Feature Learning in Infinite-Width Neural Networks

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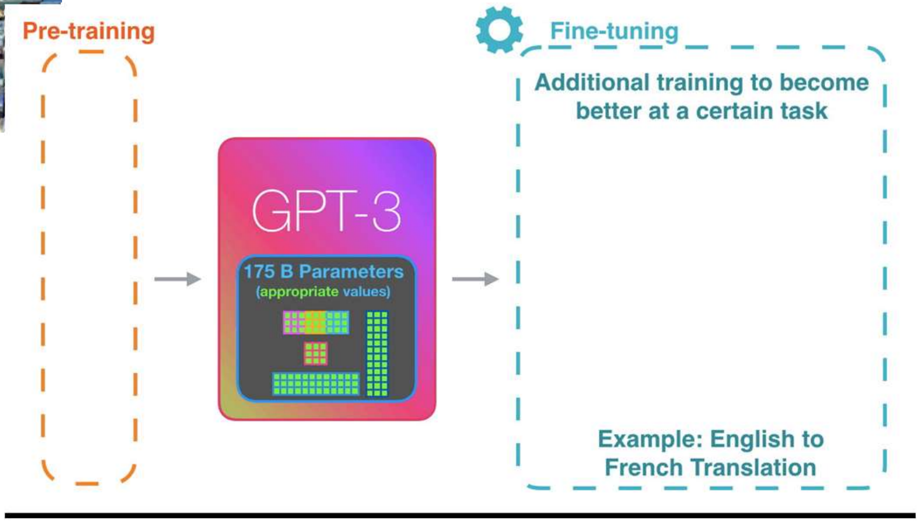
Presenting the 4th Paper of the *Tensor Programs* Series

Joint work with ex-Microsoft AI Resident Edward Hu

Feature Learning is Crucial in Deep Learning

Imagenet and Resnet

BERT and GPT3



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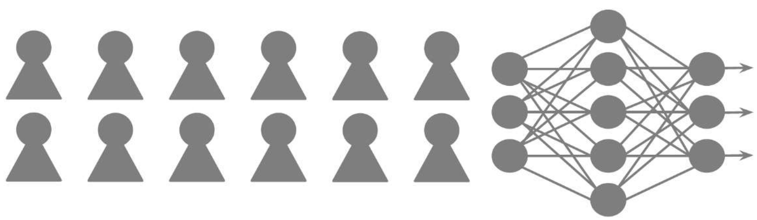
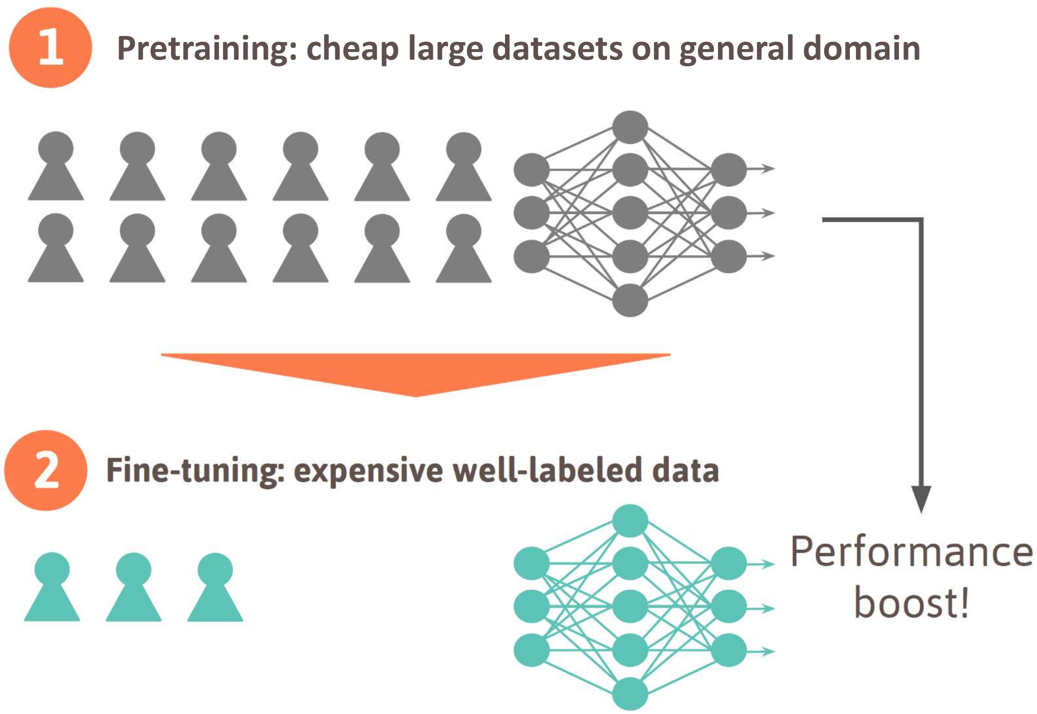
Pretraining and Transfer Learning
Cannot Happen without Feature Learning!

Pretraining and Transfer via Finetuning

1 **Pretraining: cheap large datasets on general domain**



Pretraining and Transfer via Finetuning



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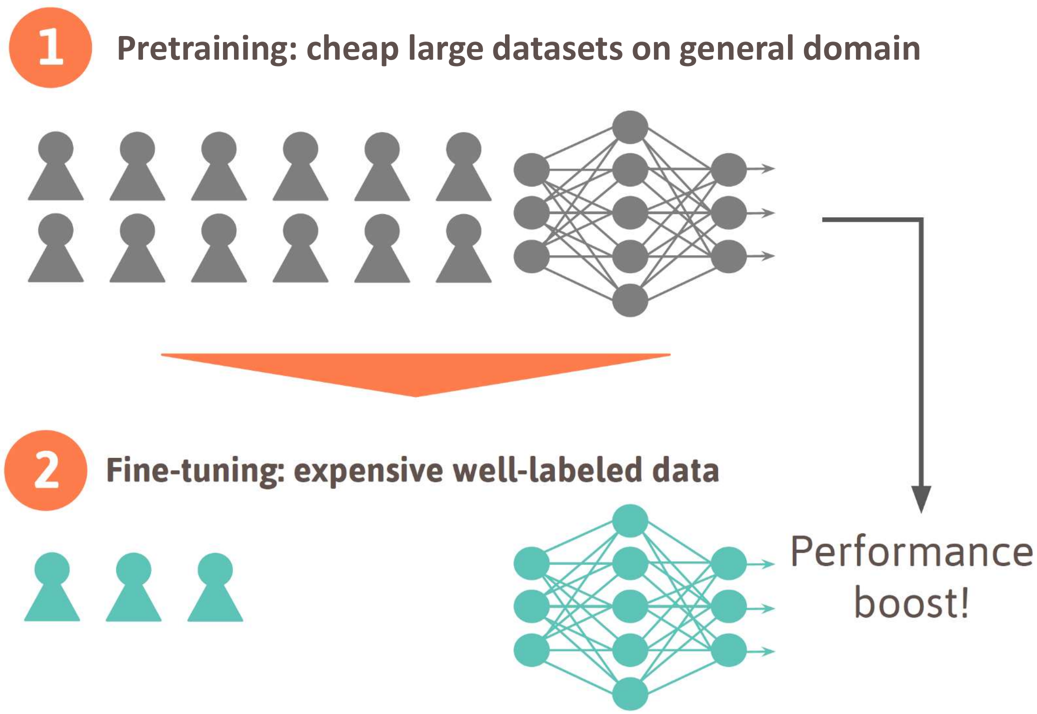

- Discard readout layer from pretraining

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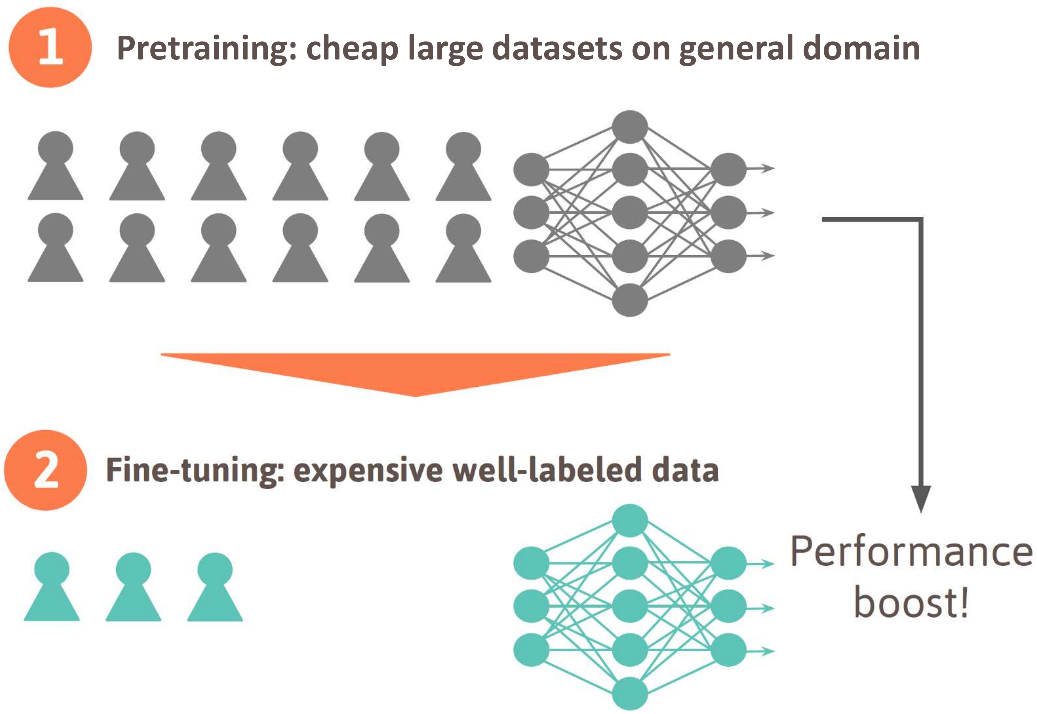

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- *Linear Finetuning*: Train new readout layer only

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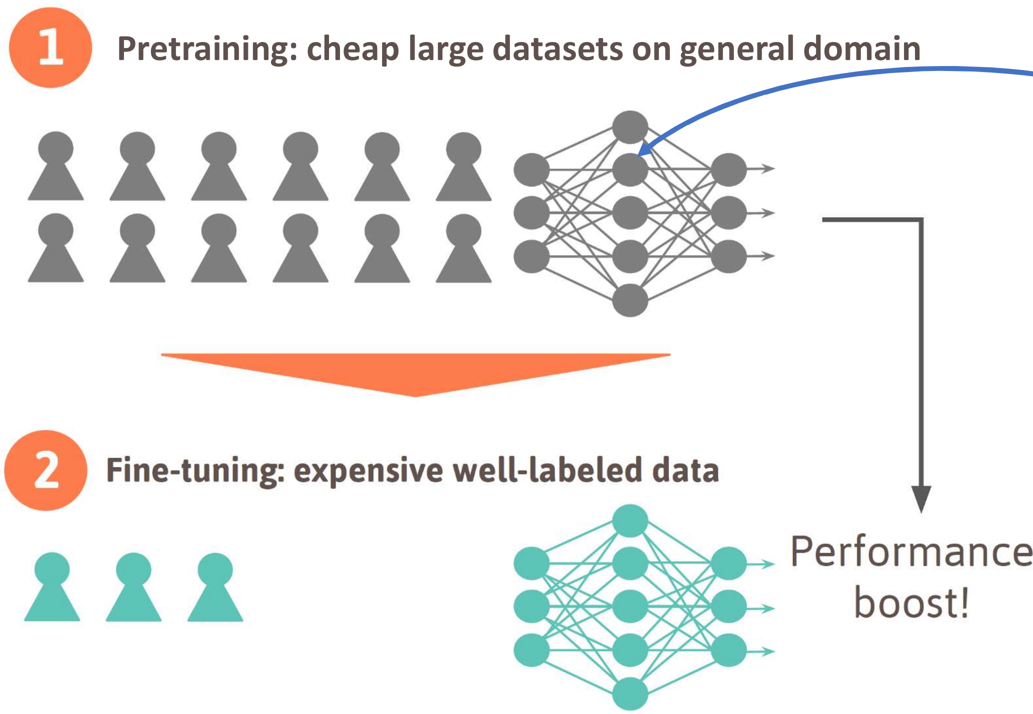

If pretraining improves linear finetuning, then the embeddings (i.e. features) of inputs must change during pretraining!

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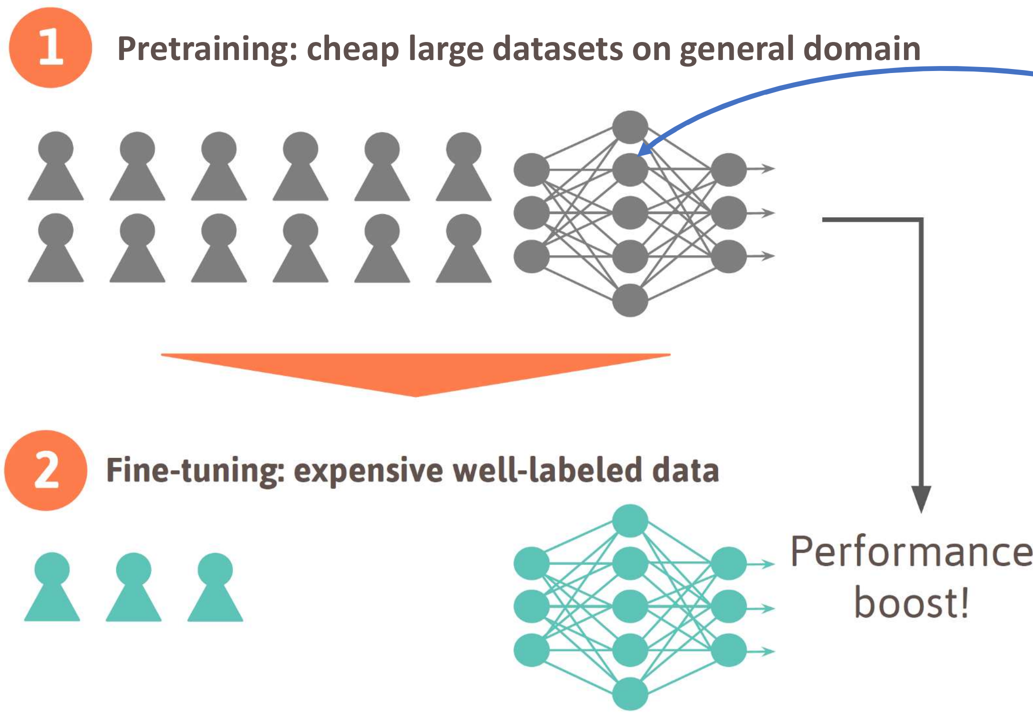

If pretraining improves linear finetuning, then the embeddings (i.e. features) of inputs must change during pretraining!

