# Machine Learning and Optimization

## Lecture 16: Training Deep Networks

CSCI 4140/6960 — Spring 2026

Course website: `cs.rpi.edu/~gittea/.../mlandopt.html`

# Learning Objectives

By the end of this lecture, you should be able to:

1. **Identify** vanishing and exploding gradients as manifestations of poorly conditioned Jacobian products, and **state** the spectral norm bound on gradient norms.
2. **Explain** how weight initialization (Xavier, He) stabilizes forward and backward signal propagation at the start of training.
3. **Compare** activation functions (sigmoid, tanh, ReLU, Leaky ReLU, GELU) in terms of saturation, derivative behavior, and gradient flow.
4. **State** the batch normalization transform and **distinguish** its training and inference behavior.

# Learning Objectives (continued)

5. **Distinguish** batch normalization and layer normalization and **identify** when each is appropriate.
6. **Explain** how residual connections provide well-conditioned gradient pathways and **state** the ResNet residual form.
7. **Describe** auxiliary losses as a mechanism for injecting gradient signal at intermediate layers.

# Lecture Roadmap

- The Vanishing/Exploding Gradient Problem
- The Multiplier Lens
- Initialization
- Activation Functions and Saturation
- Normalization Layers
- Layer Normalization
- Shortening the Gradient Path
- Auxiliary Losses
- Unifying View and Summary

# Challenges of Depth

Three main challenges come up in training deep networks:

1. **Overfitting:** too much capacity relative to data.
2. **Vanishing and exploding gradients:** slow or failed learning.
3. **Hyperparameter selection explosion:** many interacting design choices.

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1. **Overfitting:** too much capacity relative to data.
2. **Vanishing and exploding gradients:** slow or failed learning.
3. **Hyperparameter selection explosion:** many interacting design choices.

This lecture focuses on the second challenge and develops a unified view:

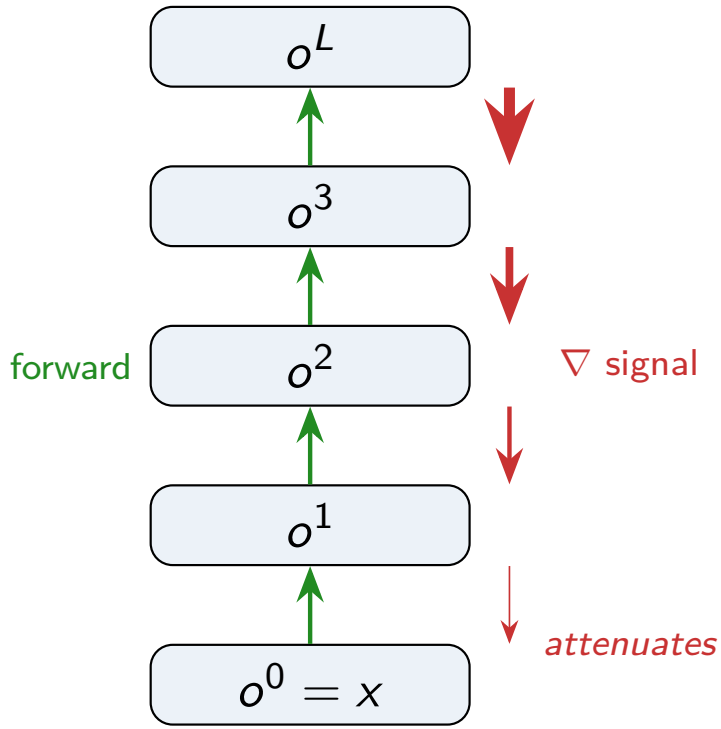
**All solutions aim to stabilize signal propagation across depth** — both forward (activations) and backward (gradients).

# Vanishing and Exploding Gradients

As backpropagation proceeds from layer $L$ toward layer 1, $\|\nabla_{o^s} f\|_2$ either:

- $\to 0$ (**vanishing**)
- $\to \infty$ (**exploding**)

Cause: the chain rule produces a *product of matrices* whose conditioning degrades with depth.



# A Two-Layer Warm-Up

Before the general formula, consider a concrete case.

**Setup:** 2-layer MLP, widths $n_0 = n_1 = n_2 = 3$, sigmoid activation.

Gradient at the input:

$$\nabla_{o^0} f = \underbrace{(W^1)^\top \operatorname{diag}(\sigma'(a^1))}_{\text{layer 1 factor}} \underbrace{(W^2)^\top \operatorname{diag}(\sigma'(a^2))}_{\text{layer 2 factor}} \nabla_{o^2} f$$

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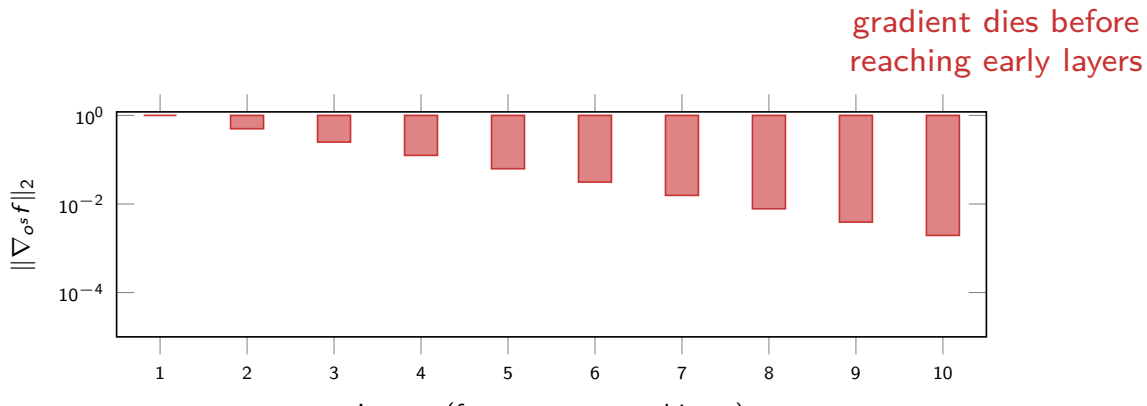
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Typical magnitudes with sigmoid: $\|W^s\|_2 \approx 0.8$, $\|\sigma'\|_\infty \leq 0.25$.

Each factor shrinks the signal by $\approx 0.8 \times 0.25 = 0.2$.

Two layers: $0.2^2 = 0.04\times$ attenuation. Now imagine **50 layers**: $0.2^{50} \approx 10^{-35}$.



