Representations in Random Deep Neural Networks

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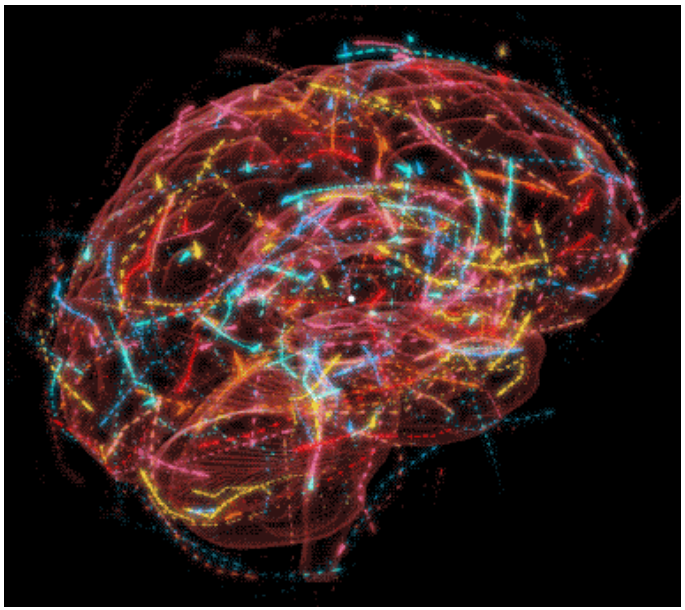
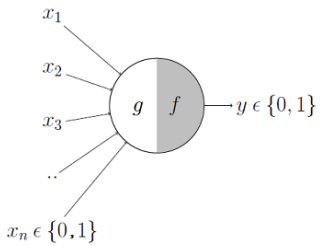
"The noisy brain"

- Brain is a collection of noisy firing neurons
- Random is essential for many brain tasks including decision-making attention[1]
- Neural synchrony causes brain dysfunctions such as schizophrenia

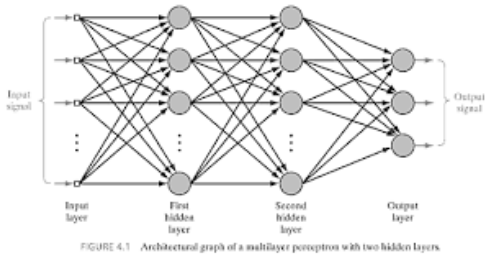


[1] **b**.

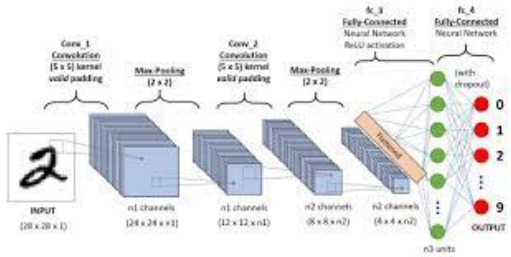
Evolution of computational neural networks



McCulloch-Pitts Neuron



MLP



Convolutional networks

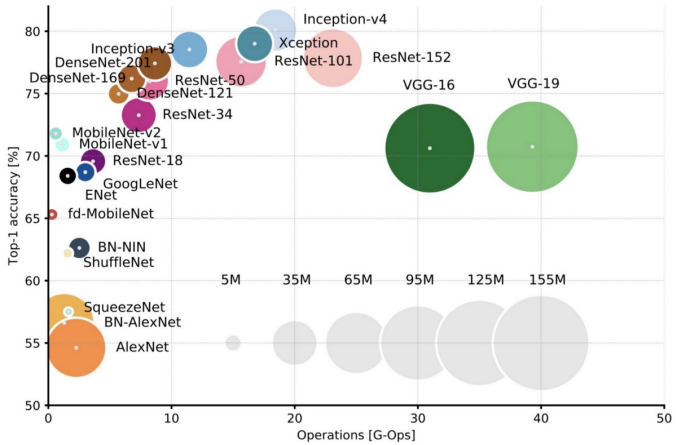


Figure: Images credit: Alfredo Canziani et. al.

Noisy computational networks

- **Historical** neural networks do not work well with random weights
- **Modern** computational neural networks perform surprisingly well with random weights if the neurons are wired well together[2].

Why?

[2] Frankle, J., Schwab, D. J. & Morcos, A. S. Training batchnorm and only batchnorm: On the expressive power of random features in CNNs. *ICLR* (2021).

Historical single-layer MLPs

$$H_1 = \frac{1}{\sqrt{\text{batchsize}}} F(W_0 H_0)$$

- $H_0 \in \mathbb{R}^{\text{width} \times \text{batchsize}}$ is a deterministic matrix
- $W_0 \in \mathbb{R}^{\text{width} \times \text{width}}$ is a random Gaussian matrix
- Empirical eigenvalue distribution (e.e.d): $\frac{1}{\text{width}} \sum_{i=1}^{\text{width}} \delta(\lambda_i(H_1^\top H_1))$
- Given the first two moments of H_1,[3] characterizes e.e.d. of H_1 as batchsize and width tends to ∞ denoted by p

[3] Louart, C., Liao, Z., Couillet, R., *et al.* A random matrix approach to neural networks. *The Annals of Applied Probability* (2018).

Historical single-layer MLPs

- Stieltjes transformation of density p on interval I:

$$S_p(z) = \int_I \frac{p(t)dt}{z-t}, \quad z \in C \backslash I$$

- Given $G = \mathbf{E}\left[H_1^\top H_1\right]$, the following holds[4]

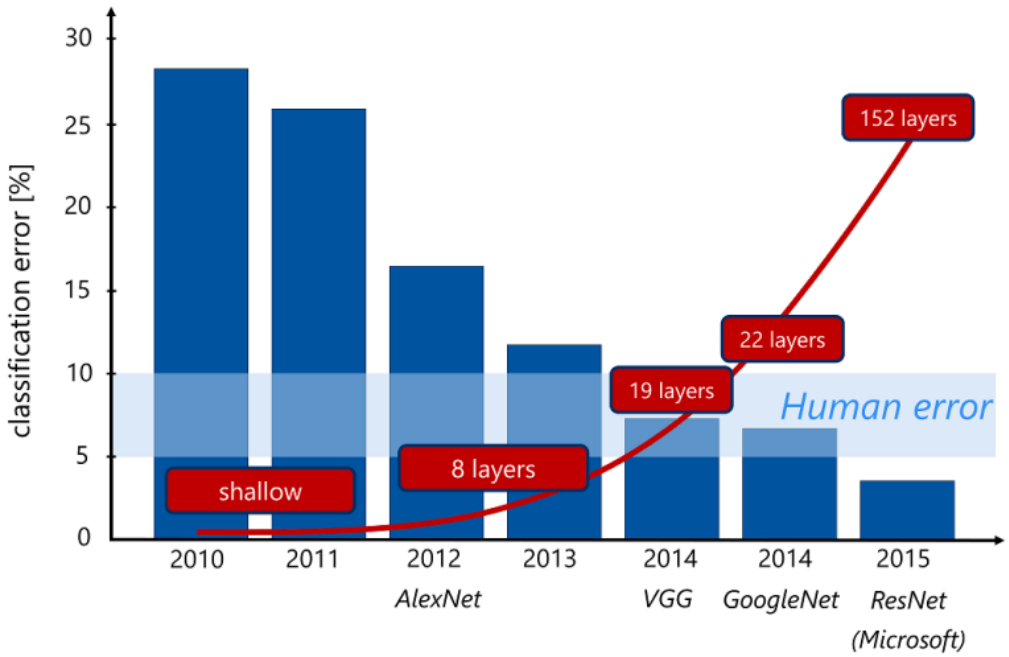
$$S_p(z) = \frac{1}{\text{batchsize}} \text{Tr} \left(\underbrace{\frac{\text{width}}{\text{batchsize}} \frac{G}{1+s(z)} - zI}_{M(s)} \right)^{-1}$$

