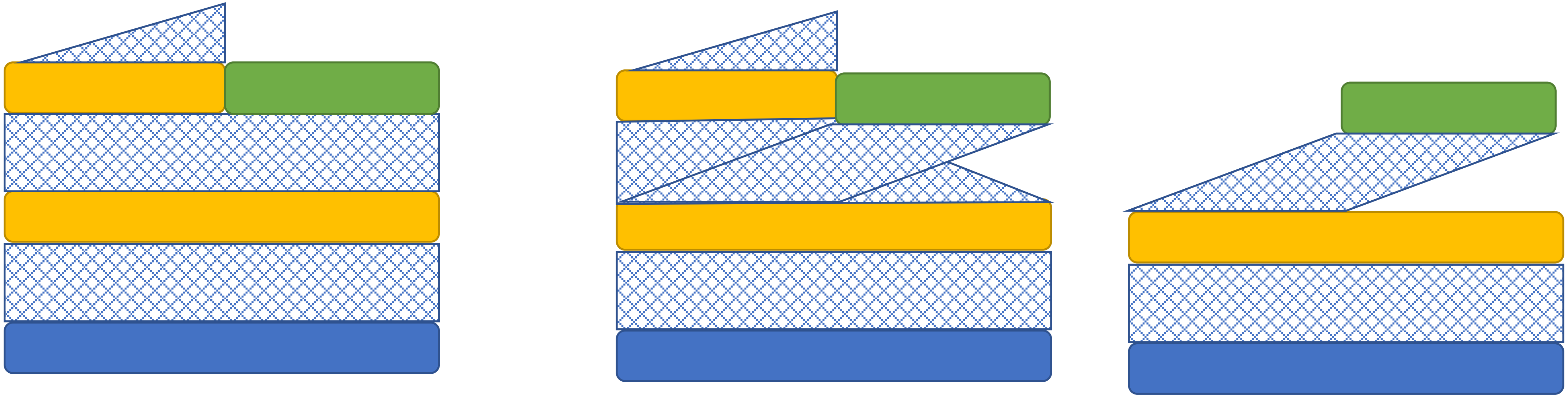




$$(1)\ \left(\begin{array}{c|c} L_3 & R_3 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline D_2 & R_2 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)$$

$$(2)\ \left(\begin{array}{c|c} \color{red}{2L_3} & 0 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline D_2 & R_2 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)\ (a)$$

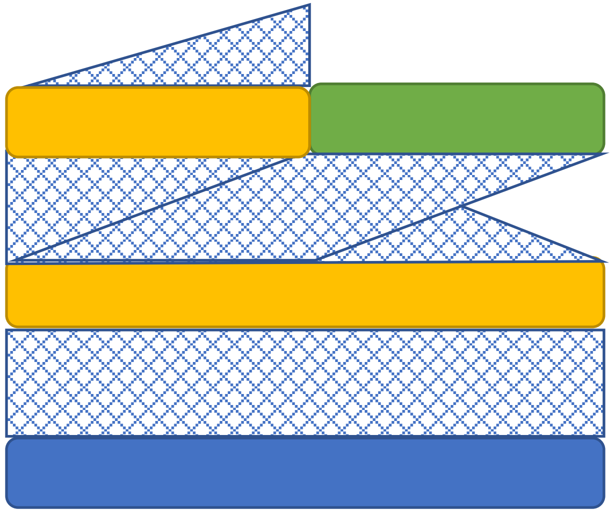
Example 3-layer path (2) -> (3)