# The Jacobian Product

Recall: $o^{s+1} = \sigma(W^{s+1} o^s + b^{s+1})$, so:

$$\nabla_{o^s} f = \left(W^{s+1}\right)^\top \operatorname{diag}\left(\sigma'(a^{s+1})\right) \cdot \nabla_{o^{s+1}} f$$

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Unrolling from layer $s$ to $L$:

$$\nabla_{o^s} f = \prod_{i=s+1}^{L} \left[\left(W^i\right)^\top \operatorname{diag}\left(\sigma'(a^i)\right)\right] \cdot \nabla_{o^L} f$$

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**Spectral norm bound:**

$$\|\nabla_{o^s} f\|_2 \;\leq\; \prod_{i=s+1}^{L} \underbrace{\|W^i\|_2 \cdot \|\sigma'\|_\infty}_{=:\, m_i} \cdot \|\nabla_{o^L} f\|_2$$

This formalizes what the warm-up showed numerically: each layer contributes a multiplicative factor $m_i$, and $L - s$ such factors compound.

# The Jacobian Product (continued)

Two mechanisms that lead to poorly conditioned Jacobian products:

1. **Activation saturation:** if $\sigma'(a^i) \approx 0$ entrywise, the $\|\sigma'\|_\infty$ factor drives $m_i$ toward zero.
2. **Weight matrix norms:** if $\|W^i\|_2$ is consistently $> 1$ or $< 1$, the product grows or shrinks exponentially in $L - s$.

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**Concrete example:** if the gradient doubles every layer, after 50 layers it grows by $2^{50} \approx 10^{15}$. If it halves every layer, it shrinks by $2^{-50} \approx 10^{-15}$.

# Consequences

**Consequence:** naively training deep architectures either fails or gives poor performance.

**Brute-force mitigation:** gradient clipping — cap $\|\nabla f\|$ at a threshold before each update. Widely used in RNN training. Treats the symptom, not the cause.

This lecture: a single diagnostic — the *per-layer multiplier* $m_s$ — and a roadmap of principled approaches widely used to mitigate this issue.

# The Per-Layer Multiplier

Define the **per-layer multiplier**:

$$m_s := \|W^s\|_2 \cdot \|\sigma'\|_\infty$$

Then the spectral bound becomes:

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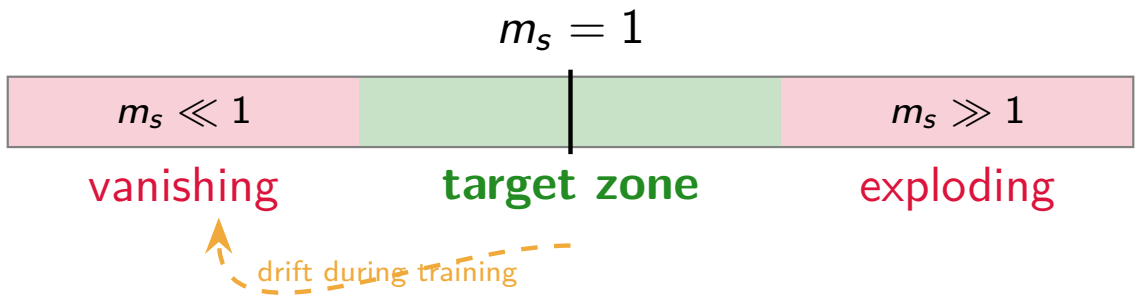
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**Goal:** keep $m_s \approx 1$ for all $s$, throughout training.




Two failure modes as $m_s$ drifts during training: $m_s < 1$ (vanishing), $m_s > 1$ (exploding).

# Roadmap Through the Multiplier Lens

Every technique in this lecture is a targeted intervention on $m_s$:

| **Method** | **Acts on** | **Effect on $m_s$** |
|---|---|---|
| Initialization | $\|W^s\|_2$ at $t = 0$ | Sets $m_s \approx 1$ initially |
| Activation choice | $\|\sigma'\|_\infty$ factor | Avoids $m_s \approx 0$ from saturation |
| Batch/Layer Norm | activations $\rightarrow$ indirectly $m_s$ | Renormalizes scale during training |
| Residual conn. | Jacobian structure | Bypasses the product: adds identity |
| Auxiliary losses | Effective product length | Shortens $\prod$ by injecting gradient |

We will revisit this table at the end of the lecture to verify each claim.

# Pause and Check

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A. Sigmoid: $\|\sigma'\|_\infty \leq 0.25$, driving $m_s$ well below 1. Poor initialization: $\|W^s\|_2$ off-scale (too large or too small).

# Controlling Both Forward and Backward Passes

It is essential to control signal propagation in *both* directions:

1. **Saturation is a forward-pass problem that poisons the backward pass.** If pre-activations $a^s$ drift into the saturating tails of sigmoid or tanh (a forward phenomenon), then $\sigma'(a^s) \approx 0$, which kills $m_s$ regardless of $\|W^s\|_2$.
2. **The backprop seed depends on forward propagation.** If $o^L$ is numerically degenerate (overflow/underflow), then $\nabla_{o^L} f$ — the initial condition of the backward pass — is garbage.

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Forward and backward stability are **coupled but not equivalent**. Controlling each requires its own condition on $\mathrm{Var}(W^s)$, and these conditions generically conflict — motivating the compromise that is Xavier initialization.

# Variance Propagation: Forward Pass

The original analysis (Glorot & Bengio, 2010) asks: under what condition on $\mathrm{Var}(W^s)$ does the per-coordinate activation variance stay constant across layers?

**Why this is the right question forward:** if $\mathrm{Var}(a_j^s)$ grows with depth, pre-activations leave the well-behaved region of $\sigma$ and saturate. If it shrinks, activations collapse to zero.

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Preserve per-coordinate variance: $\boxed{\mathrm{Var}(W_{jk}^s) = 1/n_{s-1}}$.

**Bias terms:** $b^s = 0$ at init contributes nothing; during training, bias drift is handled by normalization layers.

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Glorot & Bengio (2010) instead preserved per-coordinate gradient variance in both directions (applying the same algebraic template as the forward pass). As we will see, this leads to an apparent conflict that vanishes when you preserve the right quantity.

# Backward Pass: Per-Coordinate Calculation

Coordinate-wise backward recurrence (**assuming** $\sigma' = 1$):

$$[\nabla_{o^{s-1}} f]_j = \sum_{k=1}^{n_s} W^s_{kj} \cdot [\nabla_{o^s} f]_k$$

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This tells us how a single coordinate's second moment changes across one layer.

But we want to compare $\mathbb{E}[\|\nabla_{o^{s-1}} f\|^2]$ to $\mathbb{E}[\|\nabla_{o^s} f\|^2]$ — i.e., we need to *sum over coordinates*. To do that, we need to know whether all coordinates have the same second moment.

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Do they?