- $s(z)$ is the solution of

$$s(z) = \frac{1}{\text{batchsize}} \text{Tr}\left(GM^{-1}(s(z))\right)$$

[4] Louart, C., Liao, Z., Couillet, R., *et al.* A random matrix approach to neural networks. *The Annals of Applied Probability* (2018).

Depth in computational neural network



ImageNet Competition Summary

But, deep networks are difficult to train

Historical random deep networks

- Let $x_\ell \in \mathbb{R}^{\text{width}}$ be representation of input x_0 at layer ℓ
- The representations make a Markov chain as:

$$x_{\ell+1} = \frac{W_\ell x_\ell}{\| W_\ell x_\ell \|}$$

- Suppose the elements of $W_\ell \in \mathbb{R}^{\text{width} \times \text{width}}$ are i.i.d. Gaussian.

Information Bottleneck Principle (Tishby & Zaslavsky)

Capture relevant information

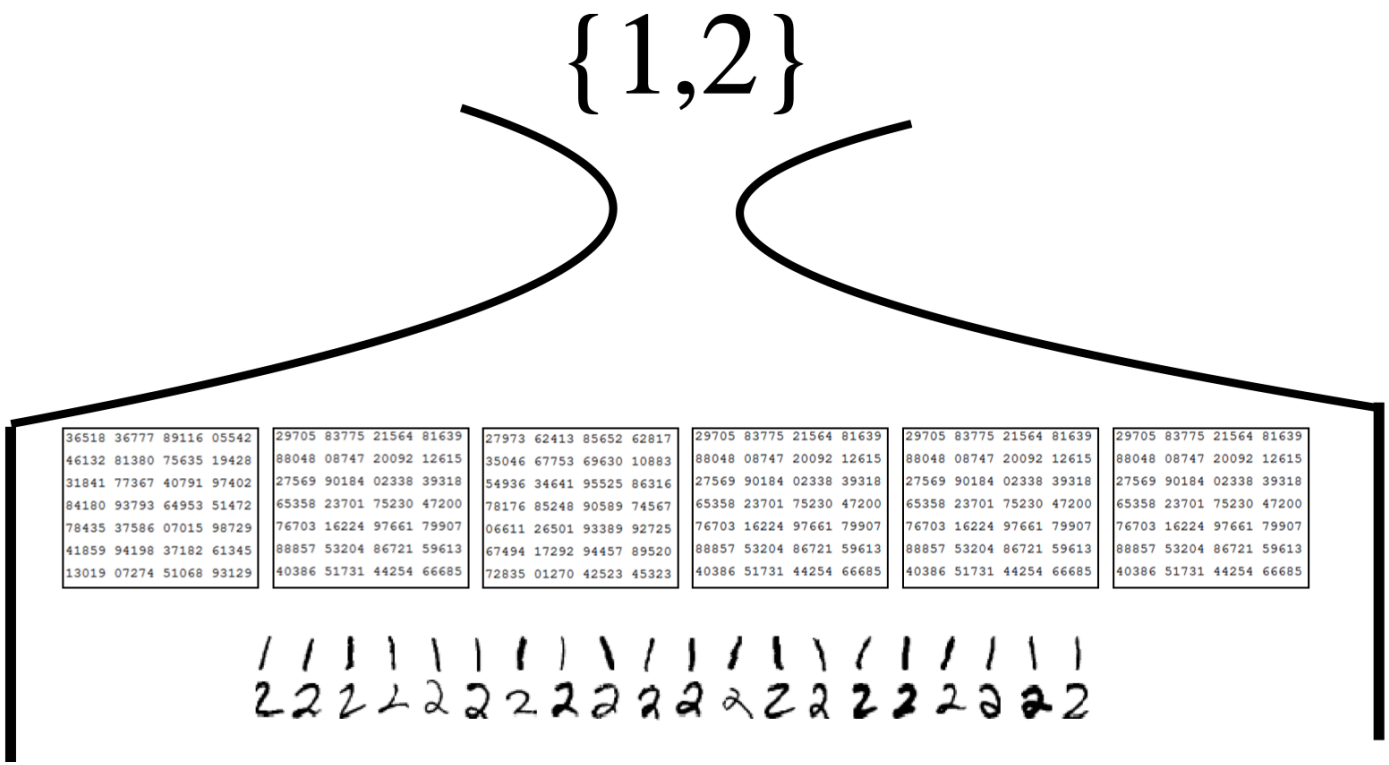
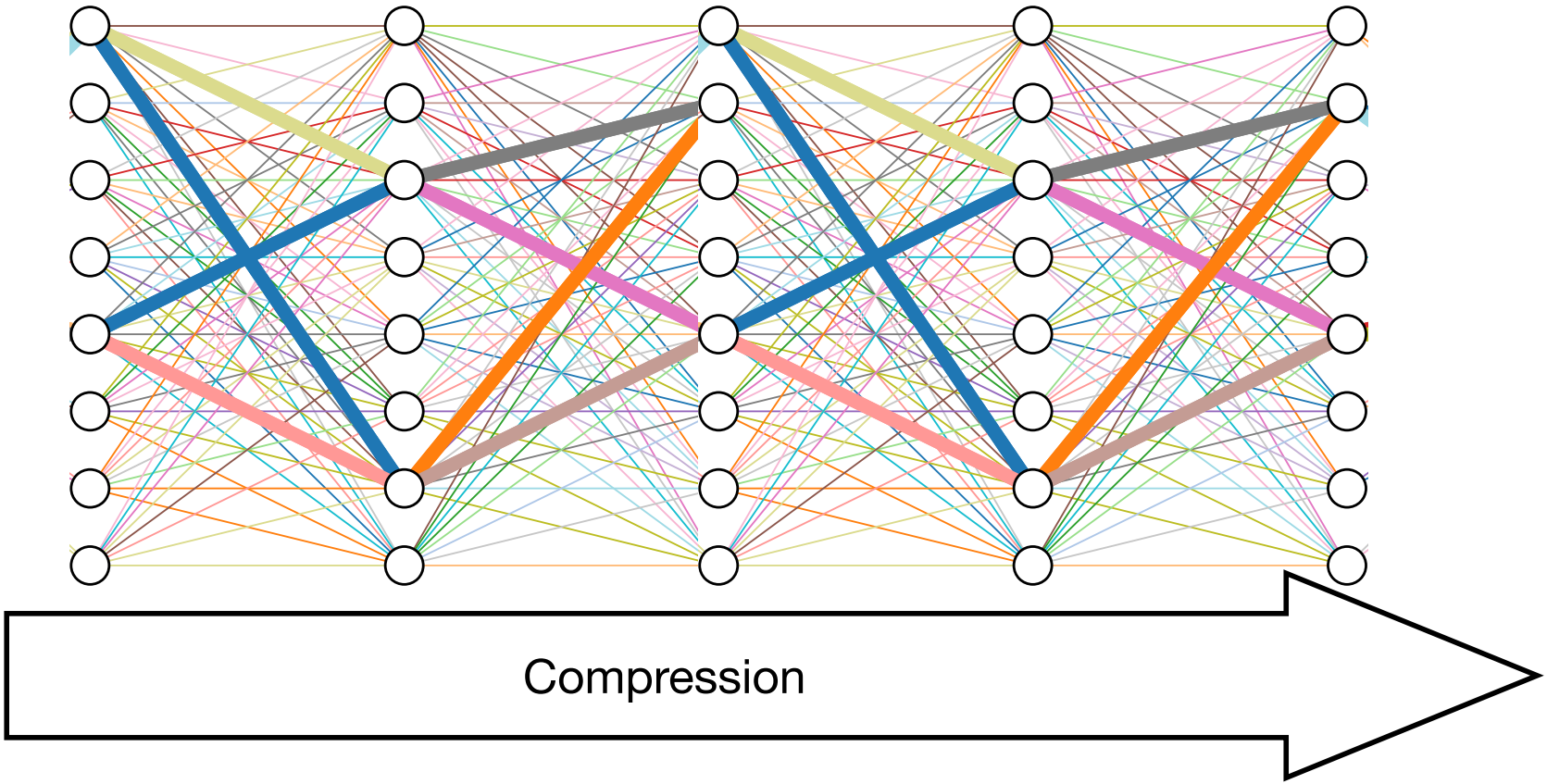