- Discard readout layer from pretraining
- *Linear Finetuning*: Train new readout layer only
- *Total Finetuning*: Train the entire network
  - Our conclusions will apply here as well

Current Theory: Neural Tangent Kernel

Naïve first order Taylor expansion

$$f(x;\theta) - f(x;\theta_0) \approx \langle \nabla_\theta f(x;\theta_0), \theta - \theta_0 \rangle$$

so

$$f_t - f_{t-1} \approx -\eta K \mathcal{L}'(f_t, y)$$

Where $\mathcal{L}$ is loss, y is label, and K is the kernel

$$K(x,z) = \langle \nabla_\theta f(x;\theta_0), \nabla_\theta f(z;\theta_0) \rangle$$

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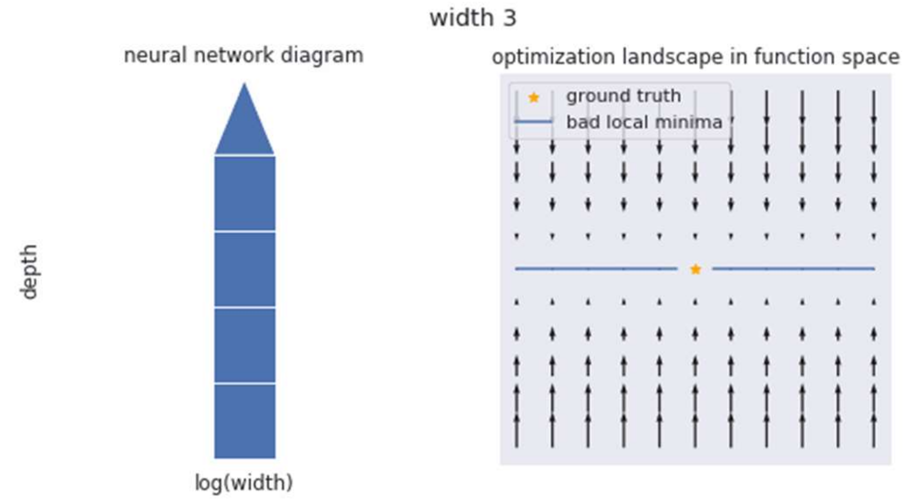

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- Linear evolution – easy to analyze
- Yields optimization and generalization results

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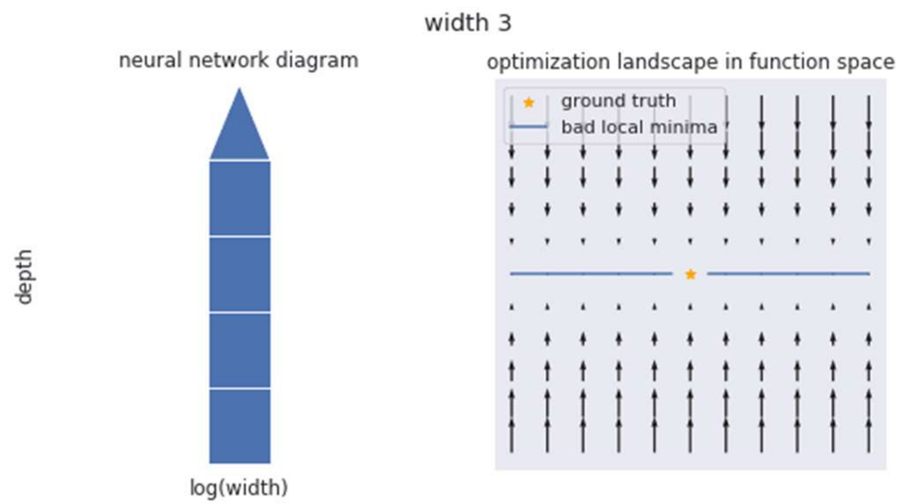

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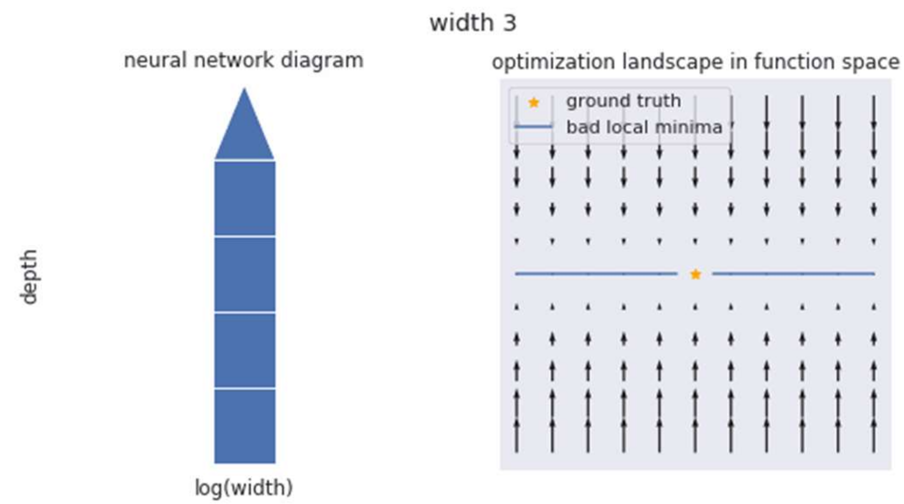


But NTK Limit Does Not Learn Features!

Word2Vec example

Will explain later

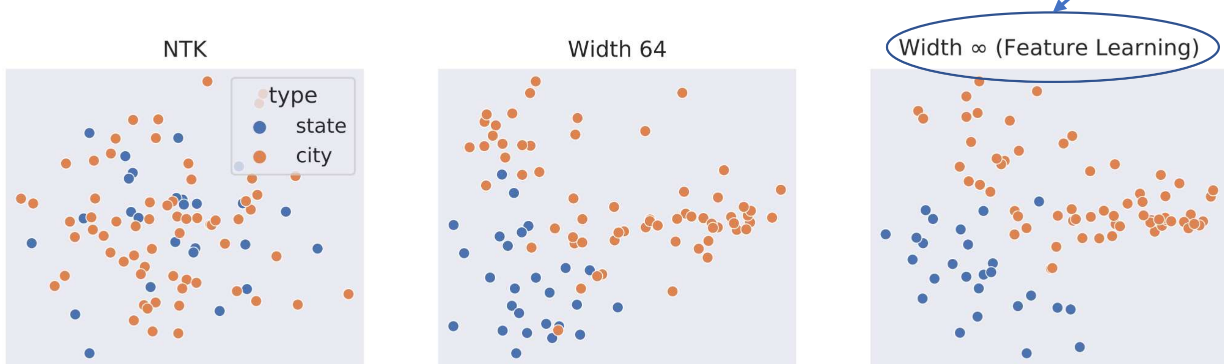
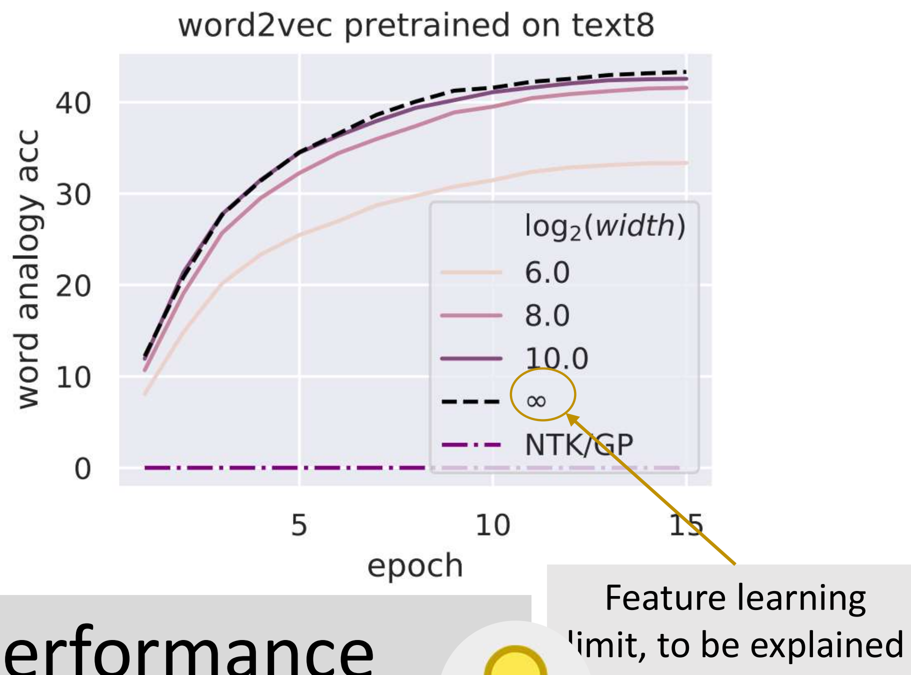


Figure 1: PCA of Word2Vec embeddings of common US cities and states, for NTK, width-64, and width-∞ feature learning neural networks. NTK embeddings are essentially random, while cities and states get naturally separated in embedding space as width increases in the feature learning regime.

Feature Learning ∞-Width NN on Real Tasks

- Word2Vec
  - Pretraining: learn word embeddings so that similar words have close embeddings, in an unsupervised manner.
  - Transfer: word analogy task, e.g. “what to a queen is as a man to a woman?”



- NTK Limit has trivial performance
- Performance is monotonic in width

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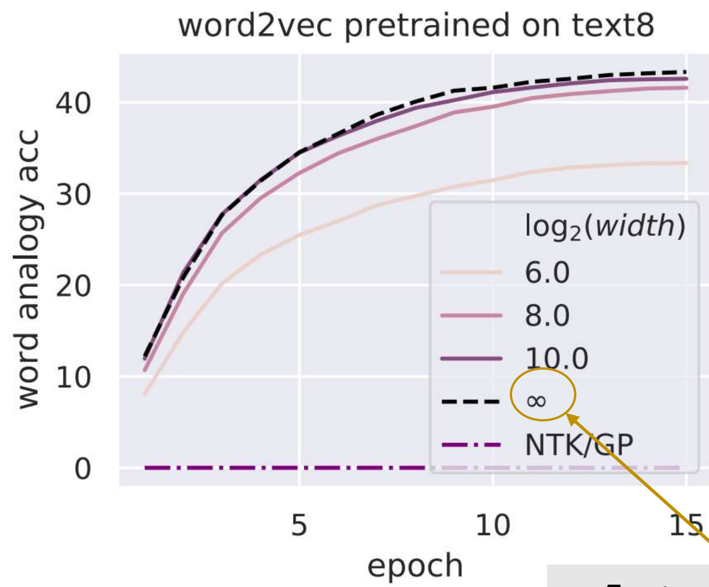

Feature learning limit, to be explained

- NTK Limit has trivial performance
- Performance is monotonic in width

Similar Results on Metalearning (MAML)

Overview

Our experiments verify this is the right limit

Our Theoretical Contributions

- Classify all "viable" ∞-width limits into feature learning and kernel limits
- Identify "*the maximal*" feature learning limit
- Propose the *Tensor Programs* technique for deriving its equations, and more generally, the limit of any neural computation

Significance

- Framework for studying feature learning in overparametrized NN
- Formulas for training feature-learning ∞-width NN in variety of settings (e.g. pretraining, metalearning, reinforcement learning, GANs, etc)
- Mostly solves the problem of taking ∞-width limits

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- Parametrizations of Neural Networks
- Dichotomy of Parametrizations
- The “Maximal” Feature Learning Limit
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abc-Parametrizations

- Consider L-hidden-layer perceptron
  - Input dim d, output dim 1, width n, nonlinearity ϕ, input $\xi \in \mathbb{R}^d$
  - Weights $W^1 \in \mathbb{R}^{n\times d}$ and $W^2, \dots, W^L \in \mathbb{R}^{n\times n}$ and $W^{L+1} \in \mathbb{R}^{1\times n}$
  - $h^1(\xi) = W^1\xi \in \mathbb{R}^n$
  - $x^l(\xi) = \phi\left(h^l(\xi)\right) \in \mathbb{R}^n, h^{l+1}(\xi) = W^{l+1}x^l(\xi) \in \mathbb{R}^n$ for $l = 1, \dots, L-1$
  - Network output (i.e. logits) $f(\xi) = W^{L+1}x^L(\xi)$

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An *abc-parametrization* is given by a set of numbers $\{a_l, b_l\}_l \cup \{c\}$ s.t.

a) Parametrize each $W^l = n^{-a_l} w^l$ where w^l is trained instead of W^l

b) Initialize each $w^l_{\alpha\beta} \sim \mathcal{N}(0, n^{-2b_l})$

c) SGD learning rate is ηn^{-c} for some width-independent η.

Examples

$$h^1(\xi) = W^1\xi \in \mathbb{R}^n, \;\; x^l(\xi) = \phi\left(h^l(\xi)\right) \in \mathbb{R}^n, \;\; h^{l+1}(\xi) = W^{l+1}x^l(\xi) \in \mathbb{R}^n, \;\;\; f(\xi) = W^{L+1}x^L(\xi)$$

	Definition	NTK	Standard (Pytorch default)	Mean Field ($L = 1$)
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By changing a_l, b_l while fixing $a_l + b_l$, we effectively give each layer l its own learning rate.

Why Do We Care About Parametrizations?

- -width limit
  - abc-parametrizations correspond to natural class of limits, including NTK, GP, Mean Field, etc
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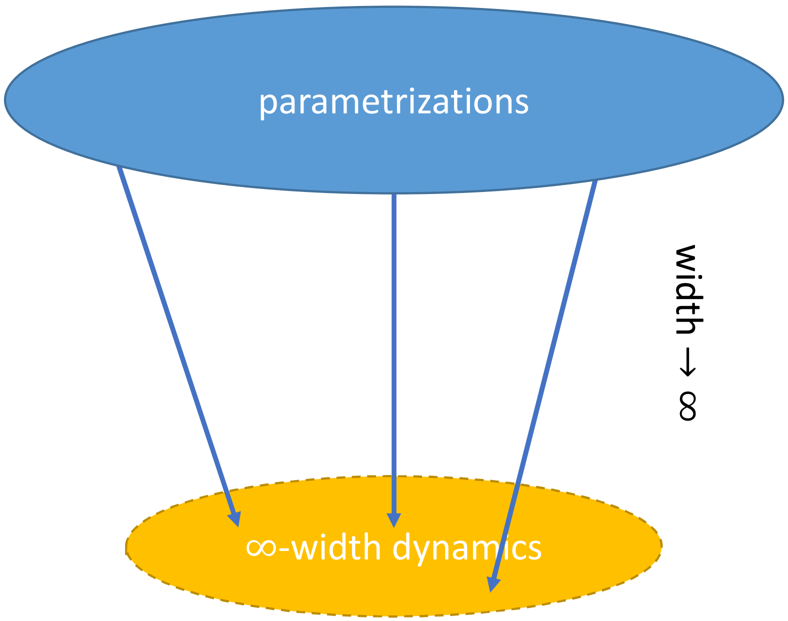

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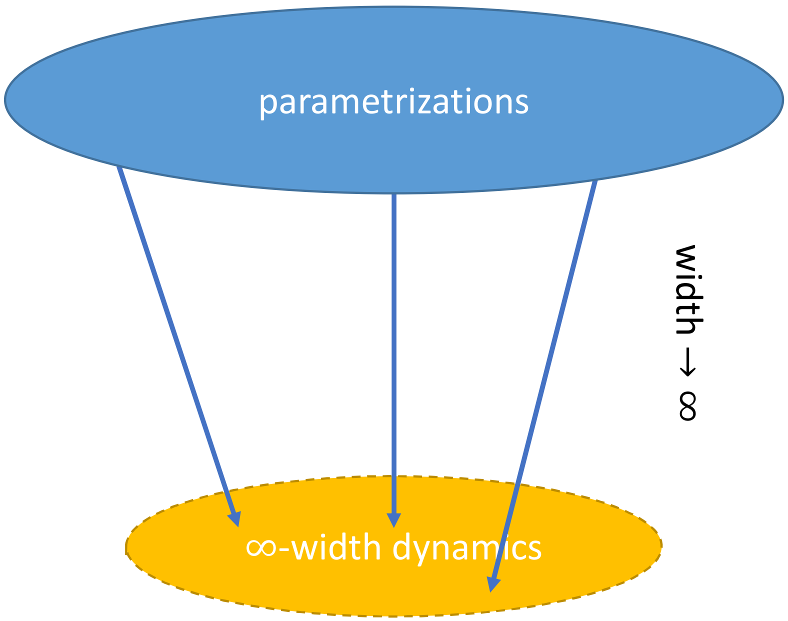
  - abc-parametrizations correspond to natural class of limits, including NTK, GP, Mean Field, etc
- Parametrizations are important practically
  - E.g. Glorot, He, Fixup



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Instability and Triviality

$LR = \eta n^{-c}$

- If LR too large w.r.t width (i.e. c too small), then logits or preactivations blow up with width during training
  - We say this abc-parametrization is $unstable$
- If LR too small w.r.t width (i.e. c too big), then the NN function doesn't evolve in the ∞-width limit
  - We say this abc-parametrization is *trivial*
- Only *nontrivial stable* abc-parametrizations are meaningful

Dynamical Dichotomy Theorem

- Any *nontrivial stable* abc-parametrization yields a (discrete-time) ∞-width limit
- When trained for any finite time, this limit either
  1. (Feature learning limit) allows the embedding $x^L(\xi)$ to evolve nontrivially or
  2. (Kernel limit) is described by kernel gradient descent in function space, but not both.