# Gradient Coordinates Are Exchangeable

## Claim (proved in Appendix A)

At initialization, the coordinates of $\nabla_{o^s} f$ are **exchangeable**: for any permutation $\pi$ of neurons at layer $s$,

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**Consequence:** all coordinates share the same second moment. Writing $c_s := \mathbb{E}\big[[\nabla_{o^s} f]_k^2\big]$ (same for all $k$):

$$\mathbb{E}\big[\|\nabla_{o^s} f\|^2\big] = \sum_{k=1}^{n_s} \mathbb{E}\big[[\nabla_{o^s} f]_k^2\big] = n_s \cdot c_s$$

# Backward Pass: Gradient Norm Preservation

From the per-coordinate calculation: $c_{s-1} = n_s \cdot \mathrm{Var}(W^s) \cdot c_s$.

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Preserve gradient norm (ratio $= 1$): $\boxed{\mathrm{Var}(W^s_{jk}) = 1/n_{s-1}}$

**This is the same condition as the forward pass!**

# There Is No Conflict

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For equal-width layers ($n_{s-1} = n_s$), the distinction vanishes entirely. In practice, Xavier's harmonic mean is close enough to $1/n_{s-1}$ that the difference rarely matters.

# Xavier and He Initialization

**Xavier/Glorot initialization** (Glorot & Bengio, 2010):

The original paper preserves per-coordinate variance in both directions, obtaining $1/n_{s-1}$ (forward) vs. $1/n_s$ (backward), then compromises:

$$W_{jk}^{s} \sim \mathcal{N}\left(0,\ \frac{2}{n_{s-1} + n_s}\right)$$

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**He initialization** (He et al., 2015) — accounts for ReLU:

ReLU zeroes out half the activations: $\mathbb{E}[(\mathrm{ReLU}')^2] = 1/2$. Both the forward (per-coordinate variance) and backward (gradient norm) conditions give the *same* answer:

$$\boxed{W_{jk}^s \sim \mathcal{N}\left(0,\ \frac{2}{n_{s-1}}\right)}$$

Applied in PyTorch via `kaiming_normal_`.

# Initialization and the Multiplier Lens

**What does initialization give us, concretely?**

For $W \in \mathbb{R}^{n \times n}$ with i.i.d. $\mathcal{N}(0, 1/n)$ entries and any fixed vector $x$:

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**What it does *not* give us:** $\|W\|_2 \approx 1$. For large $n$, $\|W\|_2 \to 2$ (Marchenko–Pastur), so the worst-case multiplier $m_s = \|W^s\|_2 \cdot \|\sigma'\|_\infty \approx 2$. The spectral bound is pessimistic because backpropagated gradients are not adversarially aligned with the top singular direction.

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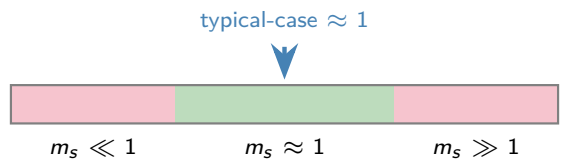
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$$\mathbb{E}[\|Wx\|^2] = \|x\|^2.$$

So $W$ acts as an **approximate isometry on typical vectors**: its RMS singular value is 1.

**What it does *not* give us:** $\|W\|_2 \approx 1$. For large $n$, $\|W\|_2 \to 2$ (Marchenko–Pastur), so the worst-case multiplier $m_s = \|W^s\|_2 \cdot \|\sigma'\|_\infty \approx 2$. The spectral bound is pessimistic because backpropagated gradients are not adversarially aligned with the top singular direction.

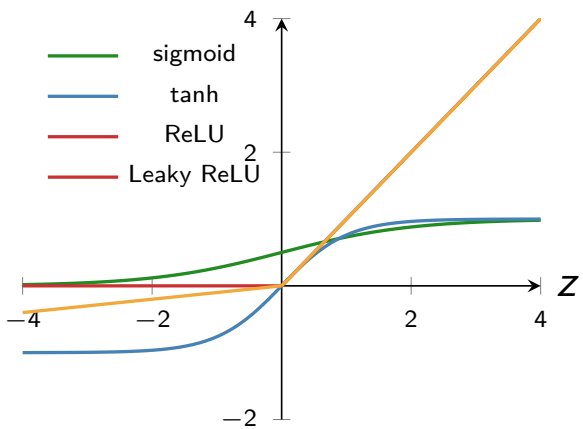
**Bottom line:** the multiplier lens gives correct *qualitative* diagnostics (is $m_s$ order-1 or not?). The variance analysis gives the correct *quantitative* initialization.



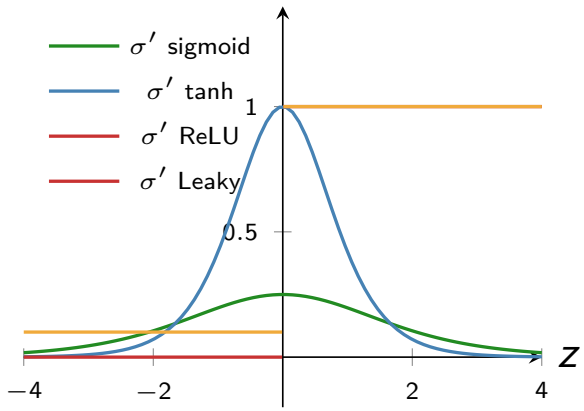
# Activation Functions: A Gradient Perspective

The activation derivative $\sigma'(\cdot)$ appears in every factor of the Jacobian product. Choice of $\sigma$ directly controls the $\|\sigma'\|_\infty$ factor in $m_s$.

**Functions $\sigma(z)$**




**Derivatives $\sigma'(z)$**



# Saturation, Sparsity, and Dead Neurons

**Sigmoid / tanh** — saturate for $|z| \gg 0$: $\sigma'(z) \approx 0$.

- Sigmoid: $\|\sigma'\|_\infty = 0.25$, so $m_s \leq 0.25 \, \|W^s\|_2$ — well below 1 even with perfect initialization.
- Saturated neurons compound: each contributes a near-zero diagonal entry.

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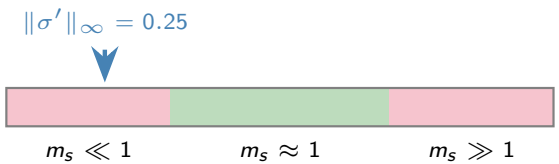
**Leaky ReLU** ($\max(\alpha z, z)$, $\alpha \approx 0.01$): $\sigma' \in \{\alpha, 1\}$, so $m_s > 0$ always.