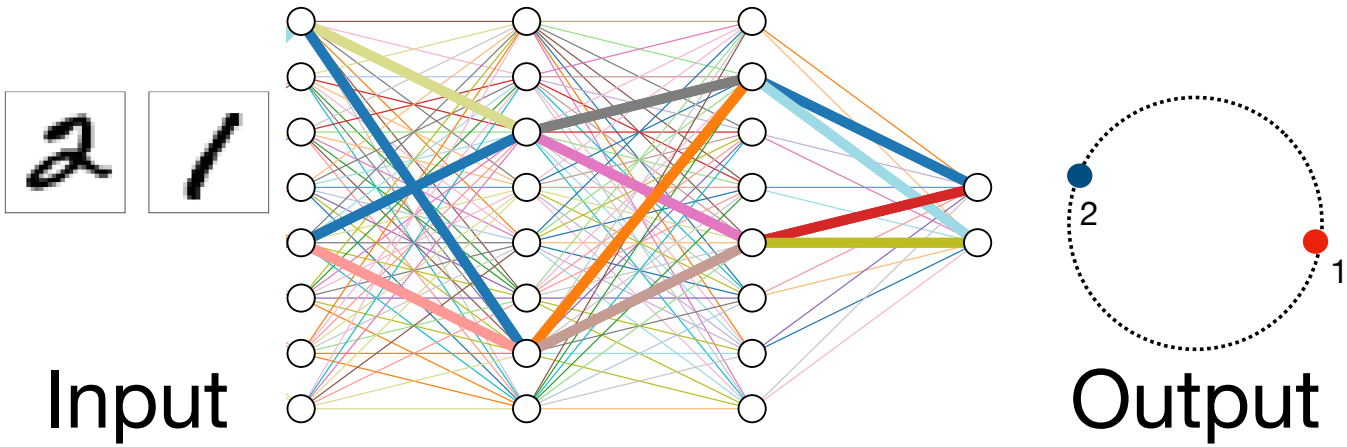
Figure: Compress irrelevant features (image idea:Xu, Tao TPAMI14)

Compression in deep learning

Random networks compress their inputs through their layers.

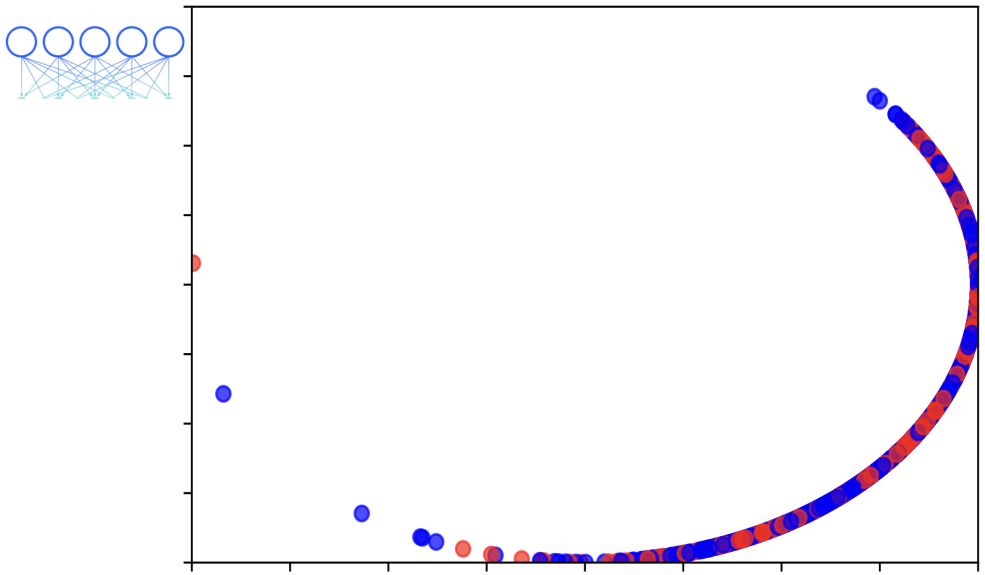


Compression study



Over-compression with depth

Deep random conventional networks compress inputs to a byte.