Example: Mean Field when $L = 1$

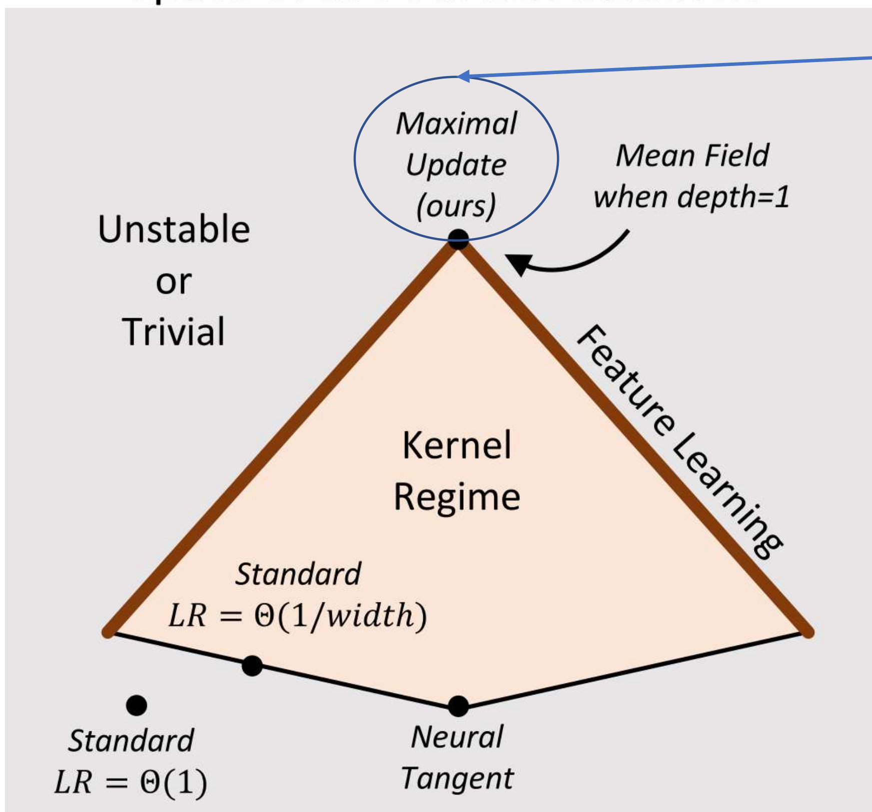
Example: NTK

for some kernel K,
$$f_{t+1} - f_t = -K\mathcal{L}'(f_t, y)$$

What is ruled out?
e.g. higher order generalizations of NTK dynamics like
$$f_{t+1} - f_t = -\langle K^{(2)}, \mathcal{L}'(f_t, y)^{\otimes 2}\rangle$$

Interesting consequence:
the NN function must be identically 0 at init in any feature learning limit

A Caricature of Space of abc-Parametrizations

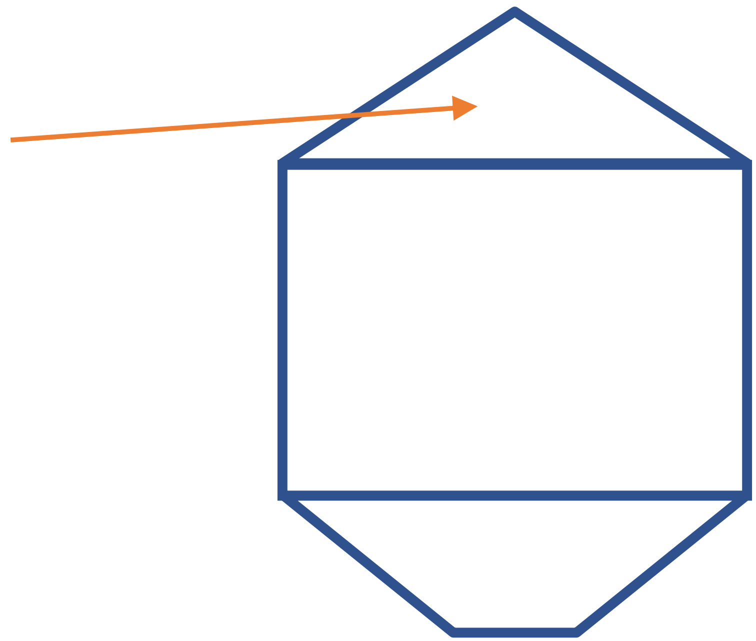


Will explain soon

- The *nontrivial stable* params form a high dimensional polytope
- Feature learning params form 2 facets
- Everything else is in kernel regime

NTK, Standard Param Don't Learn Features

- Intuition why
  - The last layer weights get too much gradient, relative to weights in the body
  - We want to use larger learning rate to enable feature learning, but then the logits would blow up.



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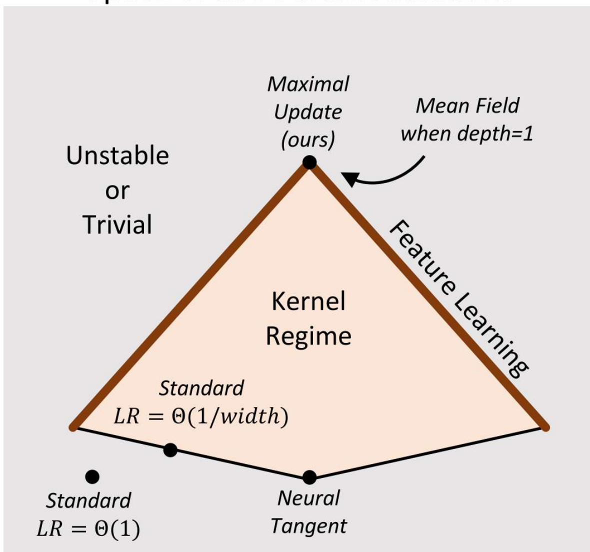
Maximal Update Parametrization (μP)

- Modify Standard Param to get Maximal Update Param
  - Last layer: divide logits by $\sqrt{n}$ and use $\Theta(1)$ learning rate
    - i.e. $a_{L+1} = \frac{1}{2}, c = 0$
    - i.e. $f(\xi) = \frac{1}{\sqrt{n}} w^{L+1} x^L(\xi)$ where $w_{\alpha\beta}^{L+1} \sim \mathcal{N}\left(0, \frac{1}{n}\right)$
    - This alone suffices to enable feature learning
  - First layer: increase the gradient by n by setting $a_1 = -\frac{1}{2}, b_1 = 1/2$
    - i.e. $h^1(\xi) = \sqrt{n} w^1 \xi$ where $w_{\alpha\beta}^1 \sim \mathcal{N}\left(0, \frac{1}{n}\right)$
    - Needed to enable feature learning in *every* layer

Maximality of Maximal Update Param

- Maximal Update Param is *Maximally Feature Learning*: *Every* layer learns features ($h^l(\xi), x^l(\xi)$ for every l will evolve during training).

Space of abc-Parametrizations

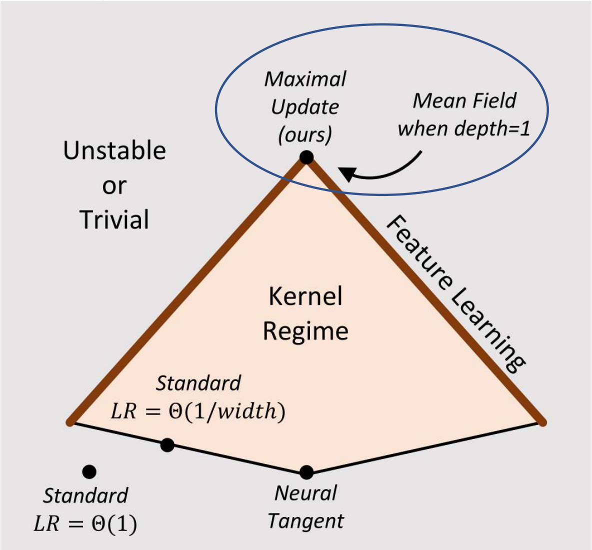


1-Dimension Degeneracy in abc

- For any $\theta \in \mathbb{R}$ and $t \geq 0$, $f(\xi)$ at time t stays fixed for all input ξ if

$$a_l \leftarrow a_l + \theta, \qquad b_l \leftarrow b_l - \theta, \qquad c \leftarrow c - 2\theta$$

Space of abc-Parametrizations



Equivalent when $L = 1$ *because, for* $\theta = 1/2$,
$a_l \leftarrow a_l + \theta, b_l \leftarrow b_l - \theta, c \leftarrow c - 2\theta$

Summary

$$h^1(\xi) = W^1\xi \in \mathbb{R}^n, \quad x^l(\xi) = \phi\left(h^l(\xi)\right) \in \mathbb{R}^n, \quad h^{l+1}(\xi) = W^{l+1}x^l(\xi) \in \mathbb{R}^n, \quad f(\xi) = W^{L+1}x^L(\xi)$$

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b_l	$w^l_{\alpha\beta} \sim \mathcal{N}(0, n^{-2b_l})$	0	$\begin{cases} 0 & \text{if } l = 1 \\ \frac{1}{2} & \text{if } l > 1 \end{cases}$	$\begin{cases} 0 & \text{if } l = 1 \\ \frac{1}{2} & \text{if } l > 1 \end{cases}$	0	1/2
c	$LR = \eta n^{-c}$	0	0	1	-1	0
Nontrivial		✔	✔	✔	✔	✔
Stable		✔	✘	✔	✔	✔
Feature Learning		✘	-	✘	✔	✔
Any depth		✔	✔	✔	✘	✔

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    - Motivating Example: Linear 1-Hidden-Layer NN
    - What is a Tensor Program?
    - Master Theorem
    - Infinite-Width Limit for All

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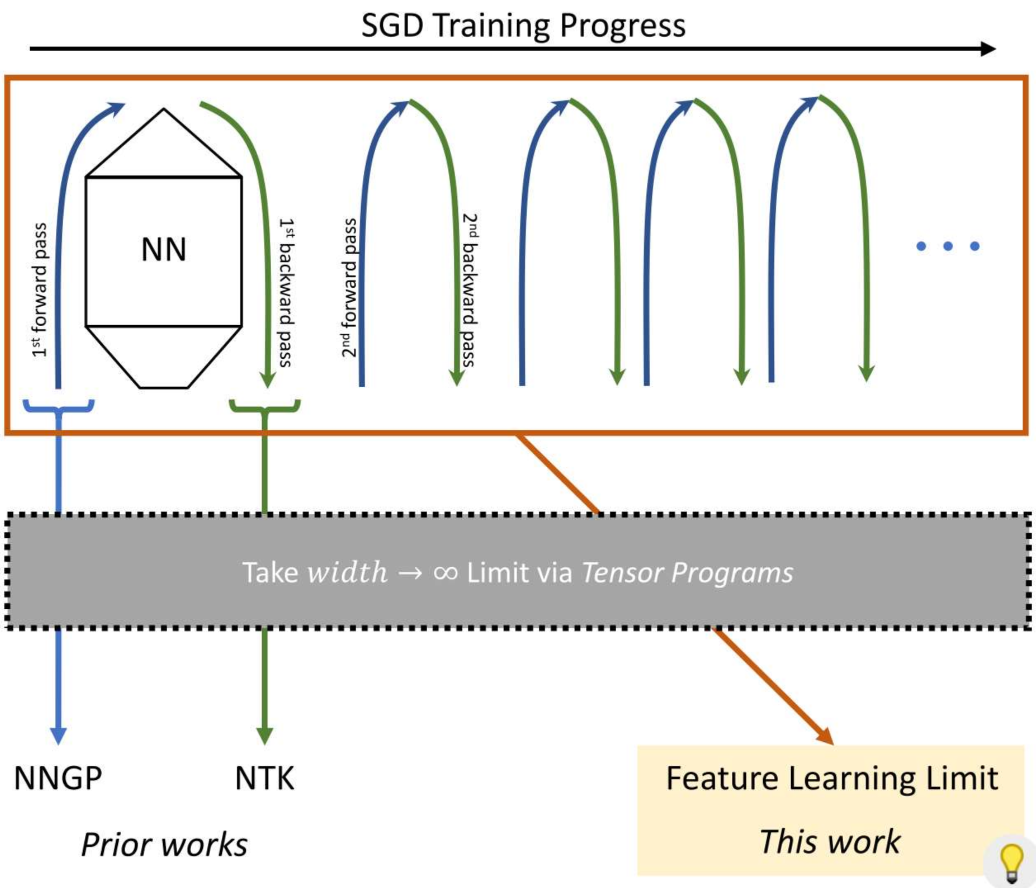
Key Theoretical Idea: Tensor Programs

When width is large, every activation vector has roughly iid coordinates, at ***any*** *time during training. Using* Tensor Programs*, we can recursively calculate such coordinate distributions, and consequently understand how the neural network function evolves.*

Key Theoretical Idea: Tensor Programs



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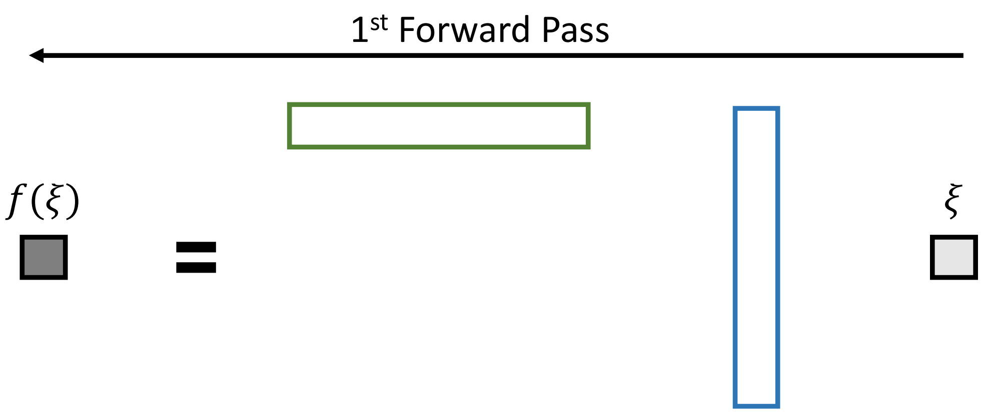
Motivating Example: Linear 1-Hidden-Layer

Assume input and output dim = 1



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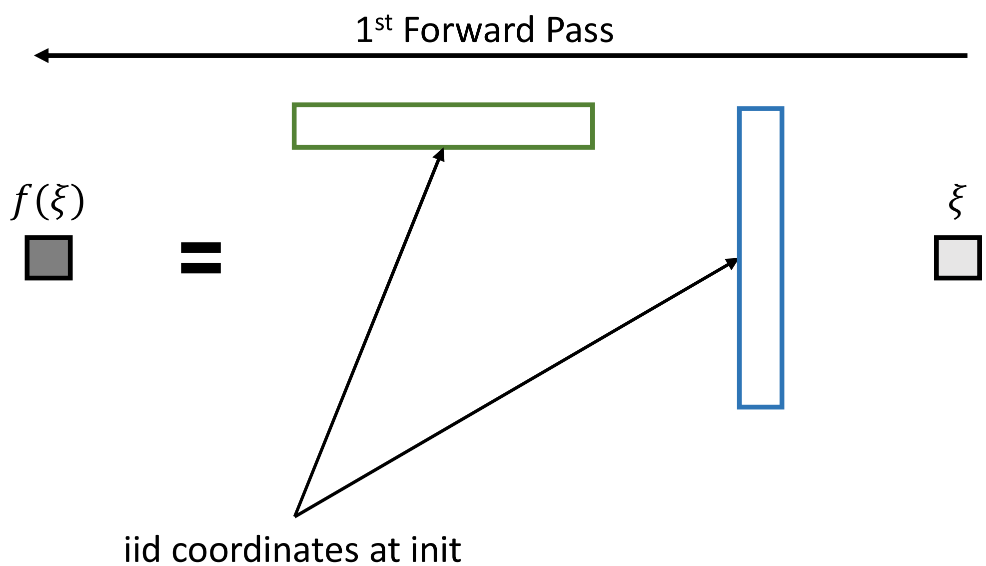

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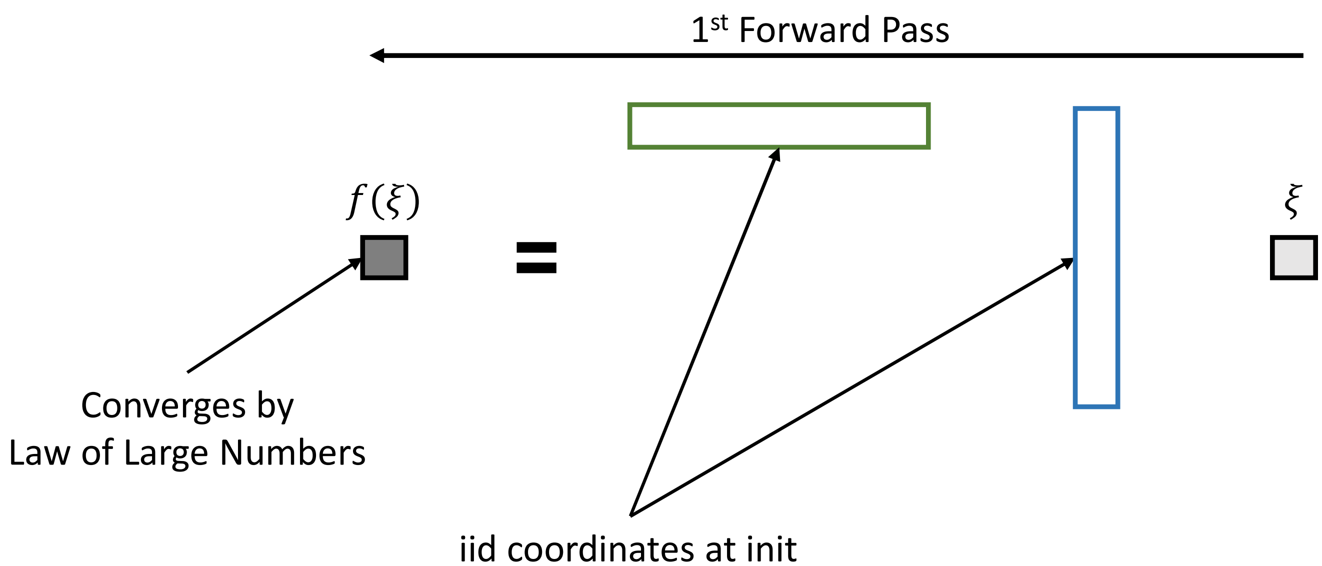
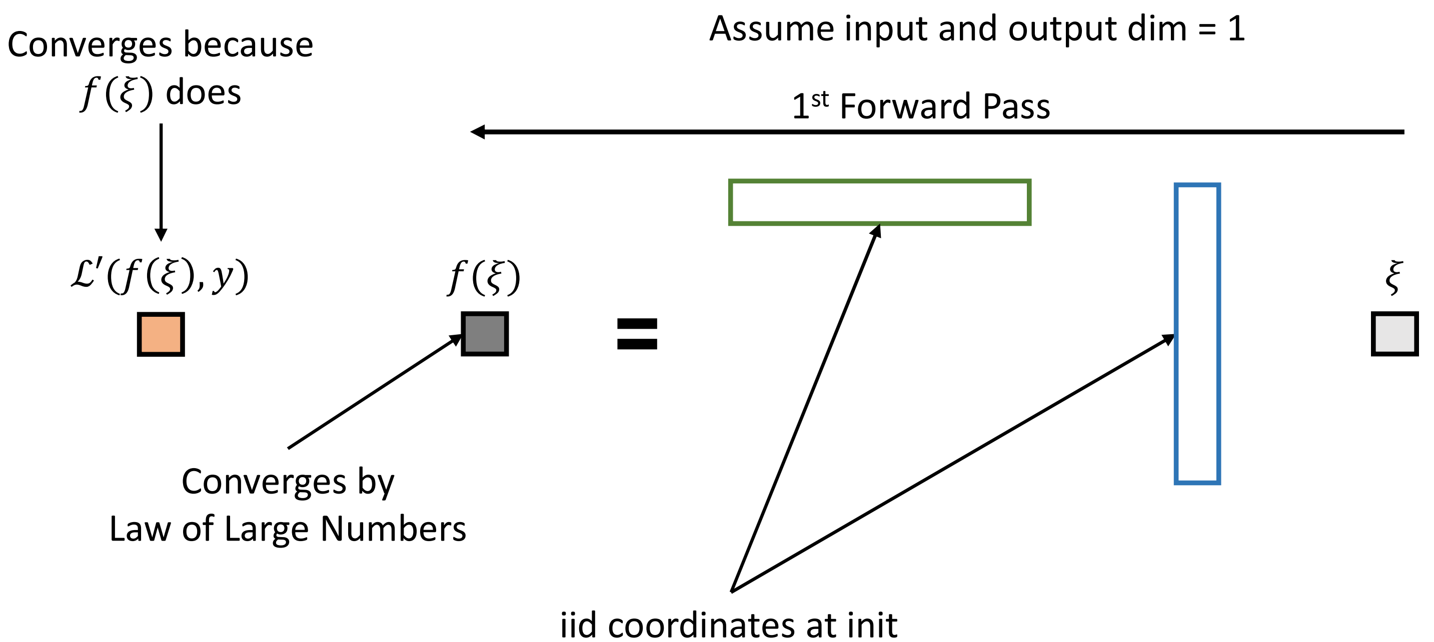