**GELU**: $\sigma(z) = z\Phi(z)$. Smooth, nonzero derivative everywhere. Default in Transformers.

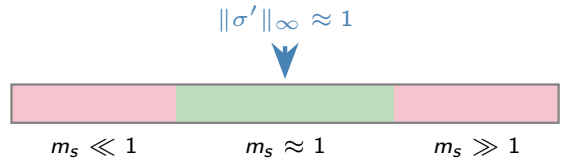
# Takeaway: Activation Choice and Gradient Flow

| **Activation** | **Saturates?** | $\sigma'$ **range** | **Dead neurons?** | **Common in** |
|---|---|---|---|---|
| Sigmoid | Yes | $(0, 0.25]$ | No | Legacy / outputs |
| tanh | Yes | $(0, 1]$ | No | Legacy / RNNs |
| ReLU | No ($z > 0$) | $\{0, 1\}$ | Yes | CNNs, MLPs |
| Leaky ReLU | No | $\{\alpha, 1\}$ | No | CNNs, MLPs |
| GELU | No | smooth, $> 0$ | No | Transformers |

Sigmoid:




ReLU / GELU:



# Pause and Check

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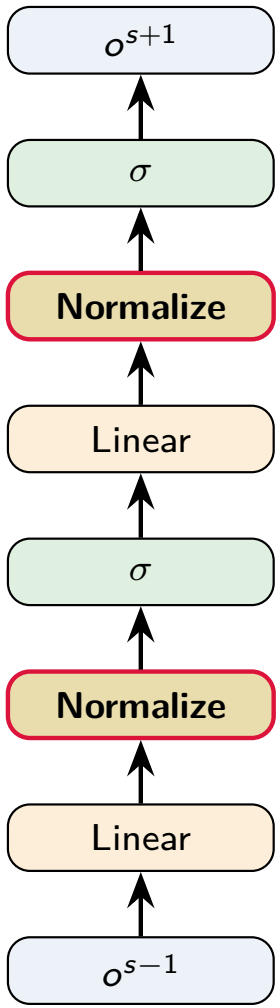
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**Q.** Now switch to ReLU with He init. Estimate $m_s$.

A. He init sets $\|W^s\|_2$ so that $m_s \approx 1$ (accounting for $\mathbb{E}[\sigma'] \approx 1/2$ via the extra factor of 2). Total attenuation: $\approx 1^{29} = 1$. Gradient propagates cleanly.

# Normalization Layers: The Idea

Initialization sets $m_s \approx 1$ at $t = 0$, but weights evolve during training and $m_s$ drifts. **Normalization layers** are modules inserted between layers that dynamically re-center and re-scale activations to maintain stable signal propagation.



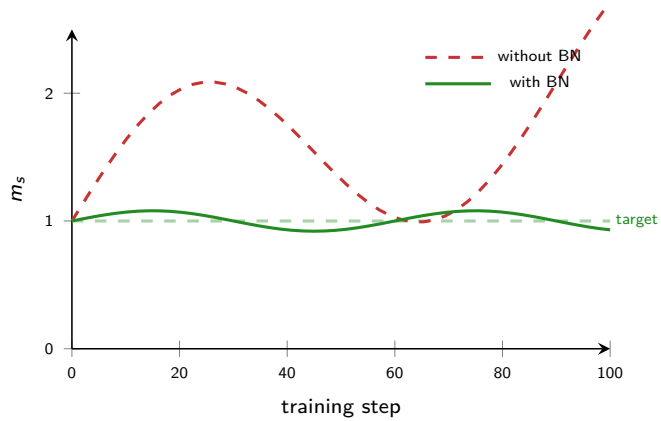

inserted between linear and activation

# Batch Normalization: Stabilizing the Multiplier During Training

**Batch normalization** (BN) (Ioffe & Szegedy, 2015) computes normalization statistics *per minibatch*: the mean and variance used to normalize each neuron's pre-activation are estimated from the $m$ samples in the current minibatch.

Effects:

- Pre-activations stay where $\sigma'$ is well-behaved
- Prevents bias accumulation
- Empirically stabilizes $m_s$ throughout training ⊙




Schematic: BN prevents multiplier drift.

# The Batch Normalization Transform

## Definition (Batch Normalization — BN)

Given a minibatch of $m$ samples, for each neuron $j$ at layer $s$:

$$\mathrm{BN}_{\gamma,\beta}(a^s) = \gamma \odot \frac{a^s - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \varepsilon}} + \beta,$$

where

$$\mu_{\mathcal{B},j} = \tfrac{1}{m}\textstyle\sum_i a^s_j(x_i) \qquad \sigma^2_{\mathcal{B},j} = \tfrac{1}{m}\textstyle\sum_i (a^s_j(x_i) - \mu_{\mathcal{B},j})^2$$

- $\gamma, \beta \in \mathbb{R}^{n_s}$: learned scale and shift (via backprop)
- $\varepsilon \sim 10^{-6}$: numerical stability constant
- Bias $b^s$ is redundant when BN precedes $\sigma$ (absorbed by $\beta$)

# Training vs. Inference

**Training** (`model.train()`)

Statistics from the current minibatch:

$$\mu_s = \frac{1}{m}\sum_{i=1}^{m} a^s(x_i)$$

$$\sigma_s^2 = \frac{1}{m}\sum_{i=1}^{m}\left(a^s(x_i) - \mu_s\right)^2$$

**Caveat:** meaningful only when $m \gg 1$.

**Inference** (`model.eval()`)

Running EMA accumulated during training:

$$\hat{\mu}^s \leftarrow \beta_1\,\hat{\mu}^s + (1-\beta_1)\,\mu_s^{\mathcal{B}}$$

$$\hat{\sigma}_s^2 \leftarrow \beta_2\,\hat{\sigma}_s^2 + (1-\beta_2)\,\sigma_{s,\mathcal{B}}^2$$

Frozen at test time $\rightarrow$ deterministic.

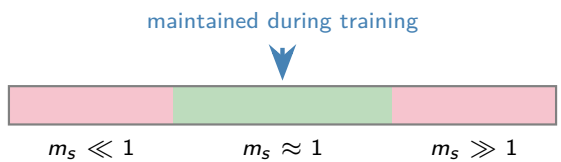
**Common PyTorch bug:** forgetting to switch `model.train()` $\leftrightarrow$ `model.eval()`.

# Batch Normalization for CNNs

Per-channel normalization: one $(\mu_c, \sigma_c^2)$ pair per channel, computed over all spatial positions and all samples in the minibatch.

For feature maps of shape $m \times C \times H \times W$: each channel's statistics use $m \cdot H \cdot W$ values.

Preserves translational equivariance: every spatial position in channel $c$ is shifted and scaled by the same $\gamma_c, \beta_c$.