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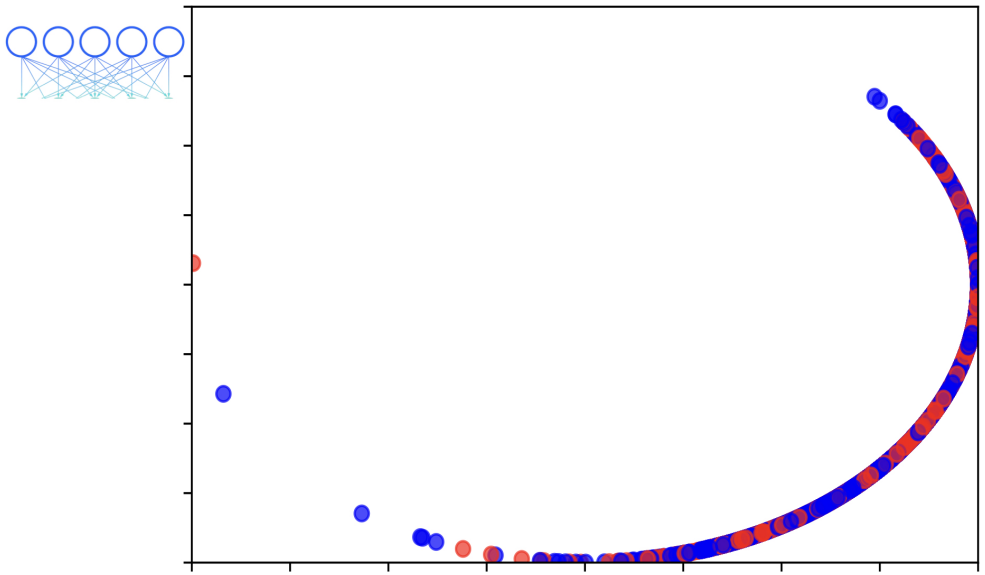
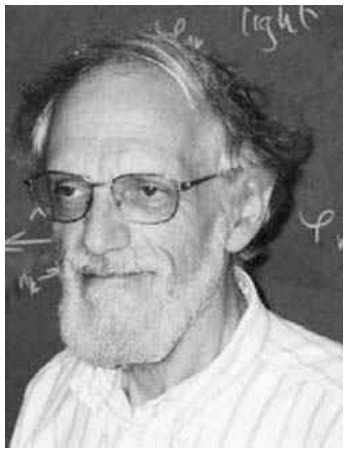
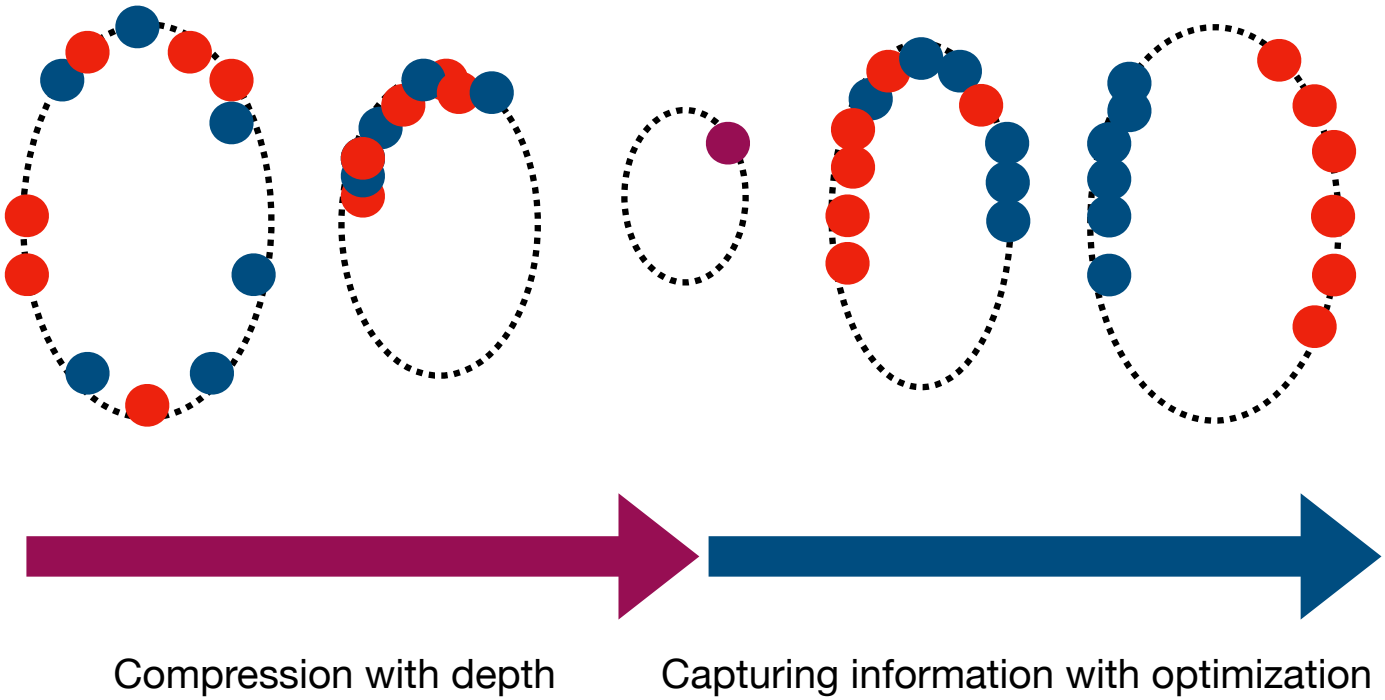




This compression is established by Markov chain studies in 1960 by Hillel Furstenberg [3]

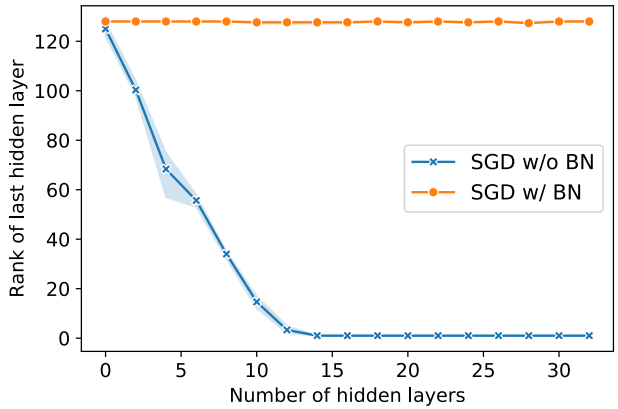
Information Bottleneck for deep learning

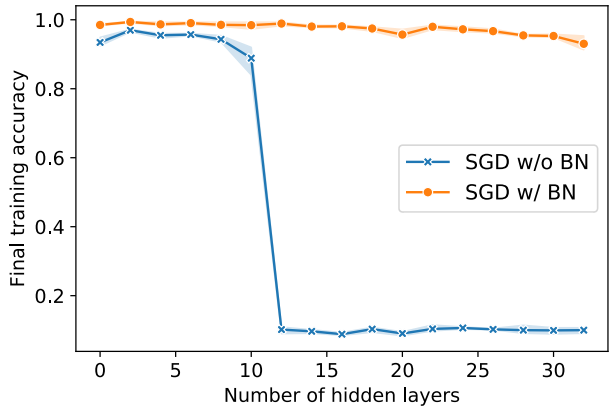
After compression in depth, networks capture relevant information during optimization.