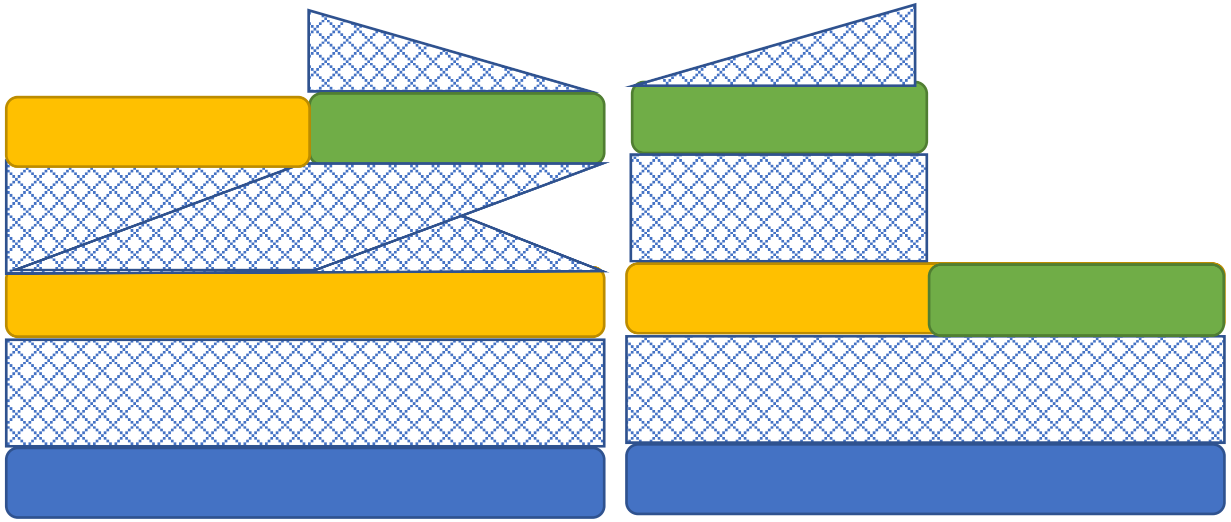


$$(2)\quad \left(\begin{array}{c|c} 2L_3 & 0 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline D_2 & R_2 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right) \quad (a)$$

$$(3)\quad \left(\begin{array}{c|c} 2L_3 & 0 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right) \quad (b)$$

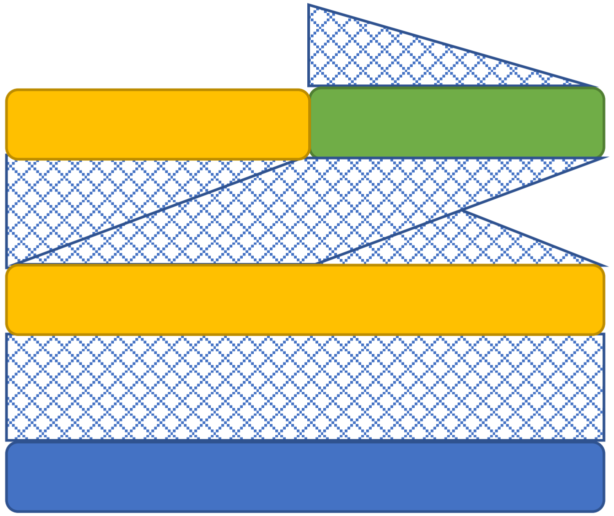
Example 3-layer path (3) -> (4)

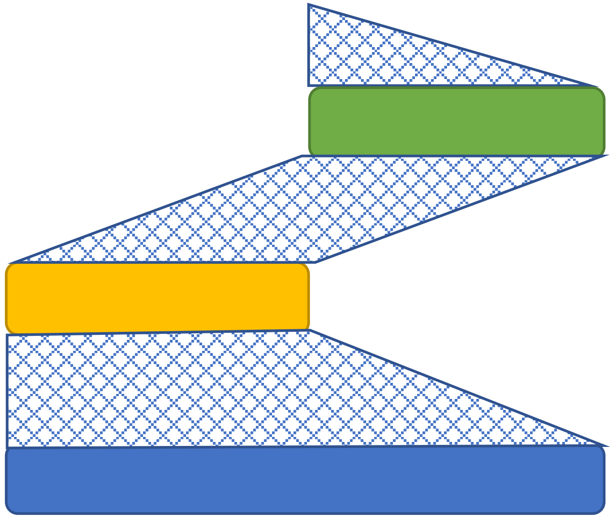




$$(3)\ \left(\begin{array}{c|c} 2L_3 & 0 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)\ (b) \qquad (4)\ \left(\begin{array}{c|c} 0 & 2L_3 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)\ (a)$$