# When Batch Normalization Breaks Down

BN requires large minibatches ($m \gg 1$). This can be problematic:

- Memory constraints may force small $m$ (large models, high-resolution inputs).
- RNNs / variable-length sequences: BN needs separate parameters per time step.

This motivates normalizing **across neurons** instead of across the batch.

# Layer Normalization

## Definition (Layer Normalization)

$$\mathrm{LayerNorm}_{\gamma,\beta}(a^s) = \gamma \odot \frac{a^s - \mu}{\sqrt{\sigma^2 + \varepsilon}} + \beta$$

where:

$$\mu = \frac{1}{n_s} \sum_{i=1}^{n_s} a_i^s(x), \qquad \sigma^2 = \frac{1}{n_s} \| a^s(x) - \mu \, \mathbf{1} \|_2^2$$

- Statistics per instance, across all neurons — no batch dependence.
- $\gamma, \beta \in \mathbb{R}^{n_s}$ learned as in BN.
- Identical behavior at training and inference (no EMA needed).

# Batch Norm vs. Layer Norm

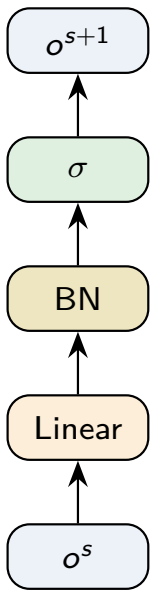
| | **Batch Norm** | **Layer Norm** |
|---|---|---|
| Stats computed over | minibatch (per neuron) | single instance (per layer) |
| Requires large $m$? | Yes | No |
| Train/test differ? | Yes (EMA at test) | No |
| Natural for CNNs? | Yes (per-channel) | Less common |
| Natural for sequences? | No | Yes |

Layer normalization is the standard in Transformer architectures over batch normalization. The **pre-norm** variant (LN applied *before* the attention/MLP sub-layer rather than after) has become dominant since GPT-2 because it provides more stable gradient flow in very deep models.

# Post-Activation vs. Pre-Activation Normalization

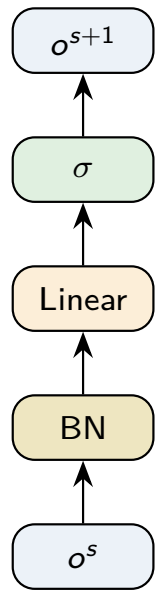
**Post-activation** (Ioffe & Szegedy, 2015):

$$o^{s+1} = \sigma\big(\mathrm{BN}(W^{s+1}o^s)\big)$$




**Pre-activation** (He et al., 2016):

$$o^{s+1} = \sigma\big(W^{s+1}\mathrm{BN}(o^s) + b^{s+1}\big)$$




Brief historical arc: BN post-activation (2015, Inception v2) $\rightarrow$ pre-activation ResNets (He et al., 2016) $\rightarrow$ pre-norm LN in Transformers (GPT-2, 2019 onward). Vanilla CNNs: post-activation BN remains standard.

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**Q.** You're training a NN with layer size 2048 and batch size 2. Why is batch normalization problematic here? What do you use instead?

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**Q.** You're training a NN with layer size 2048 and batch size 2. Why is batch normalization problematic here? What do you use instead?

A. BN computes statistics over the minibatch. With $m = 2$, the sample mean and variance are extremely noisy — the normalization does more harm than good. Use layer normalization, which computes statistics per instance across neurons and has no batch dependence.

# Beyond Per-Layer Fixes: Shortening the Gradient Path

Initialization, activation choice, and normalization all act on the per-layer multiplier $m_s$. But even with $m_s \approx 1$ at every layer, a product of 50+ factors can still drift.

An alternative strategy: **shorten the effective path length** from the output to a given layer, so that the gradient traverses fewer multiplicative factors.

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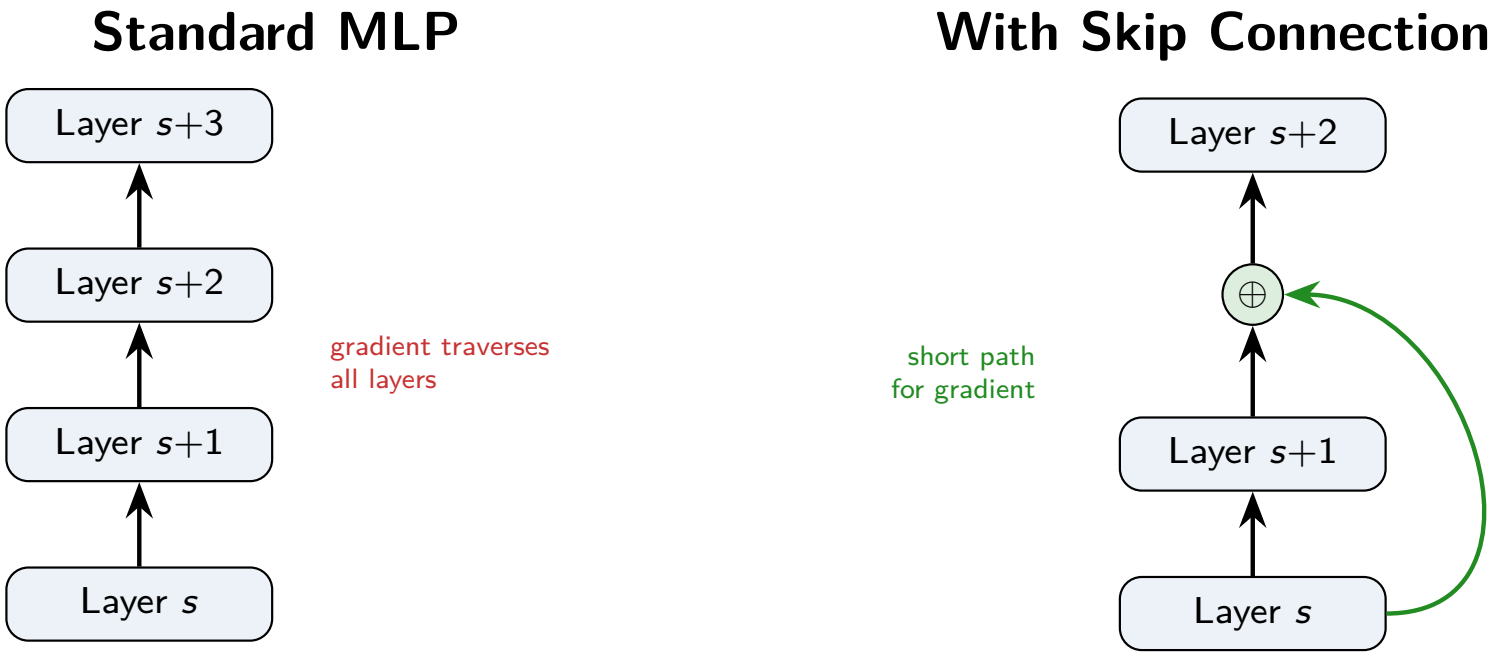
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An alternative strategy: **shorten the effective path length** from the output to a given layer, so that the gradient traverses fewer multiplicative factors.

