Average Gradient Outer Product:

A Mechanism for **Deep Neural Collapse**[1]

J. Setpal

October {10, 24}, 2024

[1]Beaglehole, Súkeník et. al. [NeurIPS 2024]

Outline

1. Background & Intuition
2. Deep Neural Collapse (DNC)
3. Average Gradient Outer Product (AGOP)
4. AGOP As a Mechanism for DNC

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Primer – Support Vector Machines (SVMs)

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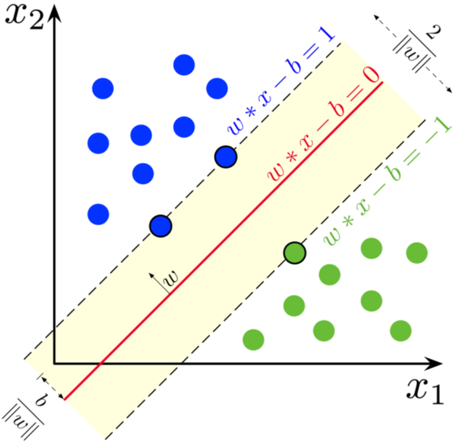

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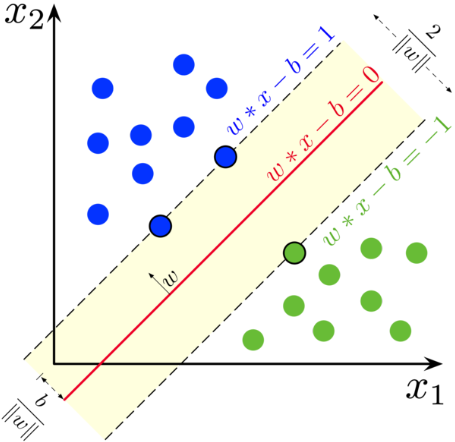

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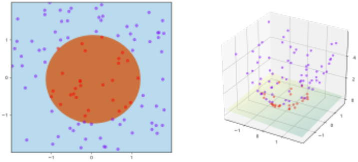

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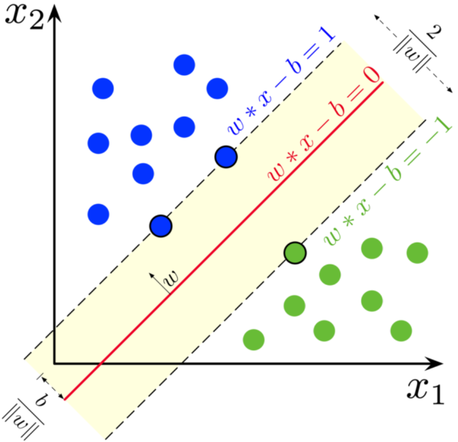

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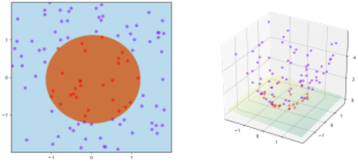

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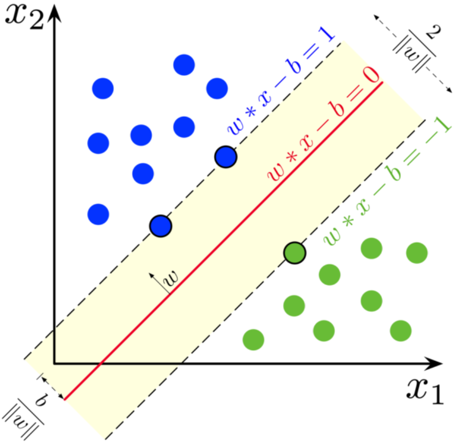

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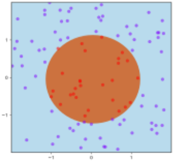

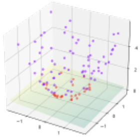

“Lazy” approaches to kernel choices include *polynomial* / *RBF* kernels.

The “laziest” kernel of all is a **deep neural network**.