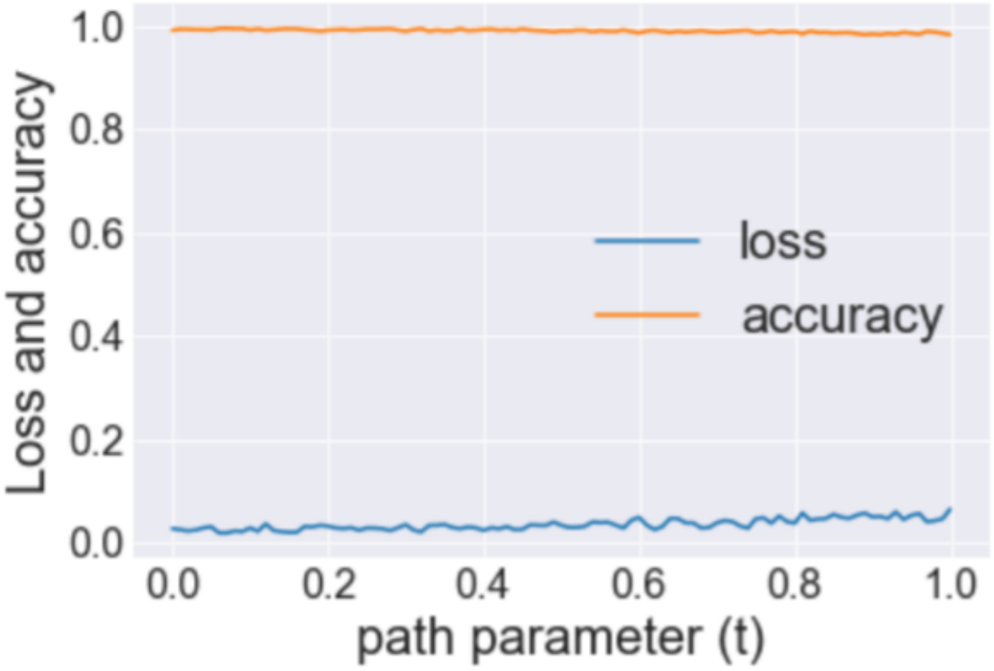
Example 3-layer path (4) -> (5)