Motivating Example: Linear 1-Hidden-Layer



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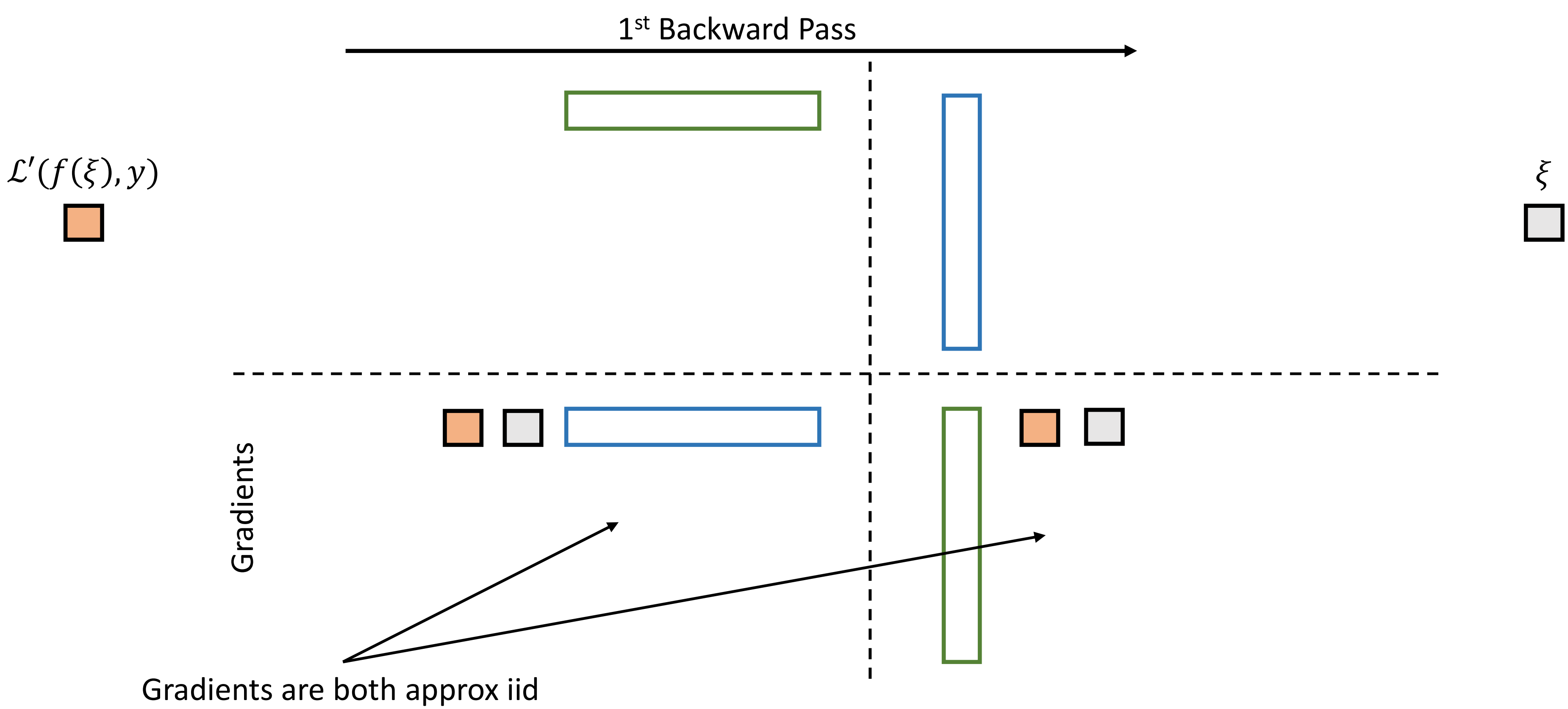
Assume input and output dim = 1



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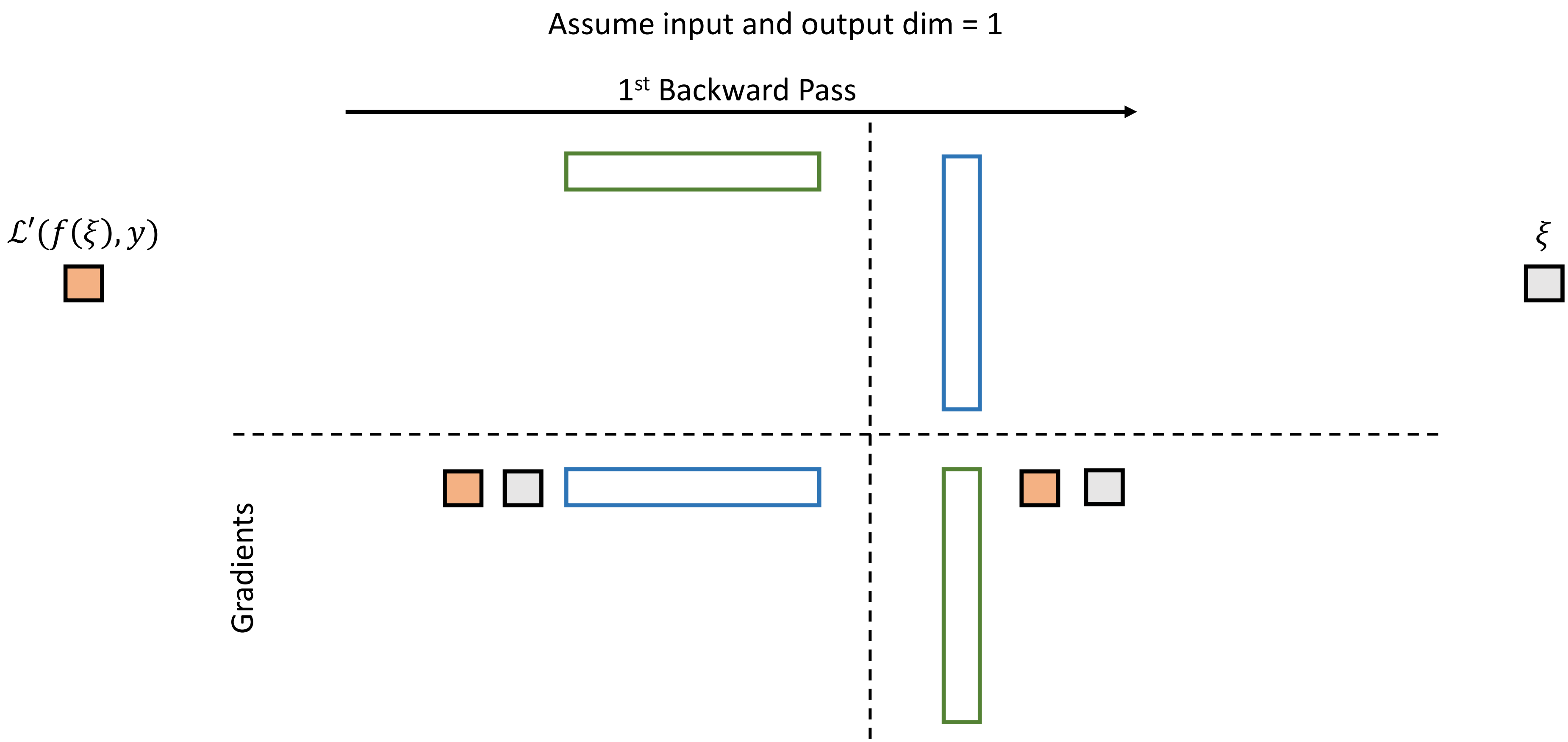

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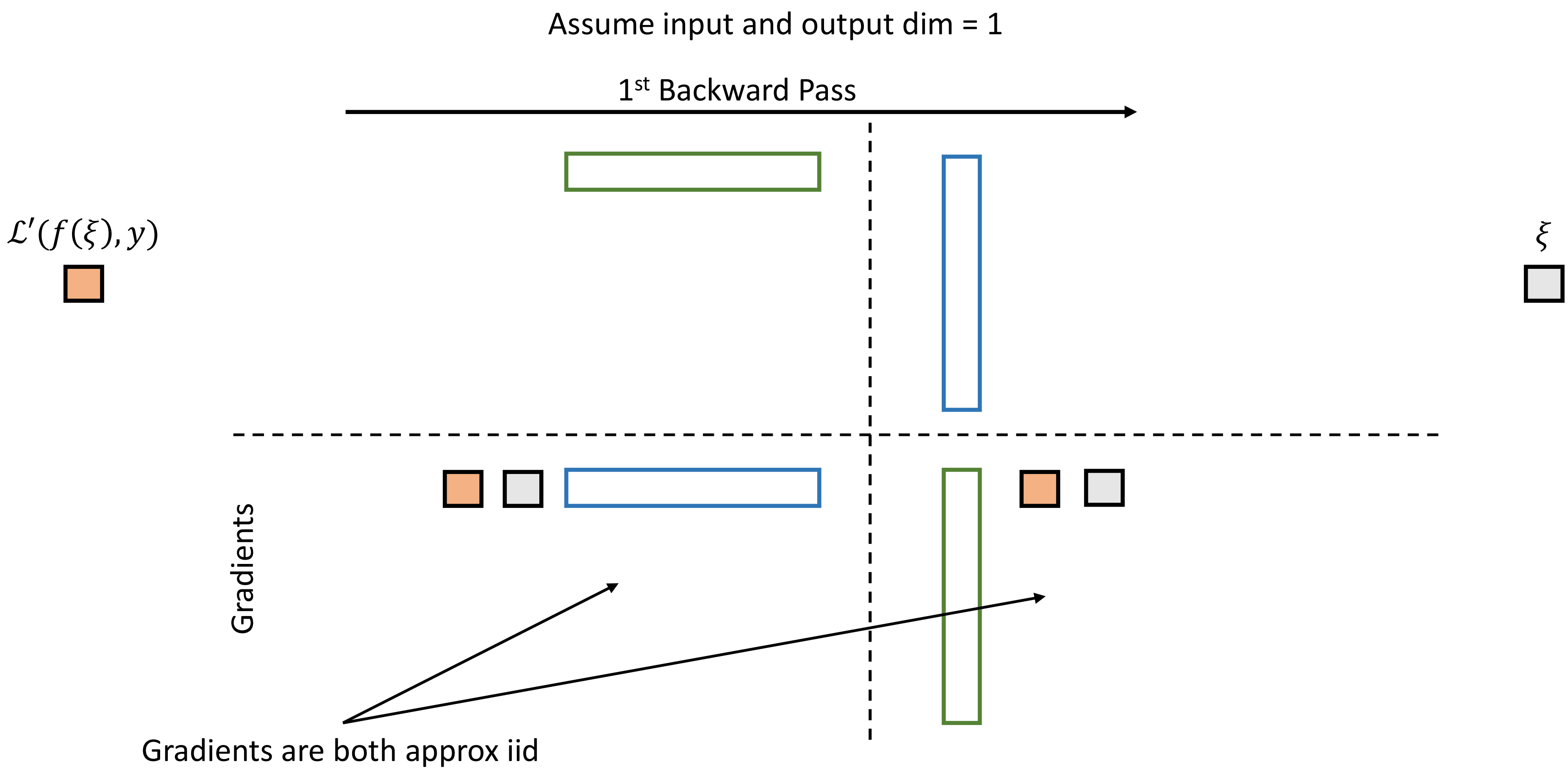

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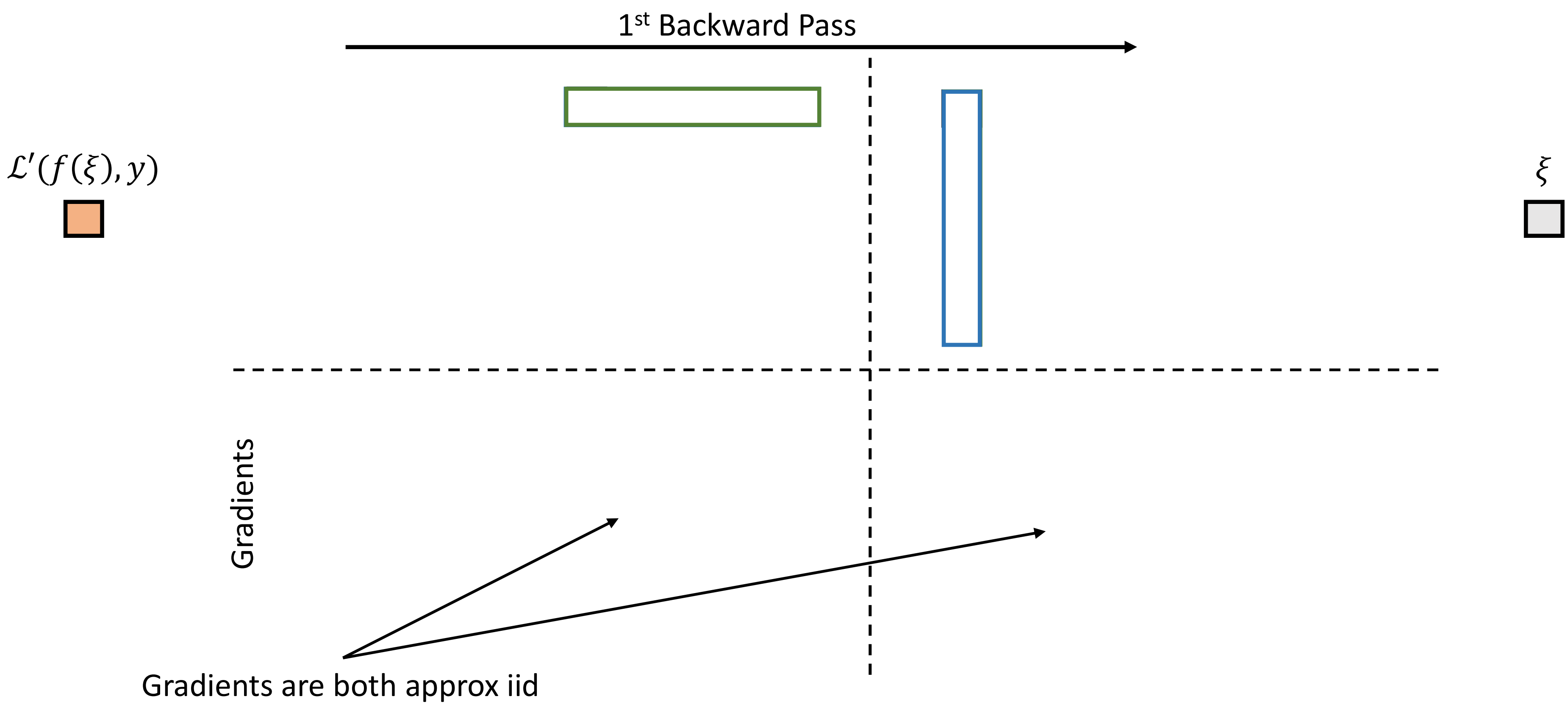