Compression influences optimization

Over-compression with depth slows optimization[5]





[5] **Daneshmand***, H. *et al.* Batch Normalization Provably Avoids Rank Collapse for Randomly Initialised Deep Networks. *NeurIPS* (2020).

Modern deep neural networks

1960

Overcompression

Slow optimization

55 years

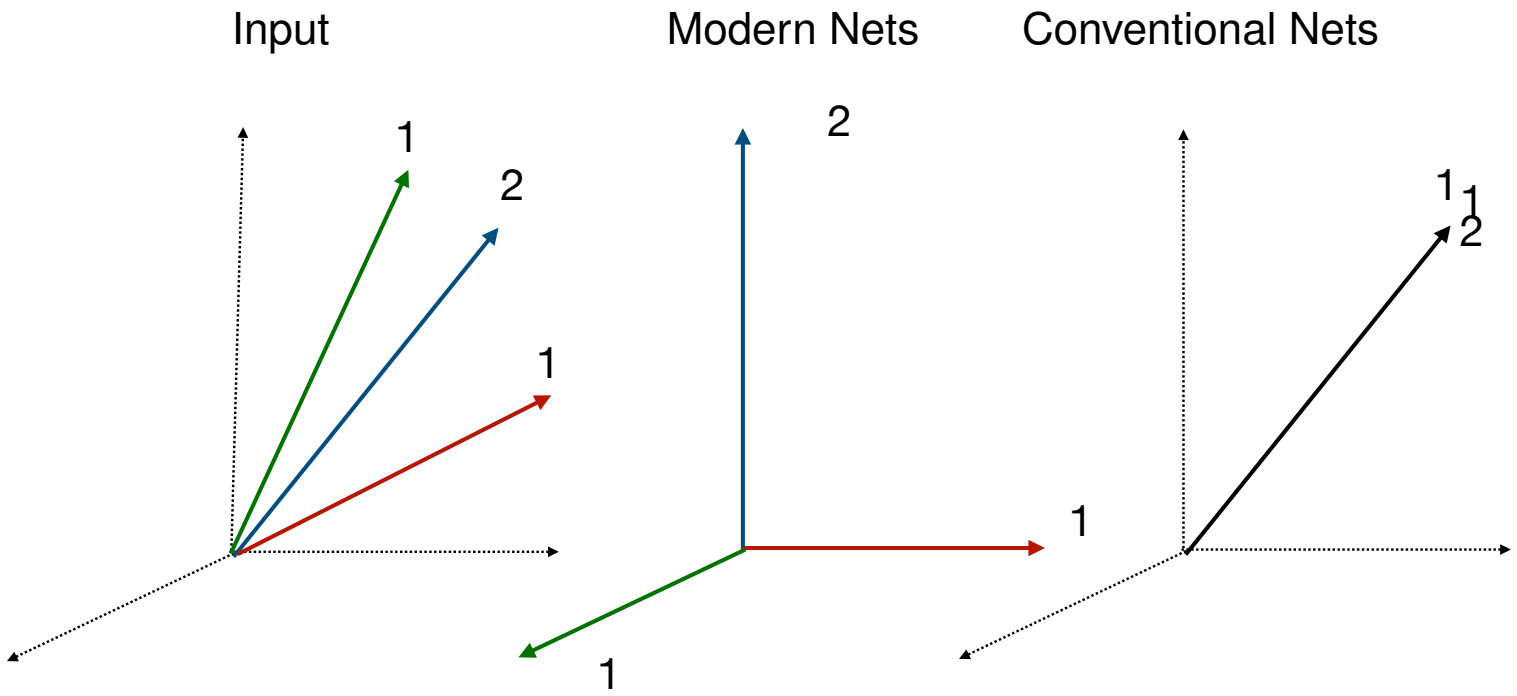
Engineering

2015

Compression?

Fast optimization

Mild compression with modern networks



Memory: $\mathcal{O}$(batchsize $\times$ dimension) $\mathcal{O}$(batchsize) $\mathcal{O}$(1)

Batch Normalization (BN)

BN is the fundamental component of modern neural networks.

[6] Santurkar et al. NeurIPS18, Bjorck et al. NeurIPS18, Arora et al. ICLR19, Yao et al. IEEE BigData20, Sun et al. AAAI20, Lubana et al. NeurIPS21

[7] **Daneshmand**, H., Joudaki, A. & Bach, F. Batch Normalization Orthogonalizes Representations in Deep Random Networks. *NeurIPS* (2021).

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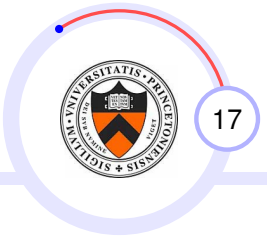

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The underlying mechanisms of BN has been

- a fundamental open problem in machine learning

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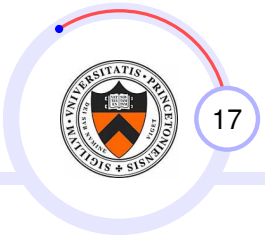


BN is the fundamental component of modern neural networks.