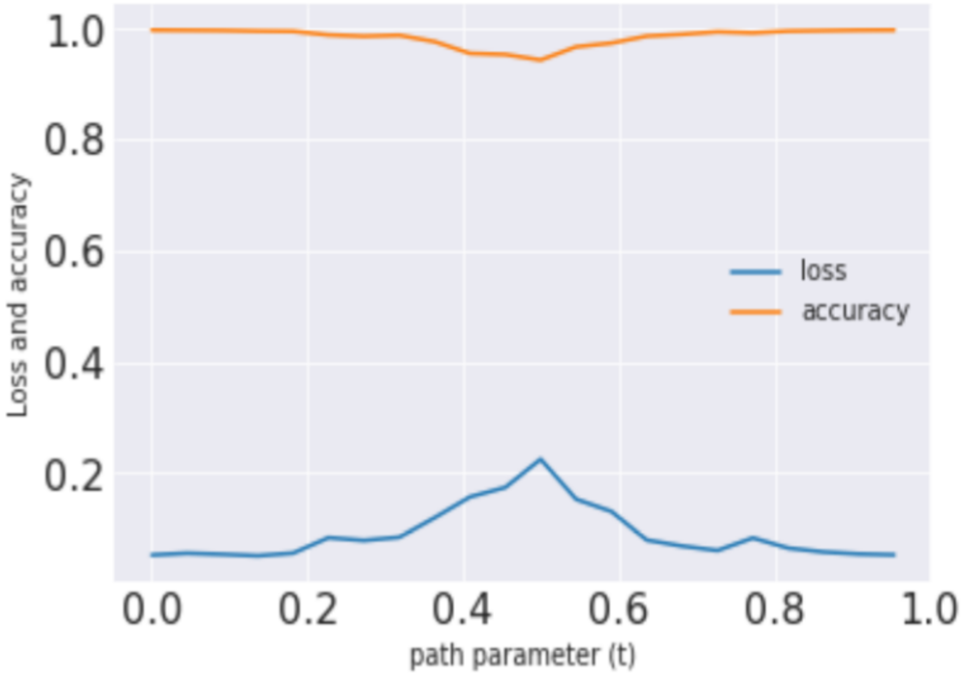


$$(4)\ \begin{pmatrix} 0 & | & 2L_3 \end{pmatrix} \left(\begin{array}{c|c} L_2 & C_2 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)\ (a)\qquad (5)\ \begin{pmatrix} 0 & | & 2L_3 \end{pmatrix} \left(\begin{array}{c|c} 0 & 0 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)\ (b)$$

Experiments



MNIST, 3-layer CNN



CIFAR-10, VGG-11

Conclusions

For neural networks, not all local/global min are connected, even in the overparametrized setting.

Solutions that satisfy dropout/noise stability are connected.

Open Problems

- Path found by dropout/noise stability are still more complicated than the path found in practice.
- Path are known to exist in practice, even if the solutions are not as dropout stable as we hoped.

- Can we leverage mode connectivity to design better optimization algorithms?

Thank you!

An example path for 3 layer network

$$(1)\quad \left(\begin{array}{c|c} L_3 & R_3 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline D_2 & R_2 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right)$$

$$(2)\quad \left(\begin{array}{c|c} 2L_3 & 0 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline D_2 & R_2 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right) \text{(a)}$$

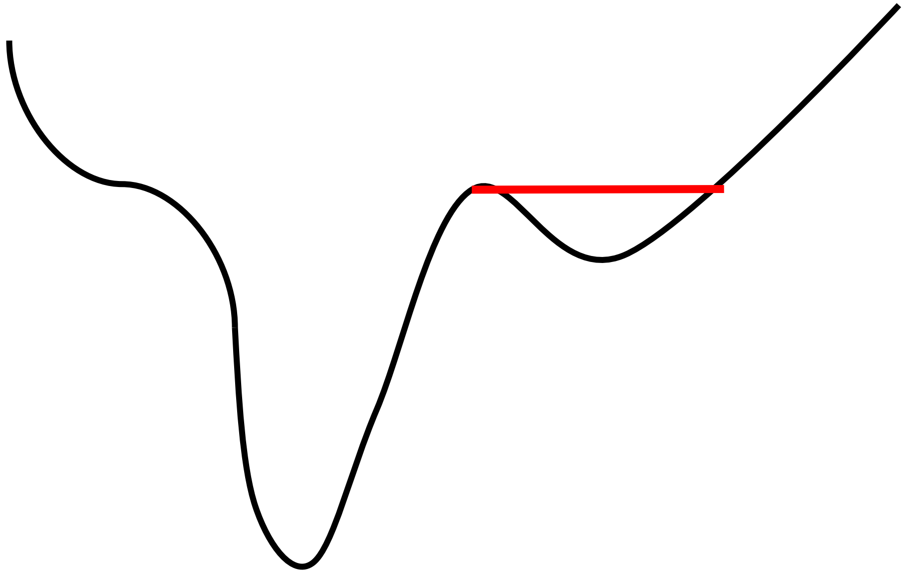
$$(4)\quad \left(\begin{array}{c|c} 0 & 2L_3 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right) \text{(a)}$$

$$(3)\quad \left(\begin{array}{c|c} 2L_3 & 0 \end{array}\right) \left(\begin{array}{c|c} L_2 & C_2 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right) \text{(b)}$$