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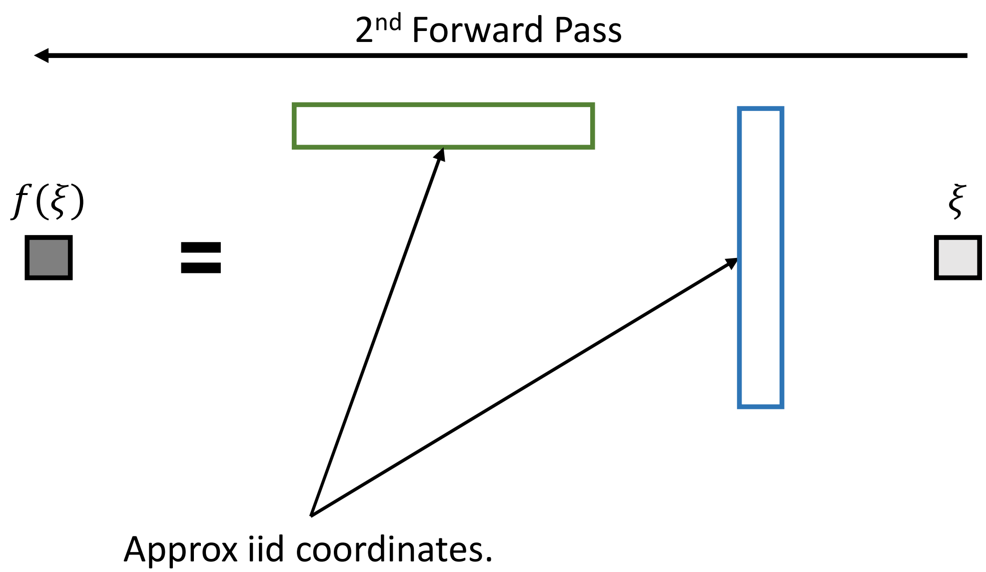

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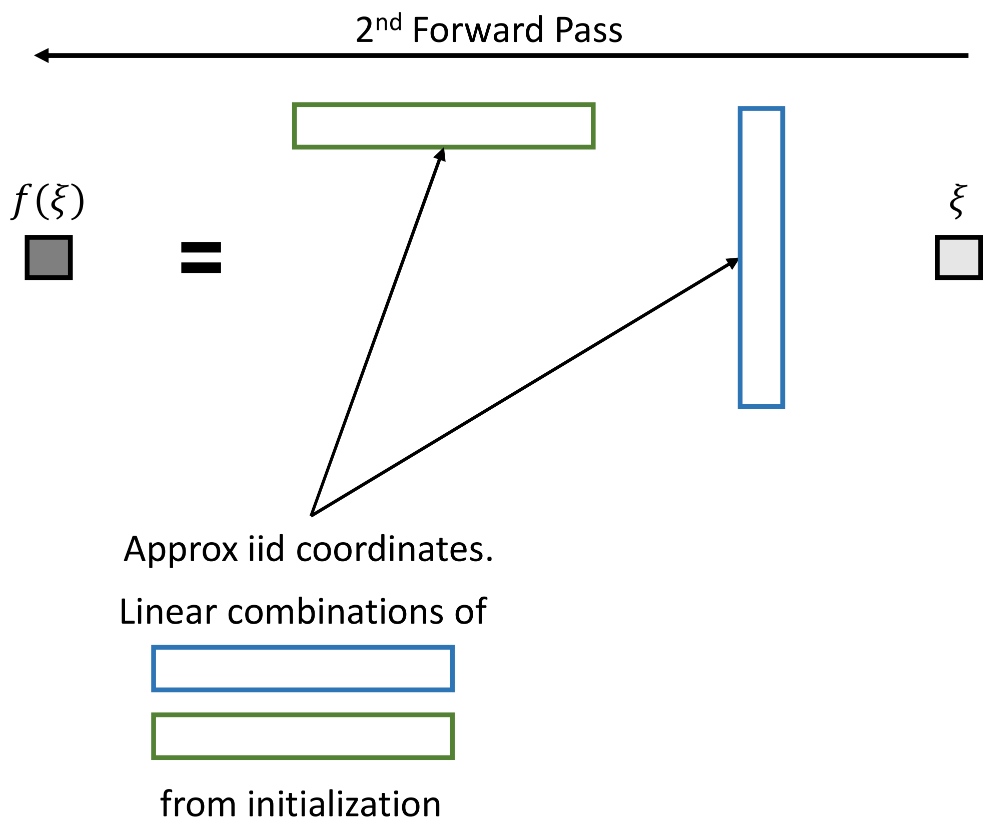

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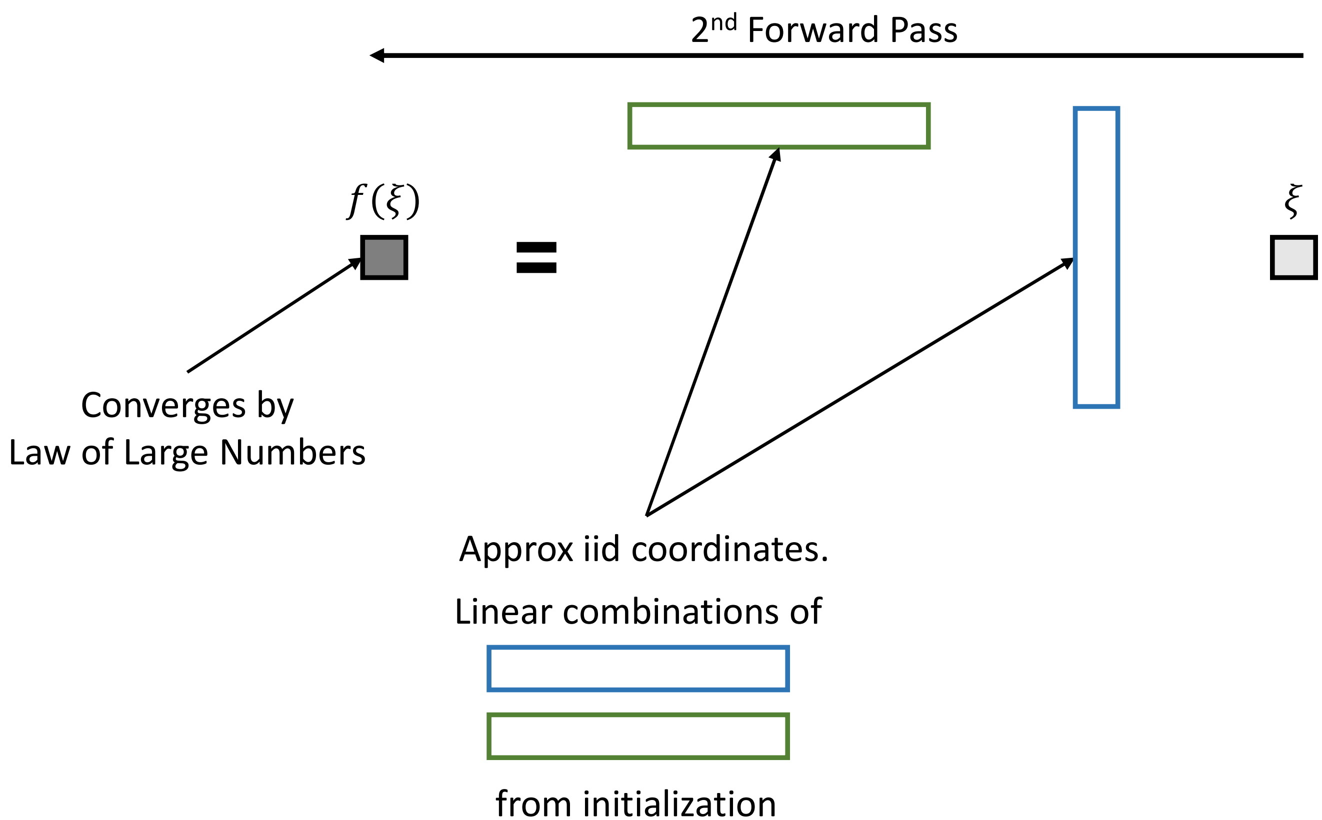

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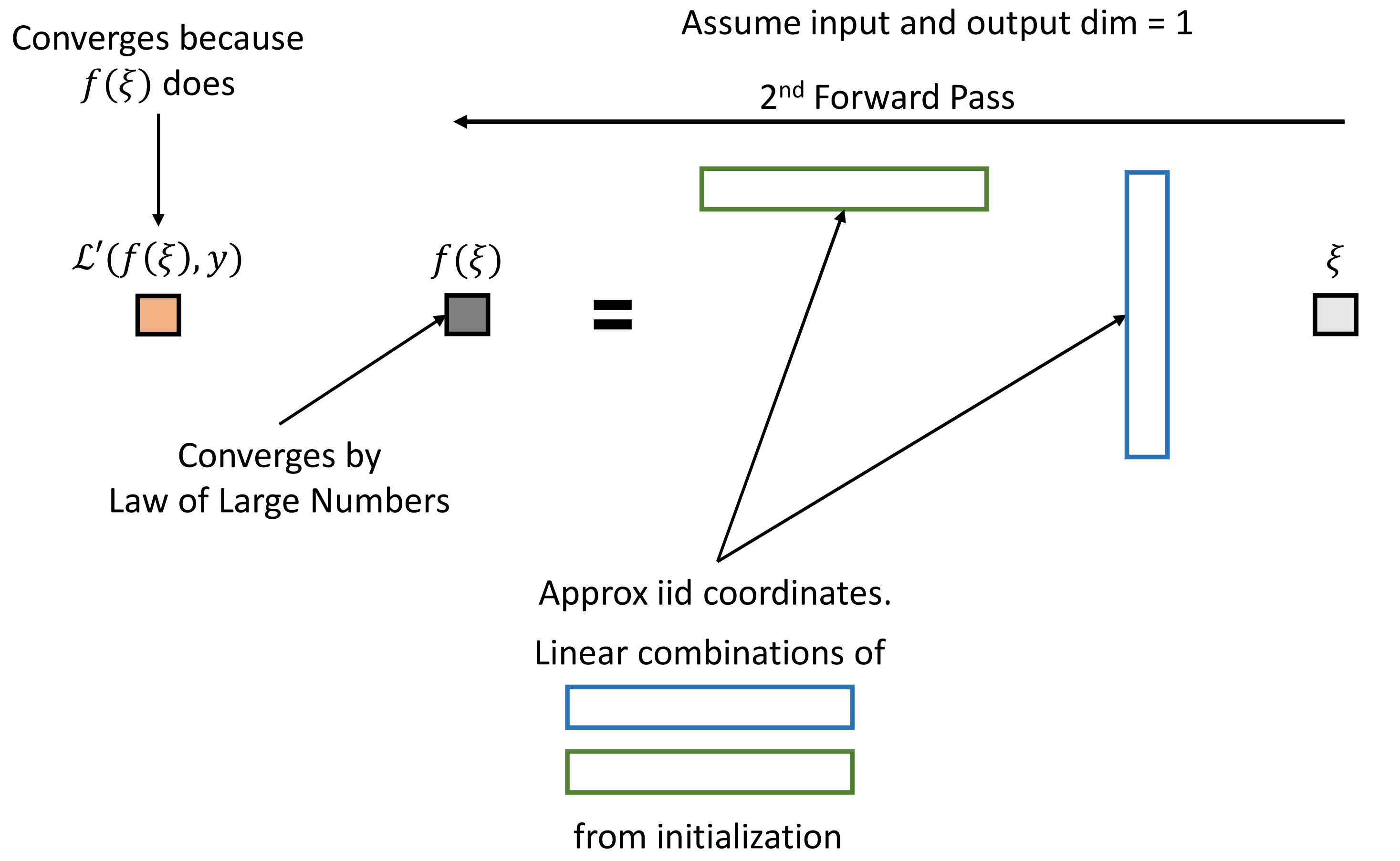

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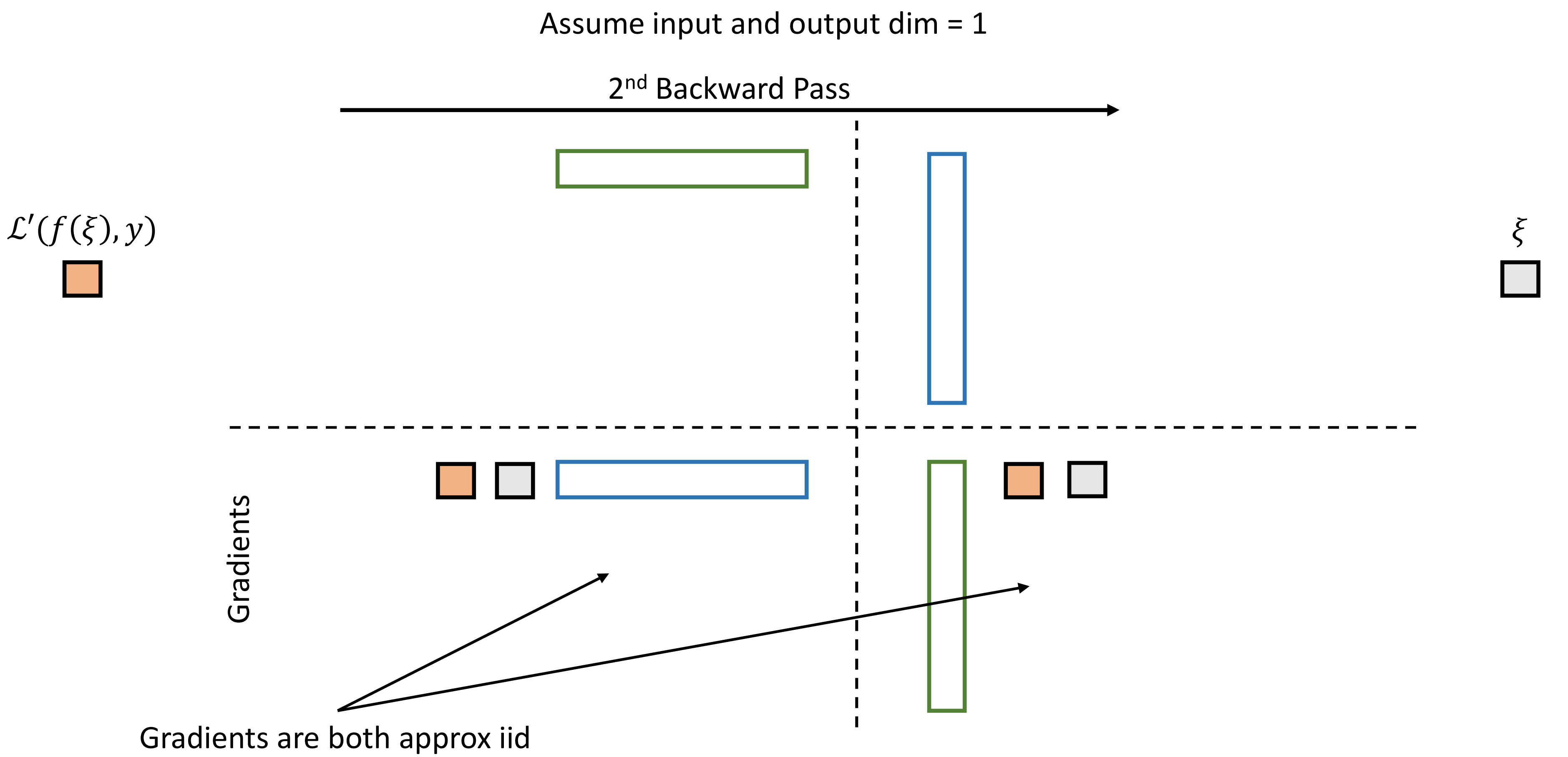

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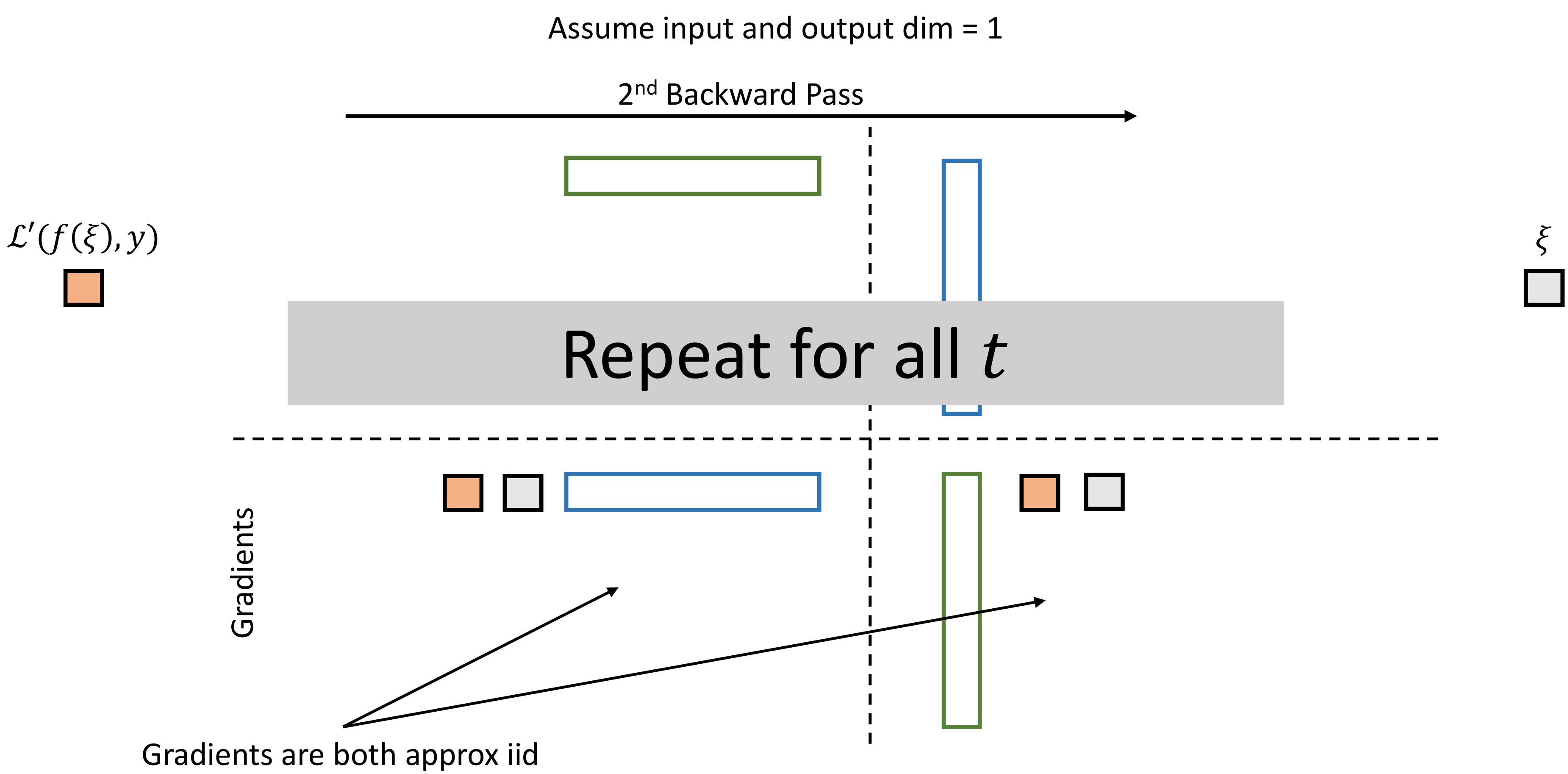