The underlying mechanisms of BN has been

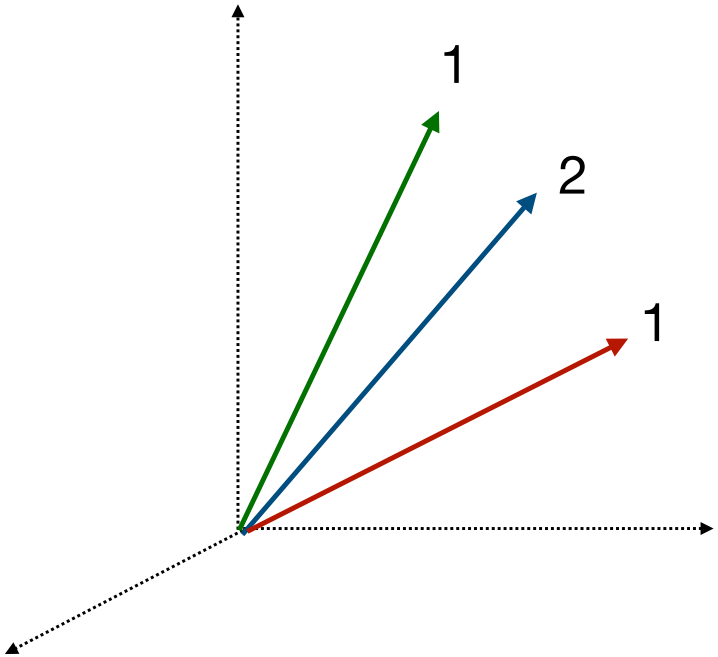
- a fundamental open problem in machine learning
- explored by recent researches in machine learning[6]

Compression. *BN makes representations increasingly orthogonal across layers*[7].

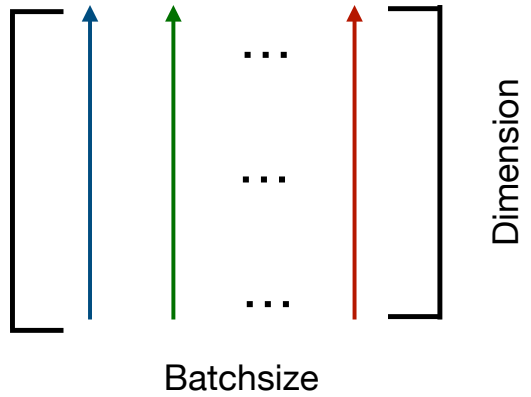
[6] Santurkar et al. NeurIPS18, Bjorck et al. NeurIPS18, Arora et al. ICLR19, Yao et al. IEEE BigData20, Sun et al. AAAI20, Lubana et al. NeurIPS21

[7] **Daneshmand**, H., Joudaki, A. & Bach, F. Batch Normalization Orthogonalizes Representations in Deep Random Networks. *NeurIPS* (2021).

The Markov chain of representations



$$H_0 =$$



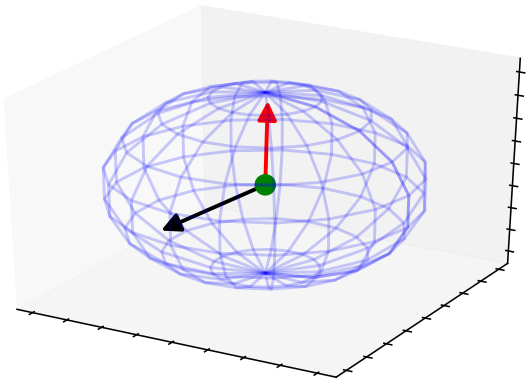
$$\overbrace{H_{\ell+1}}^{\text{Representations}} = BN(\overbrace{W_\ell}^{\textit{Gaussian}} H_\ell)$$

$$BN(M) = \left(\text{diag}(MM^\top)\right)^{-1/2} M$$

BN(.) makes the rows (features) unit norm.

Coupled representations

$$x_{\ell+1} = \frac{W_\ell x_{\ell+1}}{\|W_\ell x_{\ell+1}\|}, \qquad y_{\ell+1} = \frac{W_\ell y_{\ell+1}}{\|W_\ell y_{\ell+1}\|}$$



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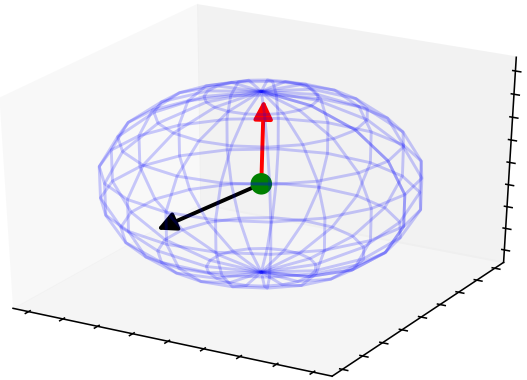
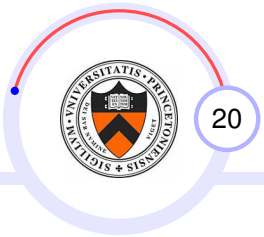


The chains contracts to a random directions independent from the starting state.

Product of random matrices



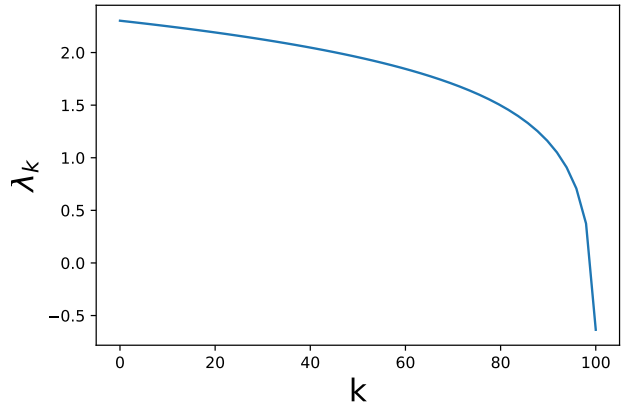
- Consider the product of Gaussian matrix as $S_\ell = W_\ell \dots W_1$
- Claim: $S_\ell / \|S_\ell\|$ becomes rank one in limit.
- Therefore, $(S_\ell x)/\|S_\ell\|$ becomes independent from x as $\ell \to \infty$.

Lyapunov exponents

- Definition:

$$\lambda_k = \lim_{\ell \to \infty} \frac{1}{2\ell} \log \left(k^{\text{th}} \text{ largest eigenvalue of} S_\ell^\top S_\ell \right)$$

- Computation[8]: $\lambda_k = \frac{1}{2}(\log(2) + \Psi\left(\frac{d-k+1}{2}\right))$



- $\lambda_1 - \lambda_2 < 0$ implies $S_\ell / \|S_\ell\|$ becomes rank one in limit.

[8] Newman, C. M. The distribution of Lyapunov exponents: Exact results for random matrices. *Communications in mathematical physics* (1986).