Two main approaches:

1. **Skip (residual) connections:** add architectural shortcuts that let the gradient bypass layers entirely, converting the Jacobian product into a sum over paths of varying length.
2. **Auxiliary losses:** attach extra loss heads at intermediate layers, injecting gradient signal directly without requiring it to traverse the full depth.

# Skip Connections: Architectural Gradient Shortcuts




Even with proper initialization and normalization, very deep networks ($L > 50$) still struggle because the product of $L - s$ factors accumulates error. Skip connections provide architecturally guaranteed short gradient paths.

# Skip Connections: Definition

**Definition (Skip Connection)**

A *skip connection* (or *residual connection*) is a connection from layer $s$ to layer $s + k$ ($k \geq 2$) that bypasses intermediate transformations.

Two rationales:

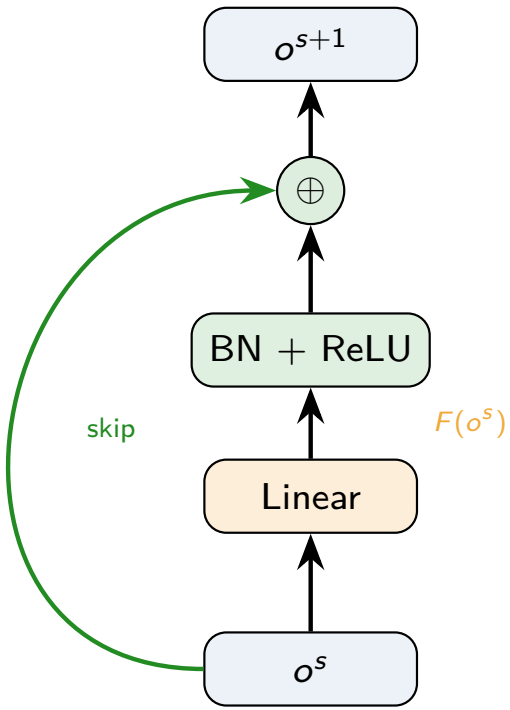
1. **Gradient flow:** short paths avoid compounding attenuation/explosion.
2. **Inductive bias:** higher layers retain access to lower-level features (e.g., U-Nets in image segmentation).

# ResNet: Skip Connections in Practice (He et al., 2015)

**Canonical residual form:**

$$o^{s+1} = o^s + F(o^s)$$

where $F$ is a small sub-network (e.g., Linear $\rightarrow$ BN $\rightarrow$ ReLU).




Important properties:

- If $F(o^s) \approx 0$: $o^{s+1} \approx o^s$ — the network easily represents the identity.
- The network learns the *residual* on top of identity.
- Requires matching dimensions; when $n_{s+1} \neq n_s$, use a projection $Po^s$ on the skip branch.

# Why Skip Connections Stabilize Gradient Flow

Gradient through a residual layer:

$$\nabla_{o^s} f = \underbrace{\nabla_{o^{s+1}} f}_{\text{skip (identity)}} + \underbrace{\nabla_{o^s} F(o^s)^\top \cdot \nabla_{o^{s+1}} f}_{\text{main branch}}$$

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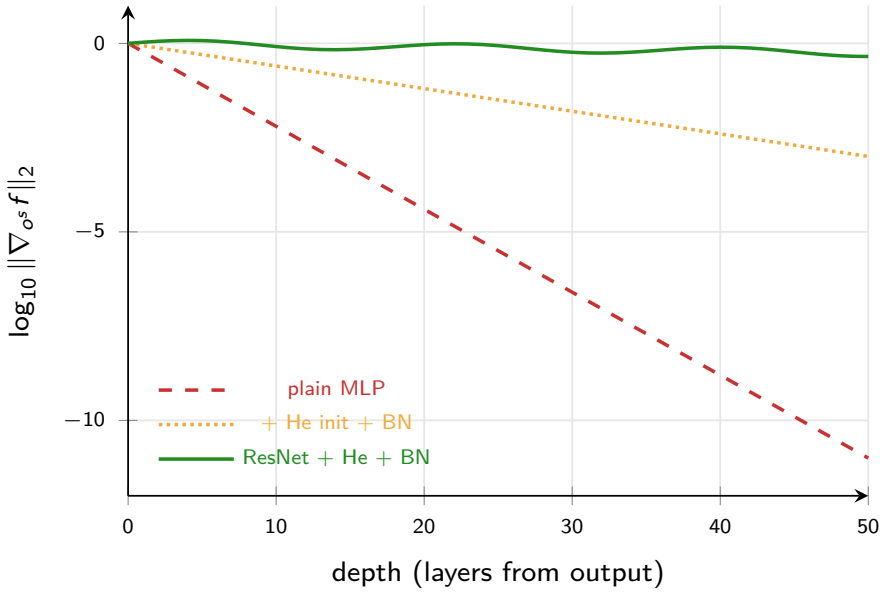
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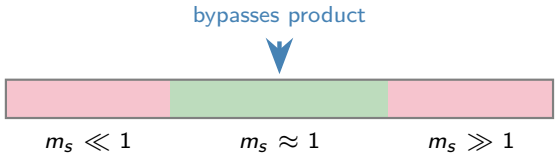
Over $k$ residual layers, the gradient is a sum of $2^k$ terms. Even if long paths (many main-branch factors) attenuate, the short paths (mostly skips) preserve gradient magnitude.