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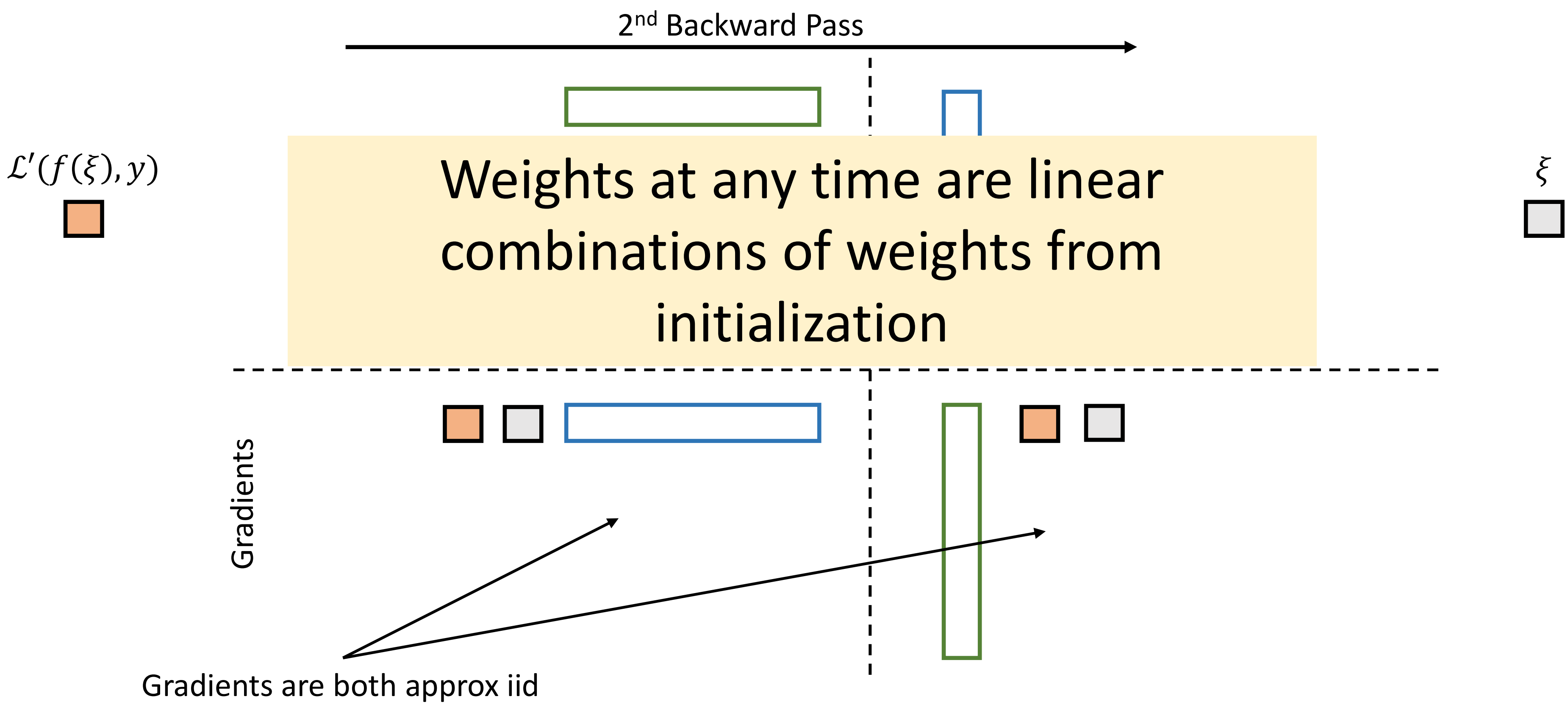

Weights at any time are linear combinations of weights from initialization

Motivating Example: Linear 1-Hidden-Layer

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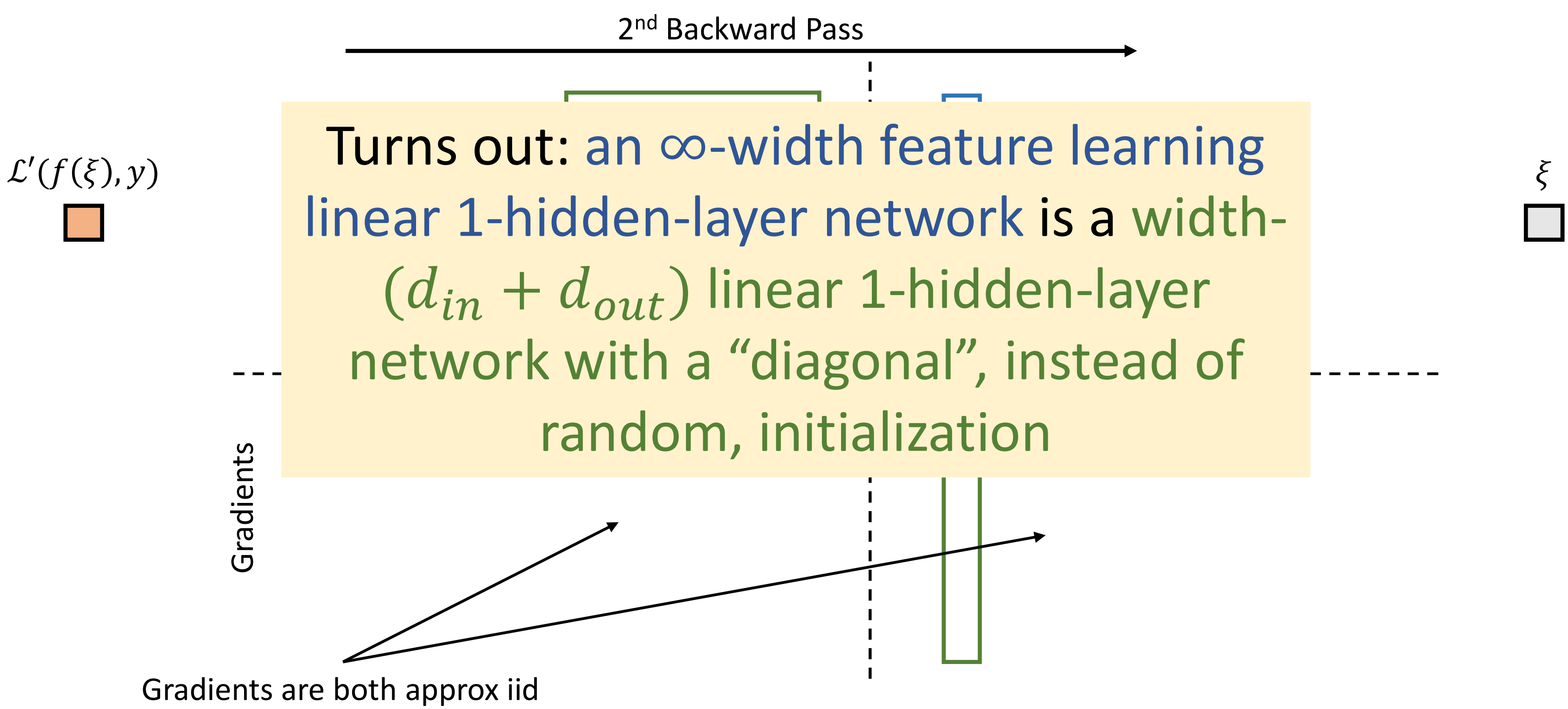
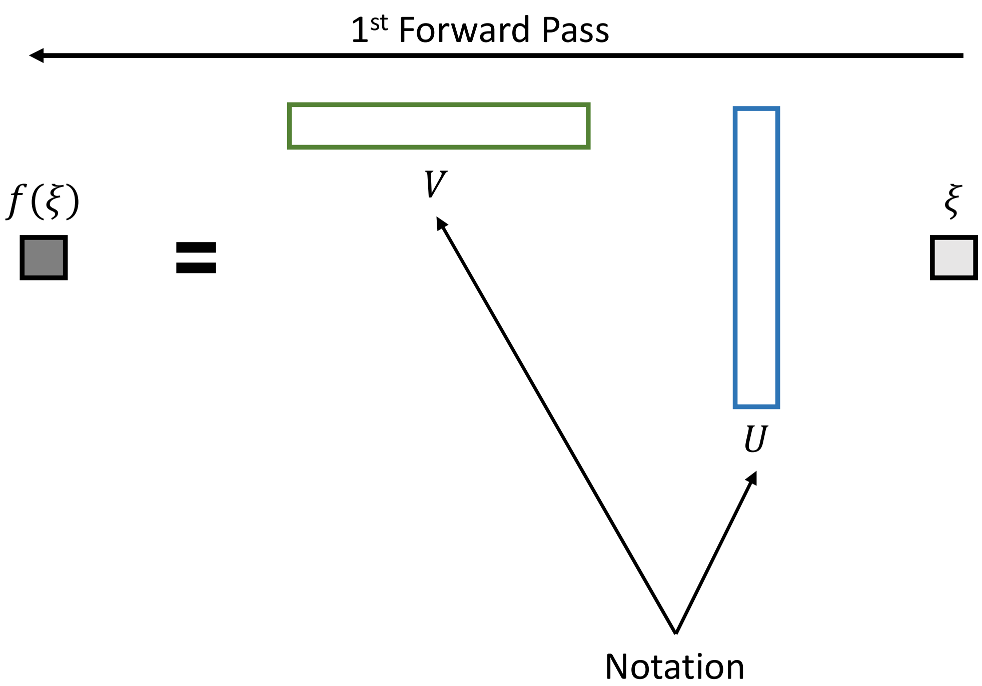


Turns out: an ∞-width feature learning linear 1-hidden-layer network is a width-$(d_{in} + d_{out})$ linear 1-hidden-layer network with a "diagonal", instead of random, initialization

Linear 1-Hidden-Layer: Taking the Limit

Assume input and output dim = 1



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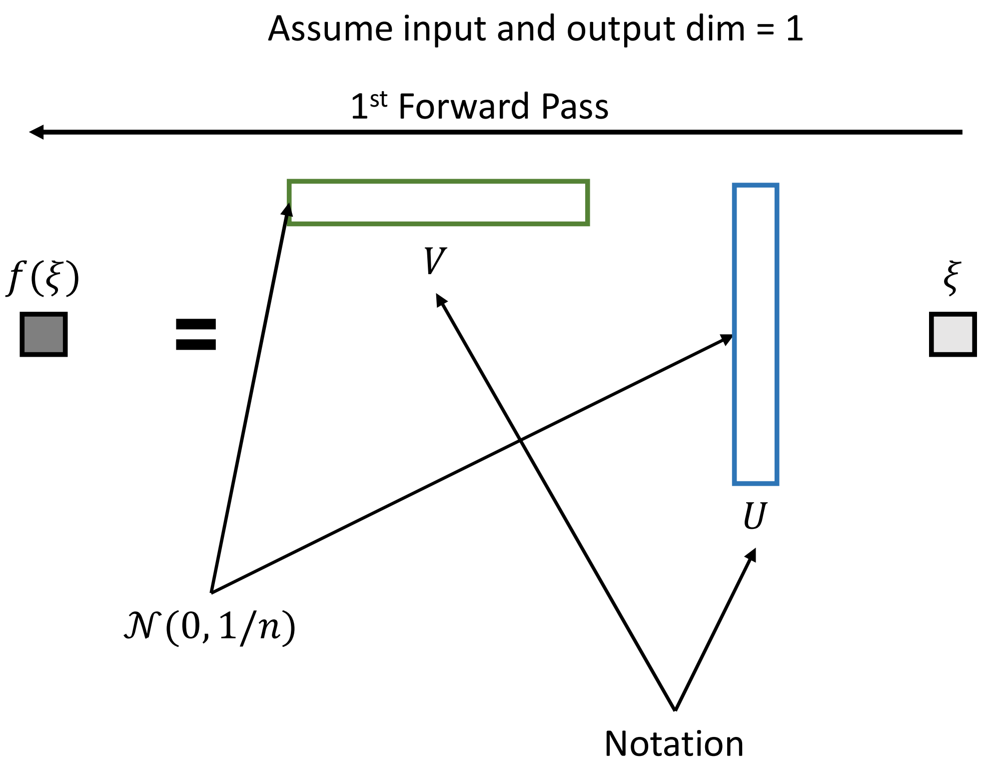

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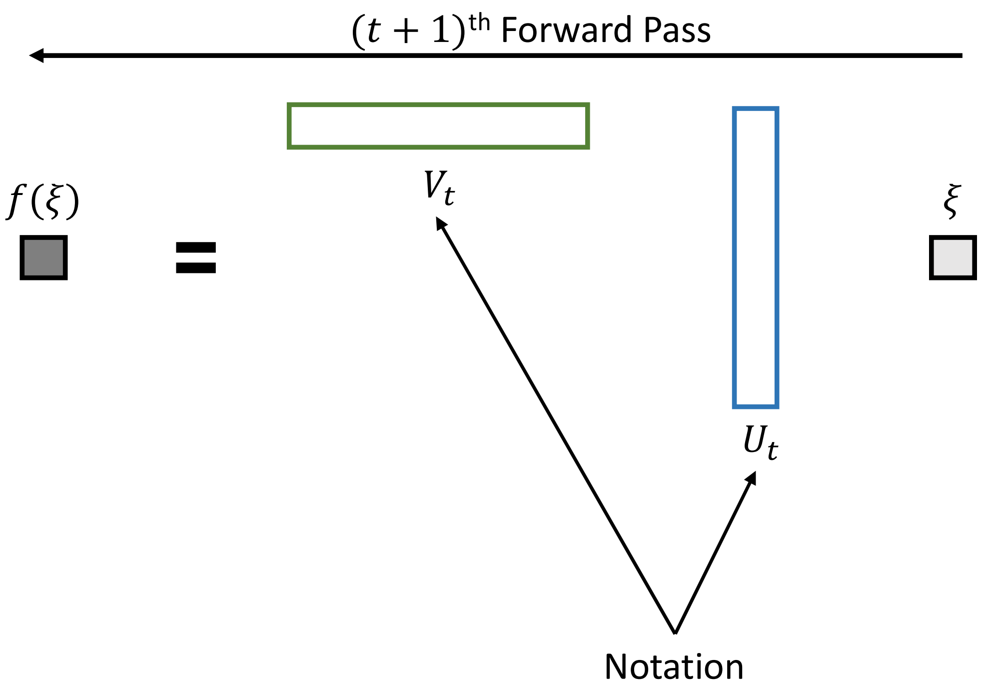