Modern NN with Batch normalization (BN)

- BN is one of the main building block of modern neural networks[9]
- Representation H_ℓ:*width* $\times$ *batchsize*.

$$H_{\ell+1} = F\left(BN_{\alpha,\beta}(W_\ell H_\ell)\right) \tag{1}$$

- $BN_{\alpha,\beta} : \mathbb{R}^{width \times batchsize} \to \mathbb{R}^{width \times batchsize}$

$$[BN_{\alpha,\beta}(M)]_{:} = \alpha_i \text{centered}(M_{i:}) + \beta_i$$

- Learning only parameters α and β (per unit) leads to surprisingly good performance[10]

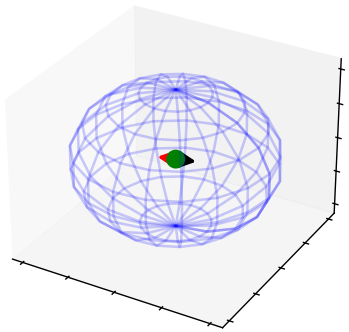
[9] Ioffe, S. & Szegedy, C. *Batch normalization: Accelerating deep network training by reducing internal covariate shift.* in *ICML* (2015).

[10] Frankle, J., Schwab, D. J. & Morcos, A. S. Training batchnorm and only batchnorm: On the expressive power of random features in CNNs. *ICLR* (2021).

The Markov chain of representations

We study the following Markov chain of matrices[11][12].

- $BN(M)$ normalizes M row-wise
- Representations:
  $H_{\ell+1} = \left(\frac{1}{\sqrt{width}}\right) BN(W_\ell H_\ell)$
- W_ℓ: $(width \times width)$ with Gaussian elements

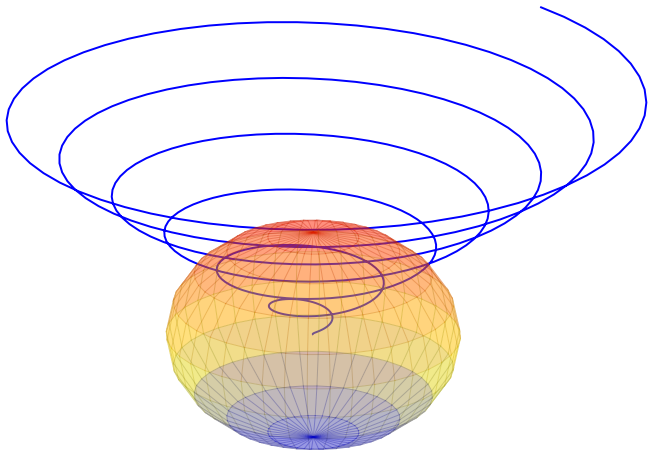


[11] **Daneshmand**, H., Joudaki, A. & Bach, F. Batch Normalization Orthogonalizes Representations in Deep Random Networks. *NeurIPS* (2021).

[12] **Daneshmand***, H. *et al.* Batch Normalization Provably Avoids Rank Collapse for Randomly Initialised Deep Networks. *NeurIPS* (2020).

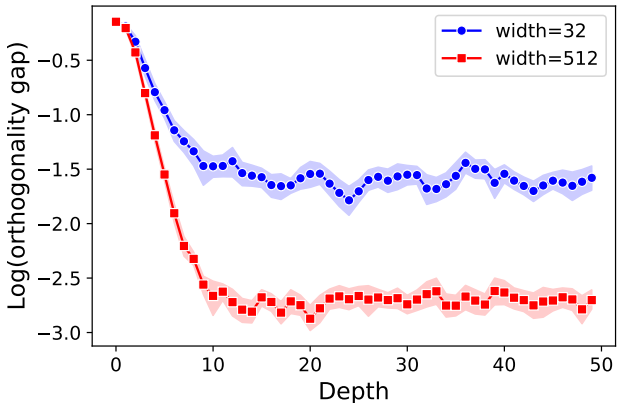
Theoretical results

- $\mathbf{E}\left[\text{orthogonality gap}(H_\ell)\right] = \mathcal{O}\left((1-\alpha)^\ell + \frac{\text{batchsize}}{\alpha\sqrt{\text{width}}}\right)$
- $\text{Wasser.}_2(W_\ell H_\ell, \text{Gaussian})^2 = \mathcal{O}\left((1-\alpha)^\ell\,(\text{batchsize}) + \frac{(\text{batchsize})^2}{\alpha\sqrt{\text{width}}}\right)$



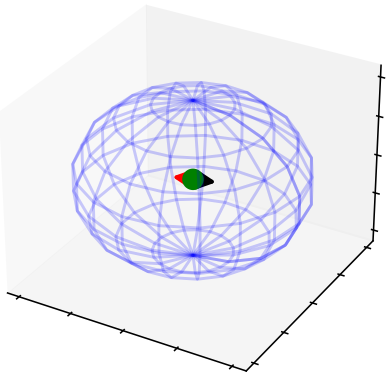
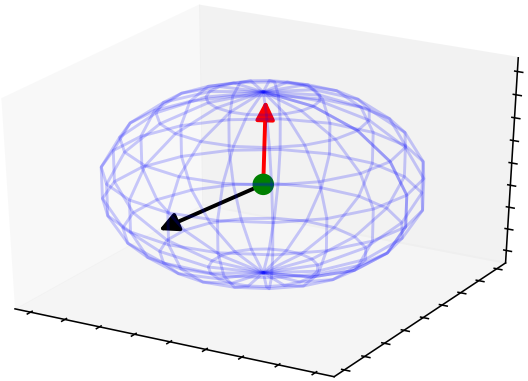
Orthogonalization

- Orthogonality gap$(H) := \left\| \left(\frac{1}{\|H\|_F^2} \right) H^\top H - \left(\frac{1}{\|I_n\|_F^2} \right) I_n \right\|_F$
- $\mathbf{E}\left[\text{orthogonality gap}(H_\ell)\right] = \mathcal{O}\left((1-\alpha)^\ell + \frac{\text{batchsize}}{\alpha\sqrt{\text{width}}}\right)$



- α is the minimum of smallest singular value of $\{H_1, \ldots, H_\ell\}$.
- To get a non-vacuous bound, we need an α independent from ℓ.