# Gradient Flow: The Payoff

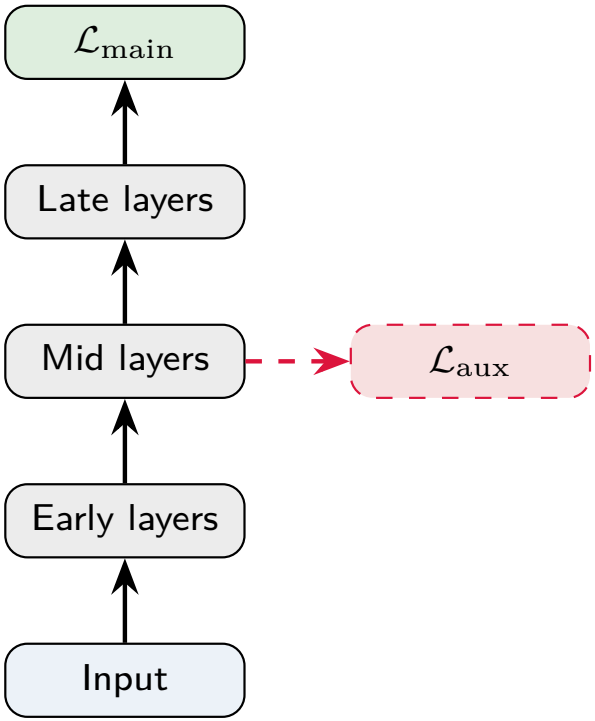



Schematic comparison (not real data):

- Plain MLP: exponential decay ($m_s < 1$ compounds)
- + He + BN: slower decay ($m_s \approx 1$ but products still accumulate)
- ResNet: roughly flat (identity paths bypass products)



# Auxiliary Losses: Direct Gradient Injection




In very deep networks (e.g., GoogLeNet, 22 layers; Szegedy et al., 2014), early layers can receive weak gradient signal even with normalization and careful initialization.

Idea: attach auxiliary classification heads at intermediate points to directly inject gradient information.

Training objective:

$$\mathcal{L} = \mathcal{L}_{\text{main}} + \lambda \mathcal{L}_{\text{aux}}$$

Through the multiplier lens: auxiliary losses don't change $m_s$ — they **shorten the effective product length** by injecting $\nabla_{o^L} f$-scale signal at an intermediate layer.

# Unifying View: Did We Deliver?

We promised to keep $m_s \approx 1$. Let's verify:

| **Method** | **Acts on** | **Effect on $m_s$** | **Status** |
|---|---|---|---|
| Initialization | typical amplification at $t{=}0$ | RMS singular value $\approx 1$ | ✓ |
| Activation choice | $\|\sigma'\|_\infty$ | Avoids $m_s \approx 0$ | ✓ |
| Batch/Layer Norm | activations $\to m_s$ | Renormalizes during training | ⊙ |
| Residual connections | Jacobian structure | Bypasses $\prod$: adds identity | ✓ |
| Auxiliary losses | Product length | Shortens $\prod$ | ✓ |

Central insight: we are studying products of random (or evolving) matrices and asking whether their singular values concentrate near 1. Initialization controls typical-case amplification; the other techniques address worst-case and dynamic drift.

# Summary

- **Vanishing/exploding gradients** arise from poorly conditioned Jacobian products $\prod_i (W^i)^\top \operatorname{diag}(\sigma'(a^i))$. The per-layer multiplier $m_s = \|W^s\|_2 \cdot \|\sigma'\|_\infty$ is a worst-case diagnostic: if $m_s \neq 1$, the effect is exponential in depth.
- **Forward and backward stability are coupled but not equivalent:** forward instability poisons $\sigma'$ and the backprop seed $\nabla_{o^L} f$.
- **Initialization** (Xavier, He): preserves per-coordinate activation variance (forward) and gradient norm (backward) — both yield $\mathrm{Var}(W) = 1/n_{\text{in}}$ (or $2/n_{\text{in}}$ for ReLU).
- **Activation choice** (ReLU, GELU): avoids saturation that drives $\sigma' \to 0$.
- **Batch normalization**: re-centers and re-scales pre-activations; prevents $m_s$ drift during training. Requires $m \gg 1$.
- **Layer normalization**: batch-independent alternative; standard in Transformers (pre-norm variant).
- **Residual connections**: $o^{s+1} = o^s + F(o^s)$. Converts

# Questions?

# Next Time: Sequence Learning

- Learning on sequences: why standard MLPs fall short
- Recurrent neural networks (RNNs): architecture and limitations
- Sequence-to-sequence architectures
- The attention mechanism
- Tokenization for NLP problems

# Gradient Coordinates Are Exchangeable at Initialization

## Theorem (Gradient Coordinate Exchangeability)

Consider an $L$-layer network with i.i.d. weight entries at each layer (e.g., Xavier or He initialization) and coordinate-wise activation $\sigma$. Fix any input $x$ and any layer index $s \in \{1, \dots, L-1\}$. Then the coordinates of $\nabla_{o^s} f$ are **exchangeable**: for every permutation $\pi$ of $\{1, \dots, n_s\}$,

$$P_\pi \, \nabla_{o^s} f \overset{d}{=} \nabla_{o^s} f$$

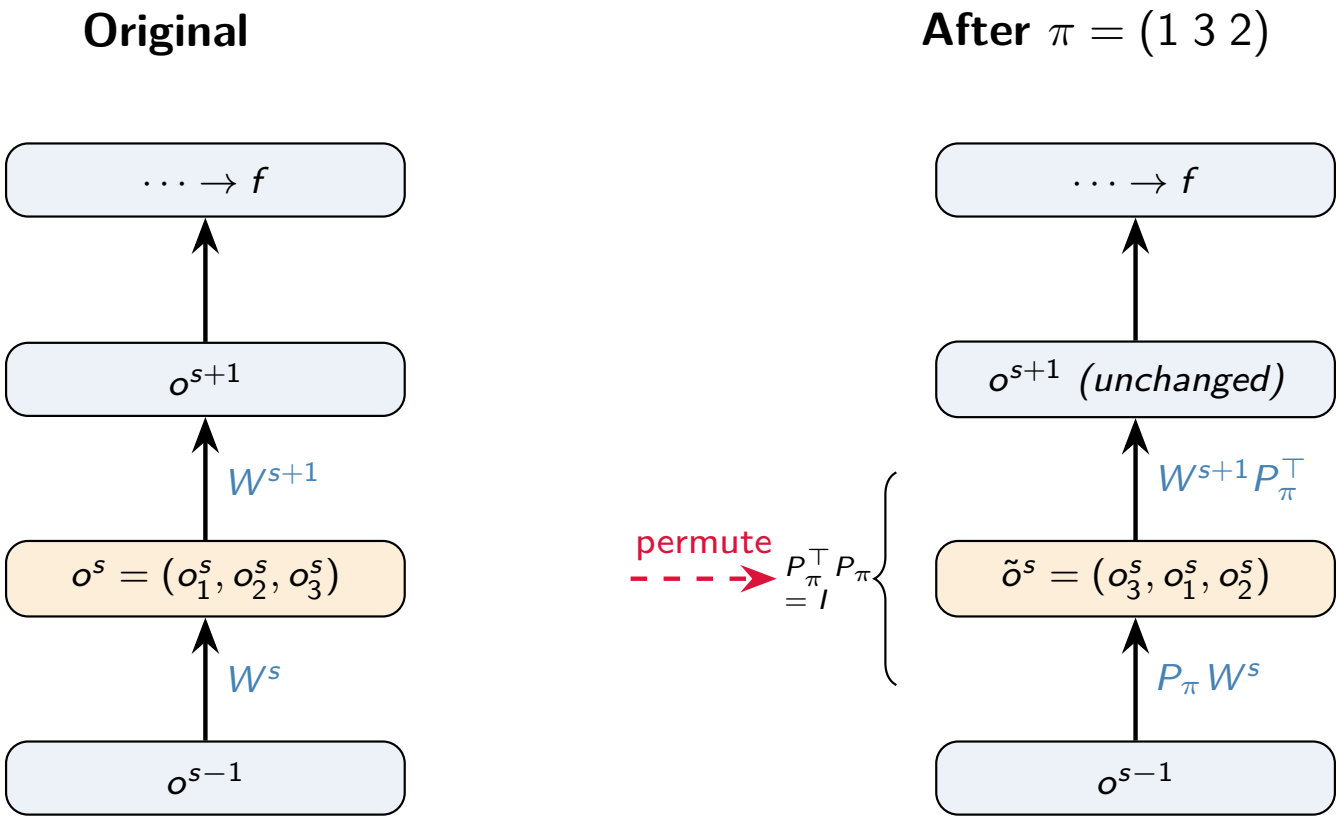
where $P_\pi$ is the permutation matrix and the distribution is over the random initialization.