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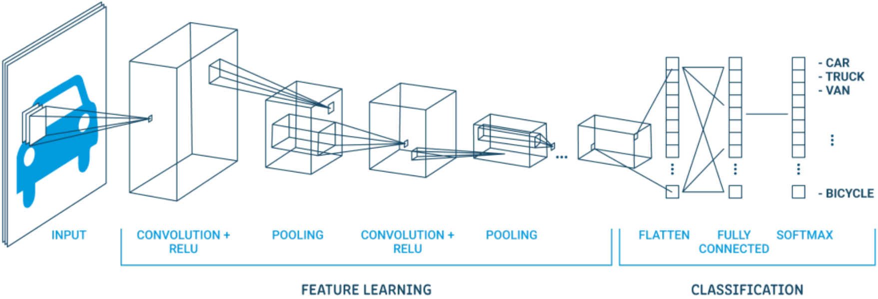

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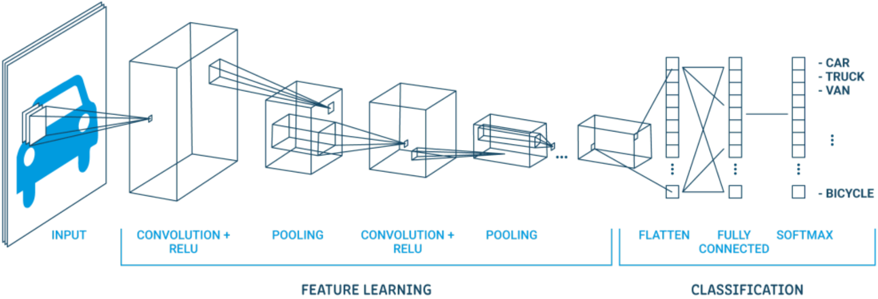

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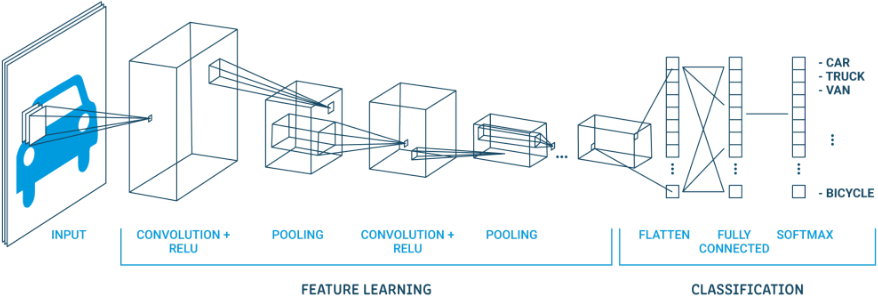

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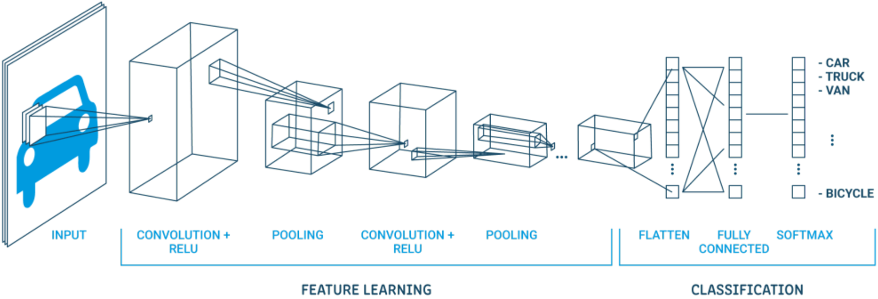

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Q: Why does overparameterized learning generalize?

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$\mathbf{A}_1$: When a sufficiently expressive network h trained to minimize $\mathcal{L}(S_n)$ satisfies $h(x_i) = y_i \ \forall i$, it reaches the **Terminal Point of Training**. When trained beyond this point, the model is overtrained.

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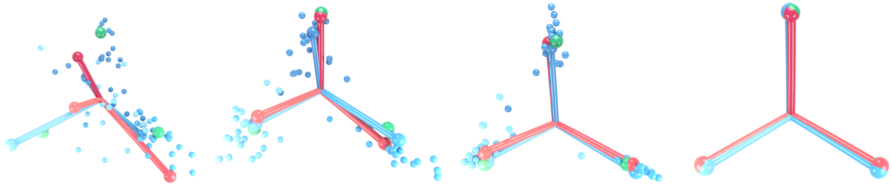
$\mathbf{Q}_{2_a}$: What are the 4 key metrics?
$\mathbf{A}_{2_a}$: Exactly what we'll discuss next!