Modern NN vs. historical NN

BN	Without BN
	

Modern NN vs. historical NN

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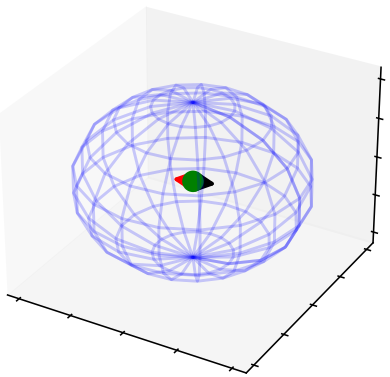
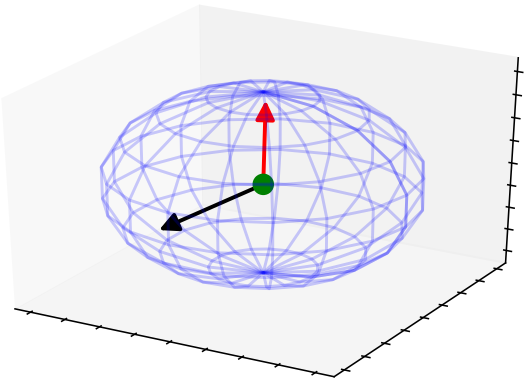
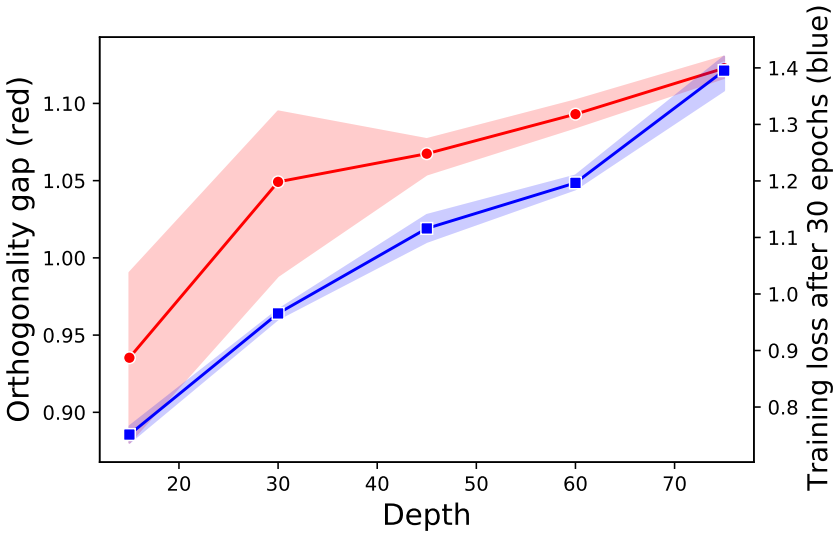
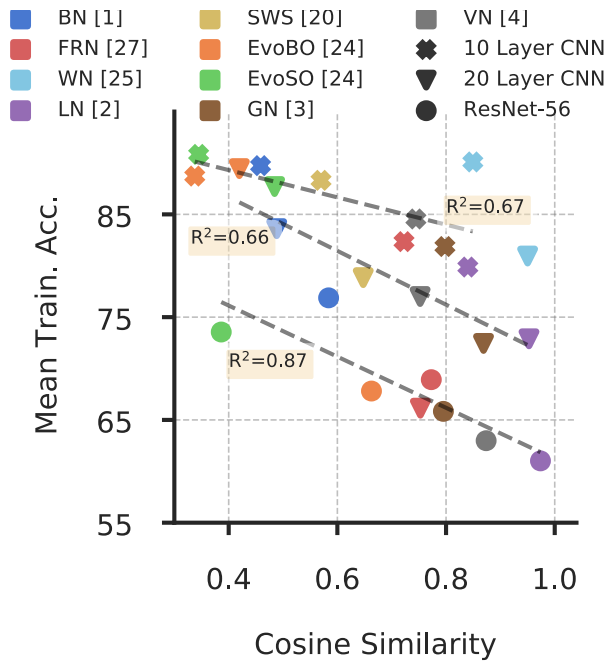
	
$\mathbf{E}\left[\text{orth. gap}(H_\infty)\right] = \mathcal{O}\left(\frac{\text{batch size}}{\alpha\sqrt{\text{width}}}\right)$	$\mathbf{E}\left[\text{orth. gap}(H'_\infty)\right] = \Theta(1)$

The orthogonality influences training



Without normalization

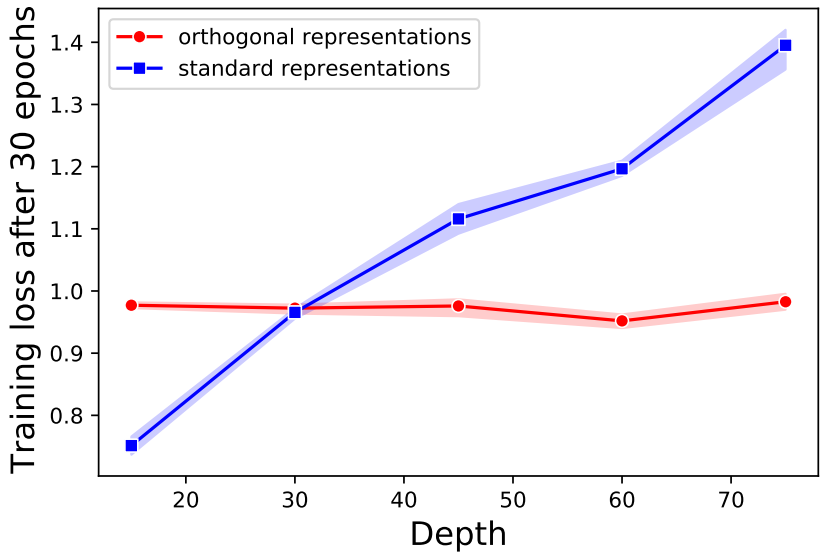


With Normalization[13]

[13] **lubana2021beyond**.

Replacing BN with orthogonalization

Saving training time by starting from orthogonal representations



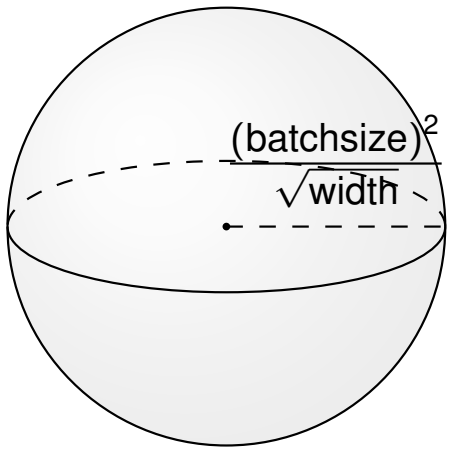
MLPs with ReLU and **without BN** for classifying CIFAR-10

Red: standard initialization with low orthogonality gaps

Blue: novel initialization ensuring orthogonal representations

Gaussian approximation

$$\text{Wasserstein}_2(W_\ell H_\ell, \text{Gaussian})^2 = \mathcal{O}\left((1-\alpha)^\ell\,(\text{batchsize}) + \frac{(\text{batchsize})^2}{\alpha\sqrt{\text{width}}}\right)$$



History of Gaussian approximation for NNs

∞-Width

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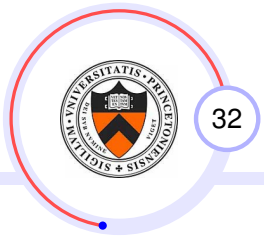
2021 Non-asymptotic (in)finite width and depth Linear MLPs.

Applications of the Gaussian approximation

Vision



Deepening our knowledge about representations in deep neural networks will allow us to design more efficient neural networks.