**Consequence:** all coordinates share the same marginal distribution, so

$$\mathbb{E}\big[\|\nabla_{o^s} f\|^2\big] = \sum_{k=1}^{n_s} \mathbb{E}\big[[\nabla_{o^s} f]_k^2\big] = n_s \cdot \mathbb{E}\big[[\nabla_{o^s} f]_1^2\big].$$

# Idea: Exploit Neuron Permutation Symmetry

The proof exploits the fact that permuting all neurons at layer $s$ leaves the joint distribution of the weights unchanged (because each $W^i$ has i.i.d. entries), but permutes $\nabla_{o^s} f$ accordingly.




The permutations of $W^s$ (rows) and $W^{s+1}$ (columns) **cancel at layer $s+1$**: $a^{s+1} = W^{s+1} P_\pi^\top \cdot P_\pi\, o^s = W^{s+1} o^s$.

# Proof

Fix a permutation $\pi$ and let $P = P_\pi$. Define the permuted weights:

$$\tilde{W}^s = PW^s, \qquad \tilde{W}^{s+1} = W^{s+1}P^\top, \qquad \tilde{W}^i = W^i \text{ for } i \neq s, s{+}1.$$

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**Step 1 (layers $\leq s$):** Since $o^{s-1}$ depends only on $W^1, \ldots, W^{s-1}$ (unchanged), $o^{s-1}$ is unchanged. Then $\tilde{a}^s = \tilde{W}^s o^{s-1} = P\, a^s$, so $\tilde{o}^s = \sigma(P\, a^s) = P\, o^s$ (coordinate-wise $\sigma$).

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**Step 2 (layers $> s$):**
$\tilde{a}^{s+1} = \tilde{W}^{s+1}\tilde{o}^s = W^{s+1}P^\top P\, o^s = W^{s+1}o^s = a^{s+1}$. So $o^{s+1}, o^{s+2}, \ldots, o^L$ and hence $f$ are all unchanged.

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**Step 1 (layers $\leq s$):** Since $o^{s-1}$ depends only on $W^1, \ldots, W^{s-1}$ (unchanged), $o^{s-1}$ is unchanged. Then $\tilde{a}^s = \tilde{W}^s o^{s-1} = P\,a^s$, so $\tilde{o}^s = \sigma(P\,a^s) = P\,o^s$ (coordinate-wise $\sigma$).

**Step 2 (layers $> s$):**
$\tilde{a}^{s+1} = \tilde{W}^{s+1}\tilde{o}^s = W^{s+1}P^\top P\,o^s = W^{s+1}o^s = a^{s+1}$. So $o^{s+1}, o^{s+2}, \ldots, o^L$ and hence $f$ are all unchanged.

**Step 3 (gradient):** $\nabla_{o^{s+1}} f$ is unchanged, and
$\nabla_{\tilde{o}^s} f = (\tilde{W}^{s+1})^\top \operatorname{diag}(\sigma'(a^{s+1}))\,\nabla_{o^{s+1}} f =$
$P\,(W^{s+1})^\top \operatorname{diag}(\sigma'(a^{s+1}))\,\nabla_{o^{s+1}} f = P\,\nabla_{o^s} f.$

# Proof

Fix a permutation $\pi$ and let $P = P_\pi$. Define the permuted weights:

$$\tilde{W}^s = PW^s, \qquad \tilde{W}^{s+1} = W^{s+1}P^\top, \qquad \tilde{W}^i = W^i \text{ for } i \neq s, s{+}1.$$

**Step 1 (layers $\leq s$):** Since $o^{s-1}$ depends only on $W^1, \ldots, W^{s-1}$ (unchanged), $o^{s-1}$ is unchanged. Then $\tilde{a}^s = \tilde{W}^s o^{s-1} = P\, a^s$, so $\tilde{o}^s = \sigma(P\, a^s) = P\, o^s$ (coordinate-wise $\sigma$).

**Step 2 (layers $> s$):**
$\tilde{a}^{s+1} = \tilde{W}^{s+1}\tilde{o}^s = W^{s+1}P^\top P\, o^s = W^{s+1}o^s = a^{s+1}$. So $o^{s+1}, o^{s+2}, \ldots, o^L$ and hence $f$ are all unchanged.

**Step 3 (gradient):** $\nabla_{o^{s+1}} f$ is unchanged, and
$\nabla_{\tilde{o}^s} f = (\tilde{W}^{s+1})^\top \operatorname{diag}(\sigma'(a^{s+1}))\, \nabla_{o^{s+1}} f =$
$P\,(W^{s+1})^\top \operatorname{diag}(\sigma'(a^{s+1}))\, \nabla_{o^{s+1}} f = P\, \nabla_{o^s} f$.

**Step 4 (distribution):** Since each $W^i$ has i.i.d. entries, $PW^s \overset{d}{=} W^s$ and $W^{s+1}P^\top \overset{d}{=} W^{s+1}$. Therefore $(\tilde{W}^1, \ldots, \tilde{W}^L) \overset{d}{=} (W^1, \ldots, W^L)$, so $P\, \nabla_{o^s} f \overset{d}{=} \nabla_{o^s} f$. □

# Visual Summary: What the Permutation Does