$NC1$ – Collapse of Variability (1/2)

At a high level, the structure of the penultimate layer collapses towards:



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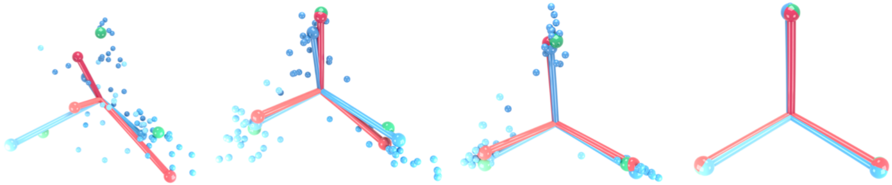

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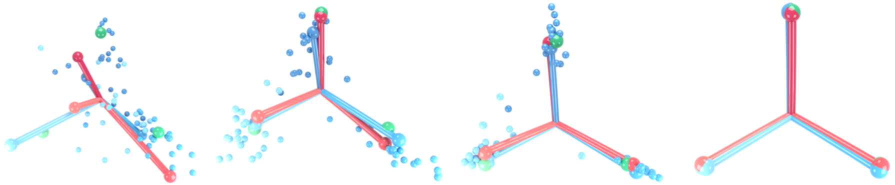

Evolution of penultimate layer outputs on VGG13 trained on CIFAR10.

For all classes $k \in [K]$, datapoints $i \in [n]$ <u>within a class</u>, & penultimate feature vector $f(k, i)$, we have class-specific & global means:

$$\boldsymbol{\mu}_k = \frac{1}{n} \sum_{i=1}^{n} f(k, i) \tag{1}$$

$$\boldsymbol{\mu}_G = \frac{1}{K} \sum_{i=1}^{K} \boldsymbol{\mu}_k \tag{2}$$

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We can use them to calculate *intra* and *inter*-class differences:

$$\mathrm{Cov}_W = \frac{1}{Kn}\sum_{k=1}^{K}\sum_{i=1}^{n}((f(k,i)-\boldsymbol{\mu}_k)(f(k,i)-\boldsymbol{\mu}_k)^T) \in \mathbb{R}^{m\times m} \qquad (3)$$

$$\mathrm{Cov}_B = \frac{1}{K}\sum_{k=1}^{K}((\boldsymbol{\mu}_k-\boldsymbol{\mu}_G)(\boldsymbol{\mu}_k-\boldsymbol{\mu}_G)^T) \in \mathbb{R}^{m\times m} \qquad (4)$$

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Which we combine to measure overall **variability collapse**:

$$NC1 := \frac{1}{K} \mathrm{Tr}\left(\mathrm{Cov}_W \, \mathrm{Cov}_B^{\dagger}\right) \tag{5}$$

Aside: Psuedoinverses

The **inverse** of a matrix A is defined s.t. it satisfies the following condition:

$$A, B, I \in \mathbb{R}^{d \times d} \text{ s.t. } AB = BA = I_d; \; B := A^{-1}, \; A := B^{-1} \tag{6}$$

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$$XX^{-1}X = X \tag{7}$$

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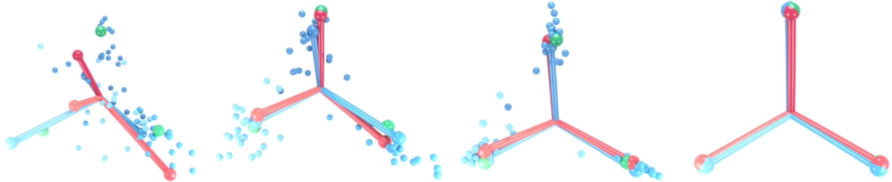
Implication: We can compute correlation b/w general matrix dimensions.

$NC2$ – The Simplex ETF (1/2)

This time, we can on focus the **structure** of the class means:



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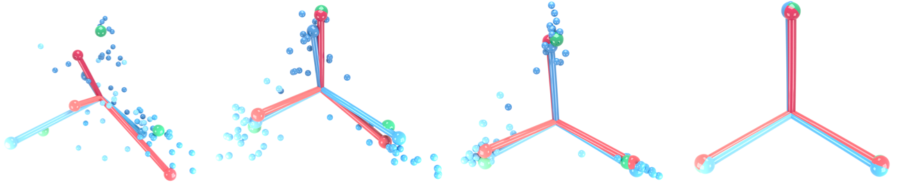

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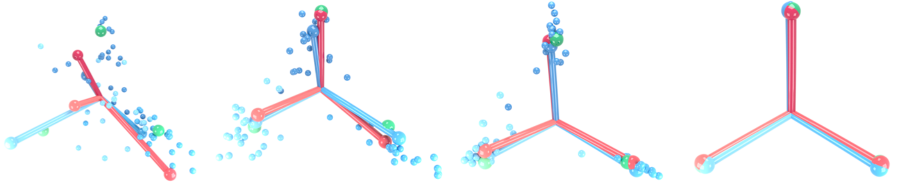