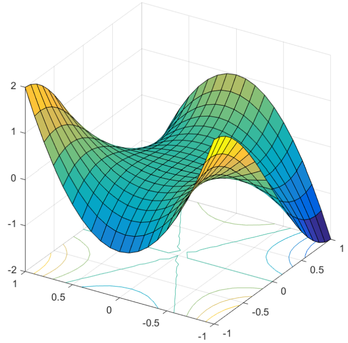
$$(5)\quad \left(\begin{array}{c|c} 0 & 2L_3 \end{array}\right) \left(\begin{array}{c|c} 0 & 0 \\ \hline 2L_2 & 0 \end{array}\right) \left(\begin{array}{c} L_1 \\ \hline B_1 \end{array}\right) \text{(b)}$$

How can we use mode connectivity?

- If all local min are connected, then all the level sets are also connected.
- If all “typical solutions” are connected (and there is a typical global min), local search algorithms will not be completely stuck.



- However, there can still be flat regions/high order saddle points.
- Can better optimization/sampling algorithms leverage mode connectivity?



Thank you!

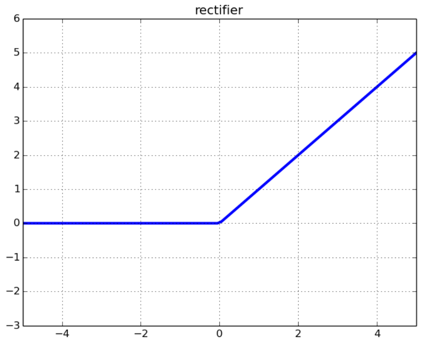
Noise stability

- A network is noise stable, if injecting noise at intermediate layers does not change the output by too much.
- Precise definition similar to [Arora et al. 2018]

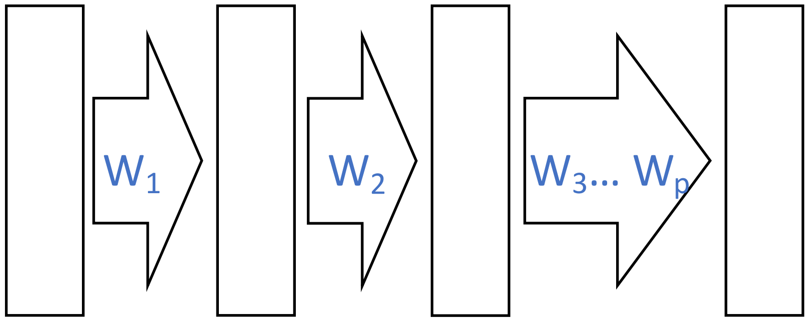
- Theorem: If both θ_A and θ_B are ε-noise stable, then there is a path between them with maximum loss $\leq \max\{L(\theta_A), L(\theta_B)\} + \varepsilon$. The path consists of 10 line segments.

- Idea: noise stability ➔ dropout stability, further, noise stability allow us to do direct interpolation between a network and its dropout.

Deep Neural Networks



- For simplicity: Fully Connected Networks
- Weights $\theta = (W_1, W_2, \ldots, W_p)$, nonlinearity σ
- Samples (x,y), hope to learn a network that maps x to y



$x^{(0)} = x$ $x^{(1)} = \sigma(W_1 x)$ $x^{(p)} = W_p x^{(p-1)}$

- Function $f_\theta(x) = W_p \sigma(W_{p-1} \sigma(\cdots \sigma(W_1 x) \cdots))$
- Objective: $L(\theta) = \frac{1}{n} \sum_{i=1}^{n} l(y_i, f_\theta(x_i))$

Convex loss function