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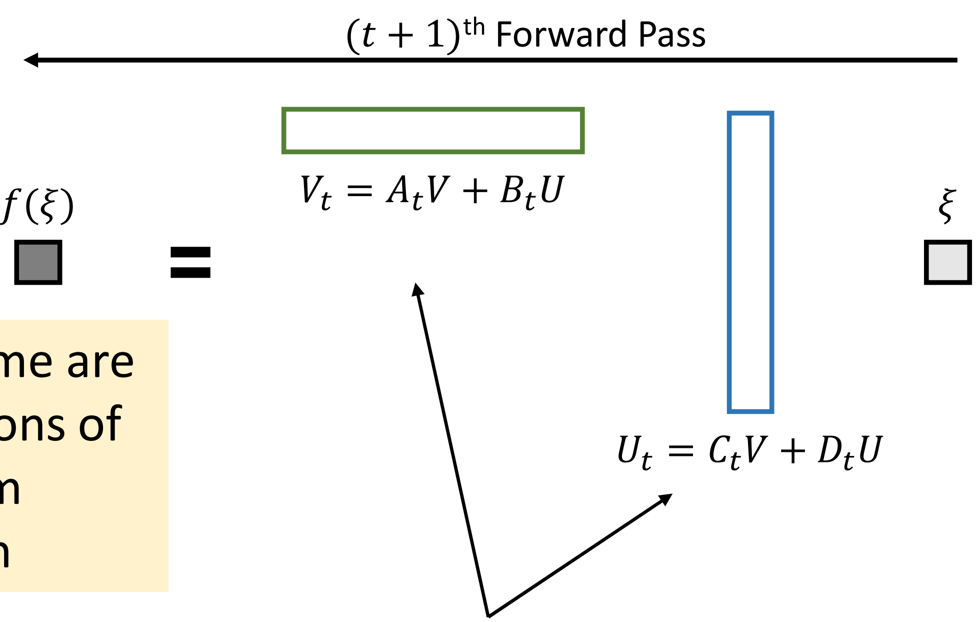
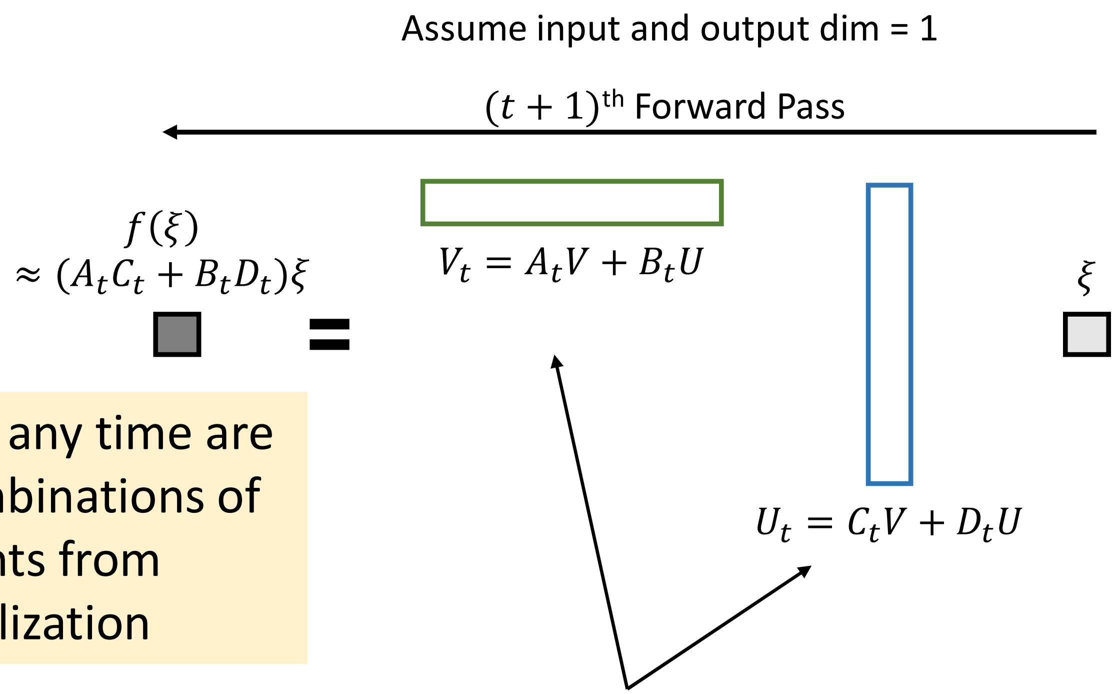


Weights at any time are linear combinations of weights from initialization

For any t, there are coefficients $A_t, B_t, C_t, D_t \in \mathbb{R}$, which converge deterministically, such that

Initial condition: for $t = 0$, $A_t = D_t = 1, B_t = C_t = 0$

Linear 1-Hidden-Layer: Taking the Limit



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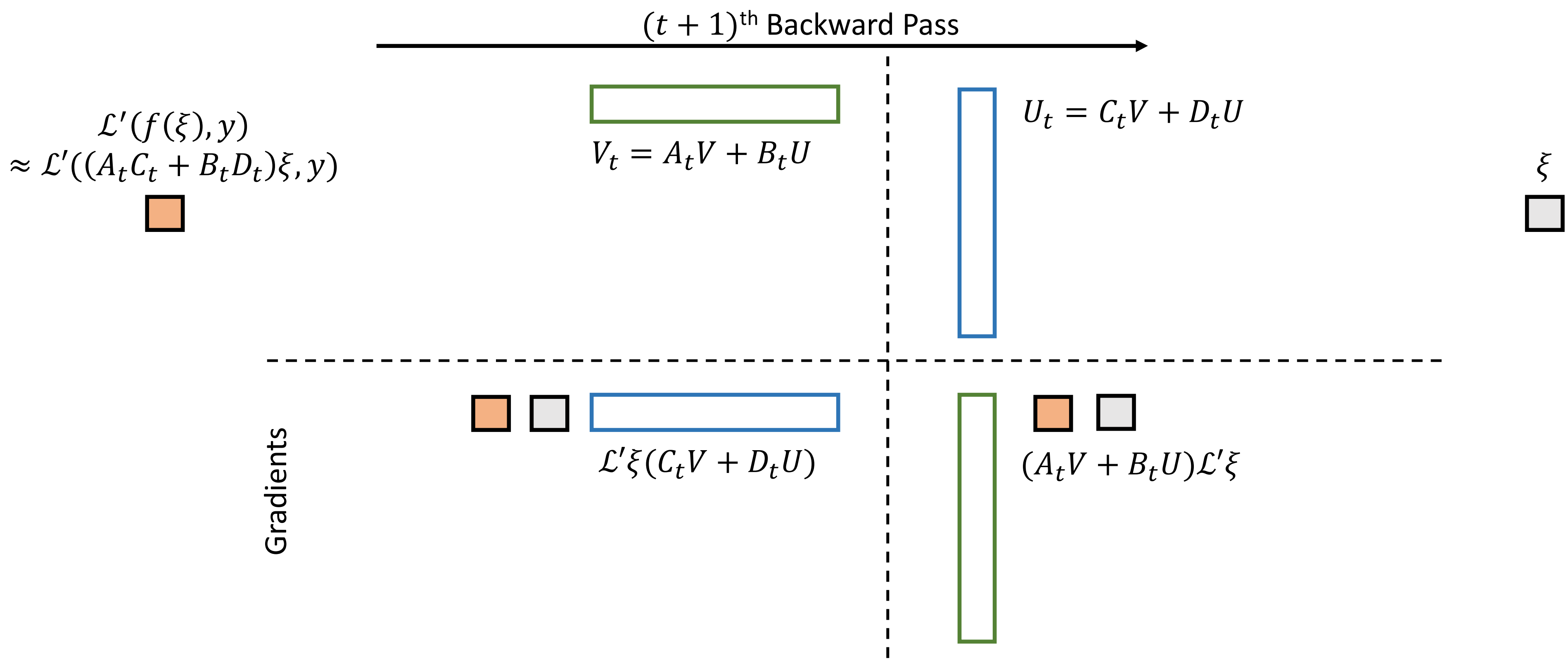

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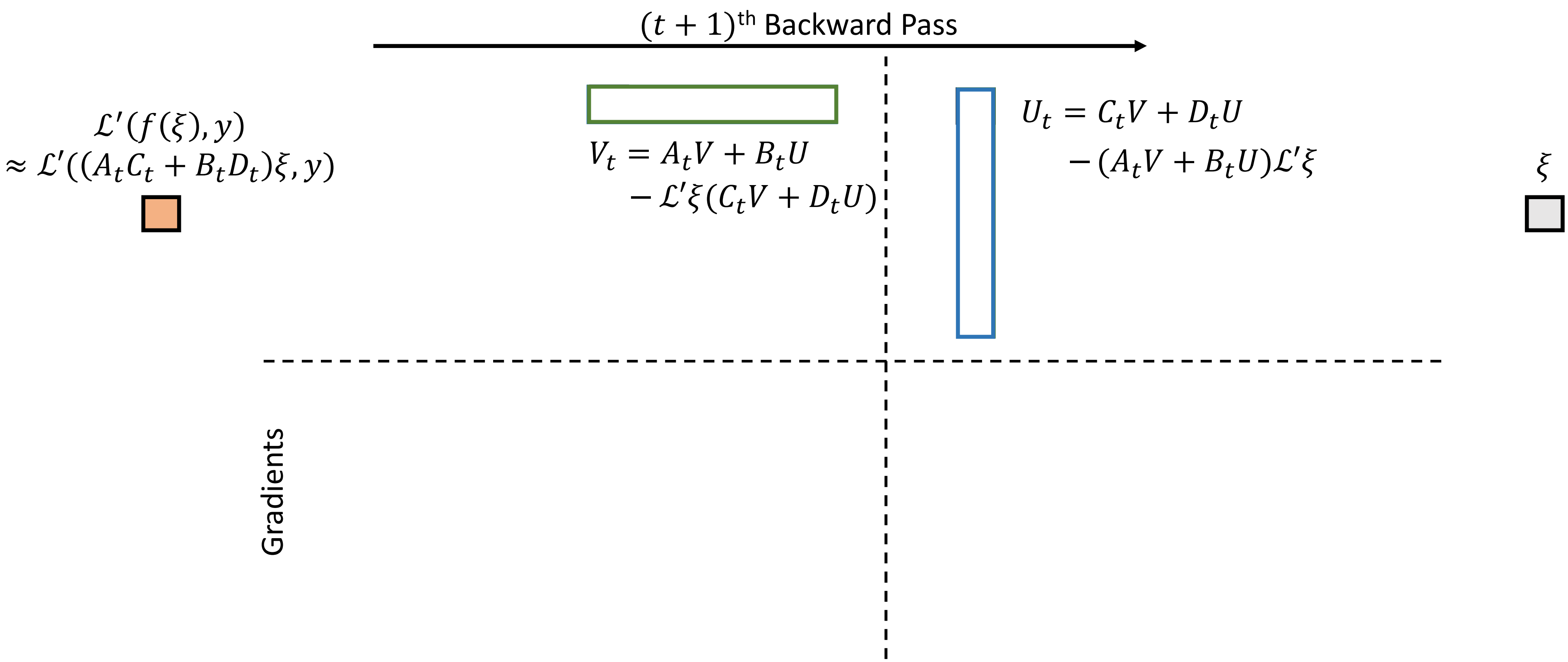

Linear 1-Hidden-Layer: Taking the Limit

Assume input and output dim = 1

$(t+2)^{\text{th}}$ Forward Pass

$f(\xi)$ =

$$V_{t+1} = A_{t+1}V + B_{t+1}U$$
$$A_{t+1} = A_t - \mathcal{L}'\xi C_t$$
$$B_{t+1} = B_t - \mathcal{L}'\xi D_t$$

$$U_{t+1} = C_{t+1}V + D_{t+1}U$$
$$C_{t+1} = C_t - \mathcal{L}'\xi A_t$$
$$D_{t+1} = D_t - \mathcal{L}'\xi B_t$$

ξ

Maximal Update Limit of Linear 1-Hidden-Layer NN

Suppose $d_{in} = d_{out} = 1$, *LR = 1. Then in* $n \to \infty$ *limit,*

$$f_t(\xi) = (A_t C_t + B_t D_t)\xi$$

$$(A_{t+1}, B_{t+1}) = (A_t, B_t) - \mathcal{L}'\xi(C_t, D_t)$$

$$(C_{t+1}, D_{t+1}) = (C_t, D_t) - \mathcal{L}'\xi(A_t, B_t)$$

where $\mathcal{L}' = \mathcal{L}'(f_t(\xi), y)$

with initial condition $A_0 = D_0 = 1, B_0 = C_0 = 0.$

Comparison with Mean Field Limit

- MF Limit expresses everything in terms of their PDF and is continuous-time
- This turns update equations into convolution equations and obscures their simplicity

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Linear 1-hidden-layer width-2 NN

Maximal Update Limit of Linear 1-Hidden-Layer NN

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Maximal Update Limit of Linear 1-Hidden-Layer NN

Linear 1-hidden-layer width-2 NN

2nd layer weights

Suppose $d_{in} = d_{out} = 1$, *LR = 1. Then in* $n \to \infty$ *limit,*

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Maximal Update Limit of Linear 1-Hidden-Layer NN

Linear 1-hidden-layer width-2 NN

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1st layer weights

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Maximal Update Limit of Linear 1-Hidden-Layer NN

Linear 1-hidden-layer width-2 NN

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"Diagonal" initialization: $\begin{pmatrix} A_0 & B_0 \\ C_0 & D_0 \end{pmatrix} = I$

Comparison with Mean Field Limit

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Maximal Update Limit of Linear 1-Hidden-Layer NN with random init **=** *Width-$(d_{in} + d_{out})$ Linear 1-Hidden-Layer NN with "diagonal" init*

Maximal Update Limit of Linear 1-Hidden-Layer NN

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$$f_t(\xi) = (A_t C_t + B_t D_t)\xi$$

$$(A_{t+1}, B_{t+1}) = (A_t, B_t) - \mathcal{L}'\xi(C_t, D_t)$$

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Linear 1-hidden-layer width-2 NN

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Maximal Update Limit of Linear 1-Hidden-Layer NN with random init

=

Width-$(d_{in} + d_{out})$ Linear 1-Hidden-Layer NN with "diagonal" init

This is what we compute for large-scale experiments like Word2Vec

$d_{in} = d_{out} = \text{vocab size}$

$d_{in} + d_{out} = 140k$ on `text8`

$d_{in} + d_{out} = 280k$ on `fil9`

1-Hidden-Layer: Summary

- The weight matrices have iid coordinates at initialization
- The function output converges due to Law of Large Numbers
- Gradients have approx. iid coordinates
- So after gradient update, weight coordinates are still approx. iid
- Repeat
- In the linear case, we express weights at any time as linear combinations of weights from initialization
  - This allows us to have efficient calculation of limit

L-Hidden-Layer: An Appetizer

- $n \times n$ Gaussian random matrix W in the middle of network
  - Central limit behavior
    - Wx is a Gaussian vector if x independent of W
  - Correlation with $W^\top$
    - Appears after 1 step of SGD
      - no effect in 1st step due to Gradient Independence Phenomenon
- See paper for details of the L-hidden-layer limit

The Tensor Program Framework
Automates All of These Derivations

Outline of This Talk

- Parametrizations of Neural Networks
- Dichotomy of Parametrizations
- The “Maximal” Feature Learning Limit
- The *Tensor Programs* technique for deriving the limit
  - Key Idea
  - Motivating Example: Linear 1-Hidden-Layer NN
  - What is a Tensor Program?
  - Master Theorem
  - Infinite-Width Limit for All

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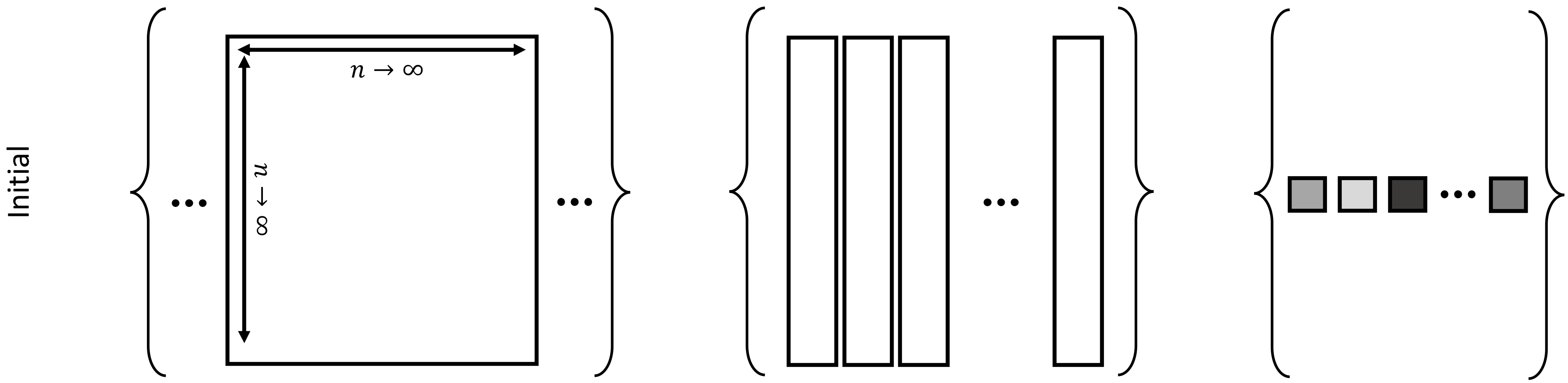
What is a Tensor Program?

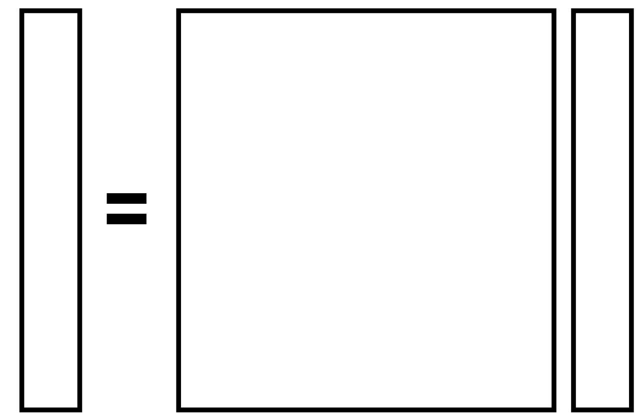
- A set of inductively generated vectors and scalars, given an initial set of matrices, vectors, and scalars



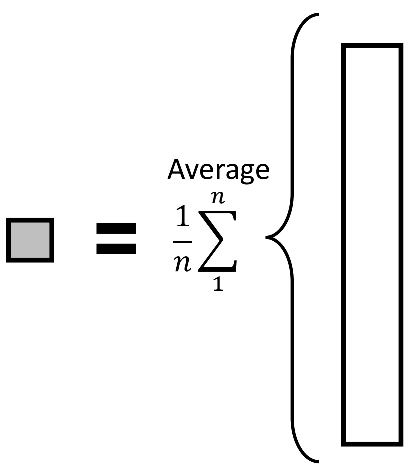
What is a Tensor Program?

- A set of inductively generated vectors and scalars, given an initial set of matrices, vectors, and scalars
- Generation rules

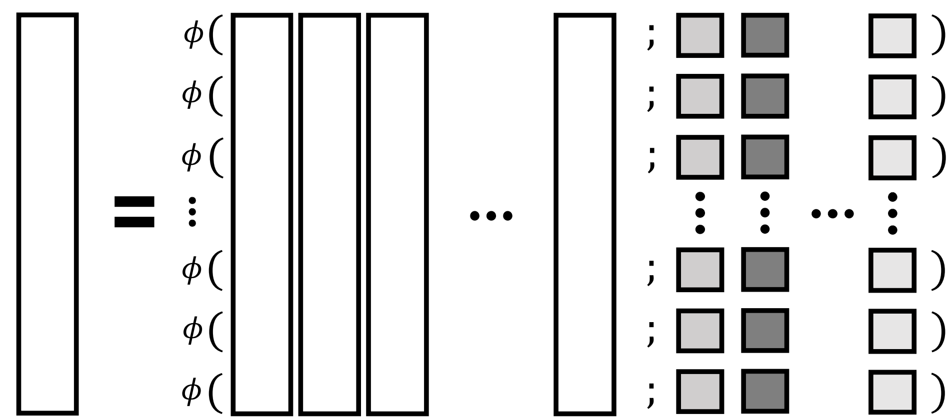
MatMul



Moment

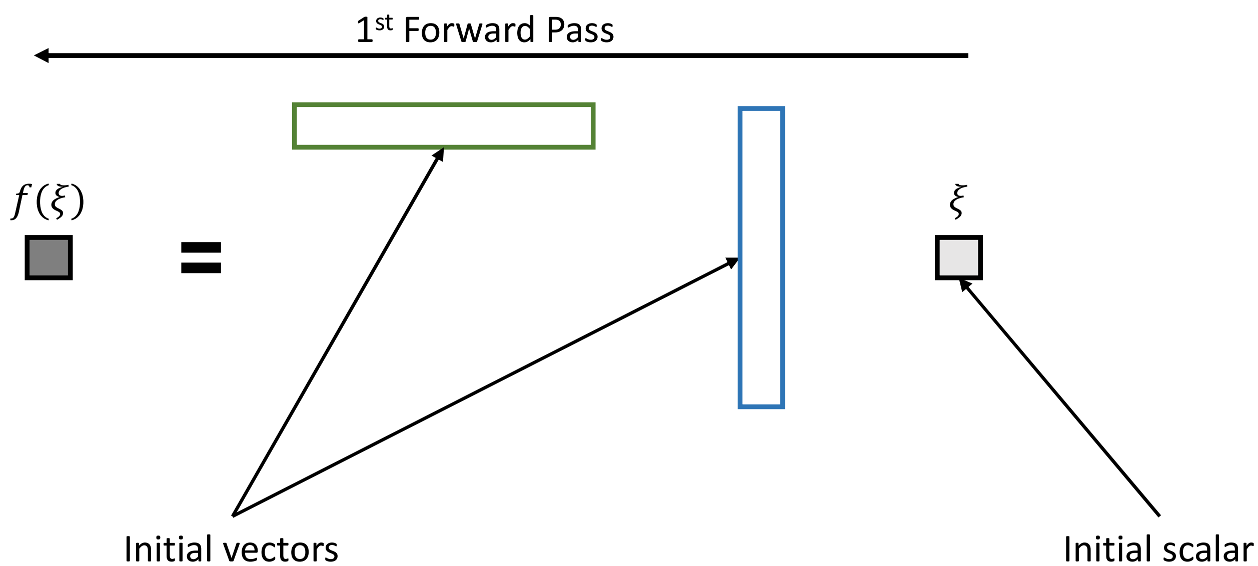


Nonlin



Linear 1-Hidden-Layer as a Tensor Program

Assume input and output dim = 1



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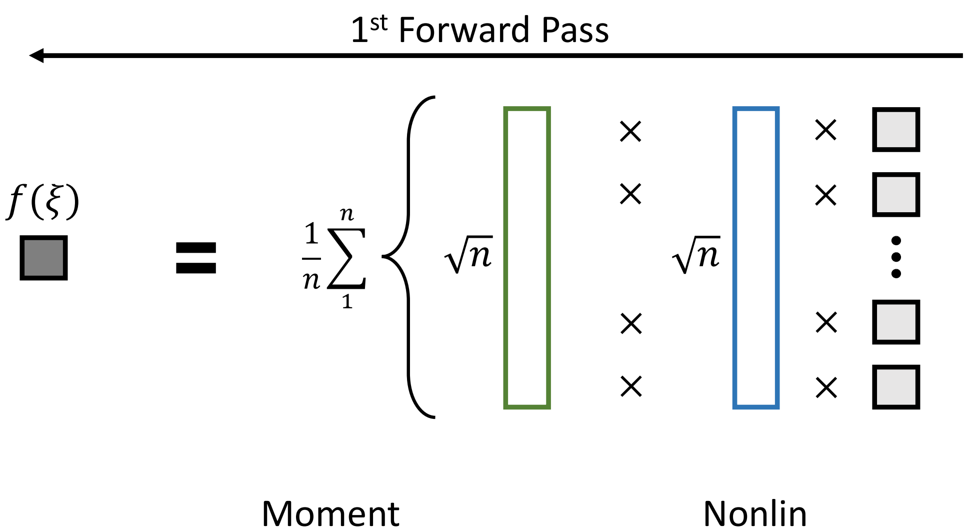

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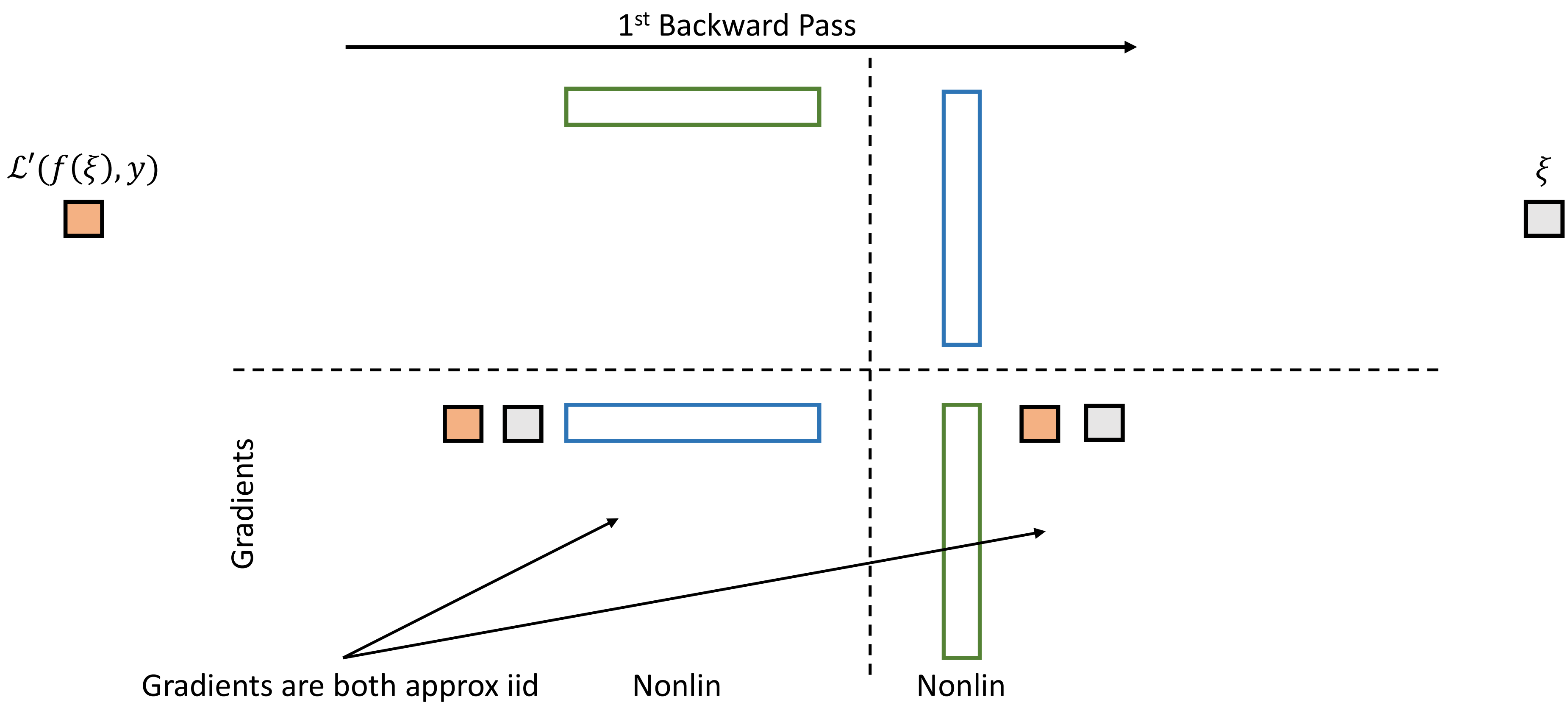
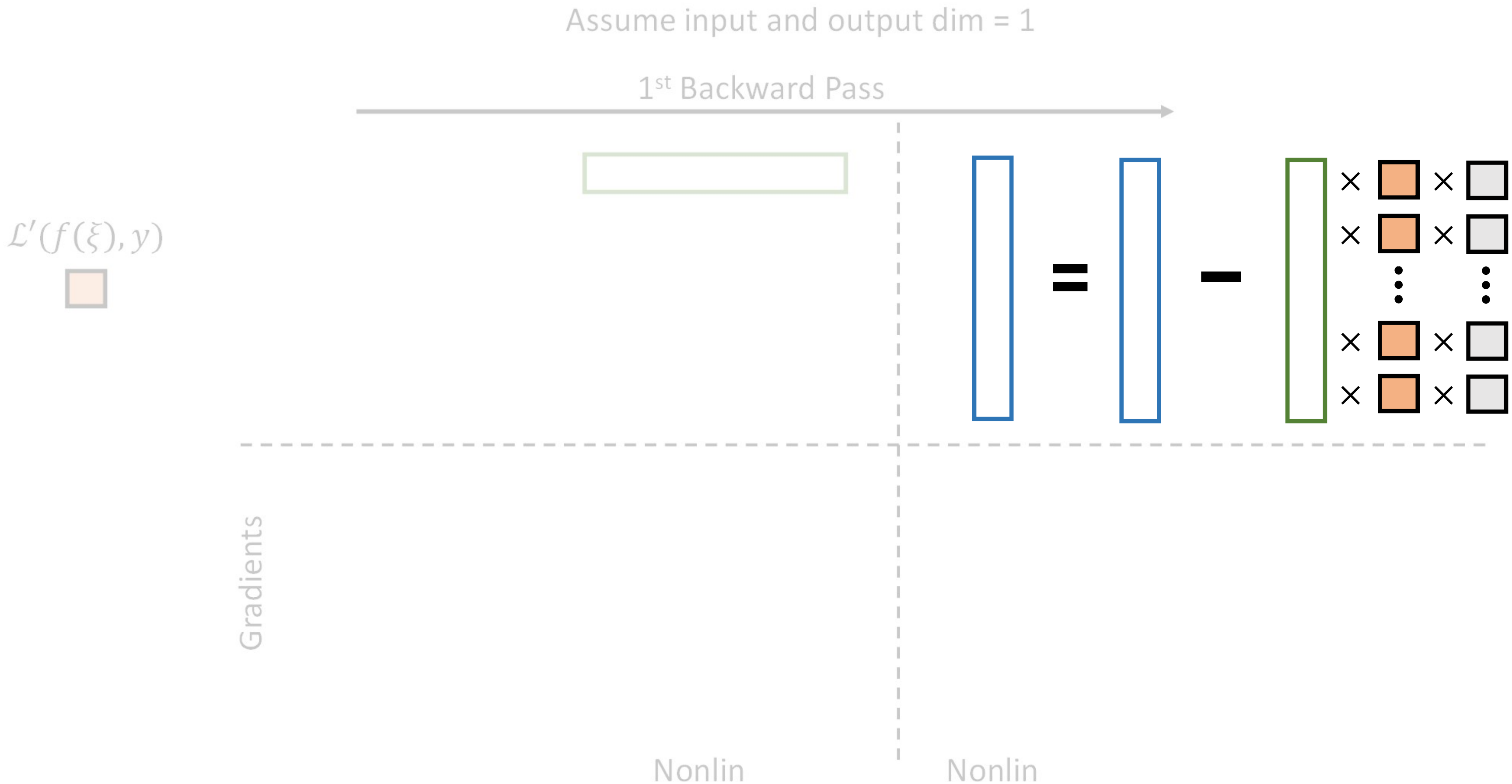


Linear 1-Hidden-Layer as a Tensor Program



SGD as a Tensor Program

- 1-hidden-layer
  - Only need to use Nonlin and Moment
- L-hidden-layer
  - Need to use MatMul because of $n \times n$ Gaussian matrix in the middle of network

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Master Theorem

Tells you how a Tensor Program behaves in the $n \to \infty$ *limit.*

Master Theorem

If 1) initial scalars converge deterministically and 2) initial matrices & vectors are sampled as iid Gaussians, then

- all vectors generated in the program have iid coordinates in the $n \to \infty$ limit, and there are rules to calculate such limit distributions.
- all scalars generated in the program converge to deterministic values, and there are rules to calculate such limit scalars.

Embedding $x^l(\xi)$ of input ξ of trained network

Output (i.e. logits) of trained network

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Church-Turing Thesis for Deep Learning

Any “useful” deep learning computation can be expressed as a Tensor Program.

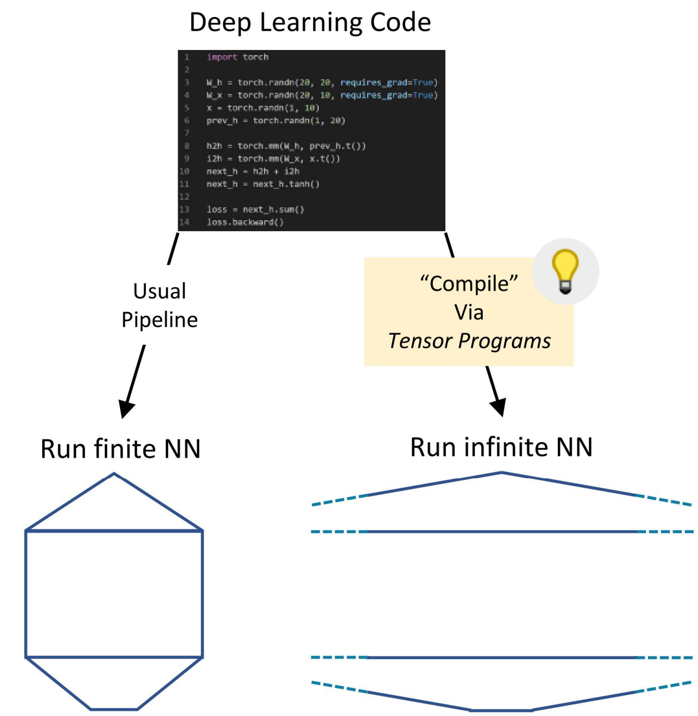
Consequence: Infinite-Width Limits for All

- SOTA architectures: ResNet, Transformers, etc
- SGD with momentum, weight decay
- Adam, Adadelta, Adafactor, etc
- Natural Gradient Descent
- Pretraining and Finetuning
- Metalearning (e.g. MAML)
- Deep Reinforcement Learning (DQN, DDPG, etc)
- Image Generation (GANs, VAEs, etc)

Tensor Programs "Compile" Finite-Width Computation to Infinite-Width Computation

To derive the infinite-width limit of **any** neural computation (e.g. SGD training),

1) express it as a Tensor Program, and
2) mechanically apply the Master Theorem.



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Summary

Our Contributions

- Classify all abc-parametrizations and their ∞-width limits
- Identify Maximal Update Parametrization for maximizing feature learning
- Propose the *Tensor Programs* technique for deriving its equations, and more generally, the limit of any neural computation

Significance

- Framework for studying feature learning in overparametrized NN
- Formulas for training feature-learning ∞-width NN in variety of settings (e.g. pretraining, metalearning, reinforcement learning, GANs, etc)
- Mostly solves the problem of taking ∞-width limits

Looking Ahead

- What kinds of representations are learned?
- How does it inform us about finite neural networks?
- How does this feature learning affect training and generalization?
- How does this jibe with the scaling law of language models?
- Can we train an infinite-width GPT…so GPT∞?
- ... and so many more questions are now ripe for the picking!

Thank you! Question?

Scan to link to paper