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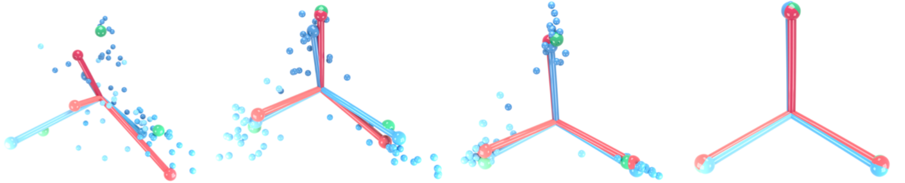

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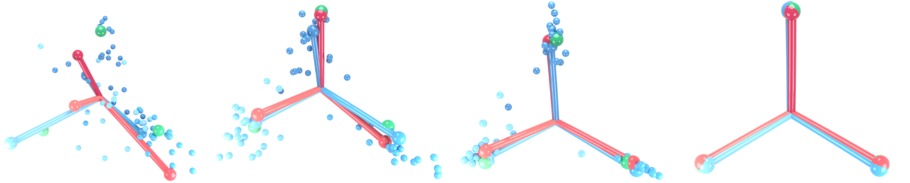

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- **Simplex** is the simplest polytope (object with flat sides).
- **Equiangular Tight Frame** is a matrix $M \in \mathbb{R}^{K \times m}$ s.t.

$$|\langle \boldsymbol{m}_j, \boldsymbol{m}_k \rangle| = \alpha \ \exists \alpha \geq 0 \ \forall j, k \text{ s.t. } j \neq k \tag{11}$$

$$MM^T = \sqrt{\frac{C}{C-1}} \left(I_C - \frac{1}{C} \mathbb{1}_{C \times C} \right) \tag{12}$$

Satisfying equiangular and tight respectively.

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$NC2$ – The Simplex ETF (2/2)

We can use this to define $NC2$. Given re-centered class means $\{\boldsymbol{\mu}_k - \boldsymbol{\mu}_G\}_{k \in [K]}$, they are **equidistant** if:

$$\|\boldsymbol{\mu}_k - \boldsymbol{\mu}_G\|_2 = \|\boldsymbol{\mu}_{k'} - \boldsymbol{\mu}_G\|_2 \ \forall k, k' \in [K] \tag{13}$$

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We then normalize each feature vector to create our simplex ETF:

$$M = \text{Concat}\left(\left\{\frac{\boldsymbol{\mu}_k - \boldsymbol{\mu}_G}{\|\boldsymbol{\mu}_k - \boldsymbol{\mu}_G\|_2} \in \mathbb{R}^m\right\}^{[K]}\right) \in \mathbb{R}^{K\times m} \tag{14}$$

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M is now compared to it's distance from the simplex ETF:

$$NC2 := \left\| \underbrace{\frac{MM^T}{\|MM^T\|_F}}_{\text{feature vector as a simplex}} - \underbrace{\frac{1}{\sqrt{K-1}}\left(I_K - \frac{\mathbb{1}_{K\times K}}{K}\right)}_{\text{canonical simplex}} \right\|_F \tag{15}$$

Setting up our second metric.

$NC3$ – Self-Dual Alignment

The final layer's weights $W \in \mathbb{R}^{K \times m}$ align with simplex ETF of M:

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We can use this to setup the third metric:

$$NC3 := \left\| \underbrace{\frac{AM^T}{\|AM^T\|_F}}_{\equiv \text{ cosine similiarity}} - \underbrace{\frac{1}{\sqrt{K-1}}\left(I_K - \frac{\mathbb{1}_{K\times K}}{K}\right)}_{\text{canonical simplex}} \right\|_F \tag{17}$$

$NC4$ – Secretly k-NN

Finally, we observe that for x_{n+1}, the classification result $\equiv$ k-NN rule:

$$\arg\max \hat{y}_{n+1} = \operatorname*{arg\,min}_{k \in [K]} \|f(x_{n+1}) - \boldsymbol{\mu}_k\|_2 \tag{18}$$

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$$NC4 : \frac{1}{Kn} \sum_{k=1}^{K} \sum_{i=1}^{n} \mathbb{1} \left[\arg\max \hat{y}_i \neq \arg\min_{k \in [K]} \|f(x_i) - \boldsymbol{\mu}_k\|_2 \right] \tag{19}$$

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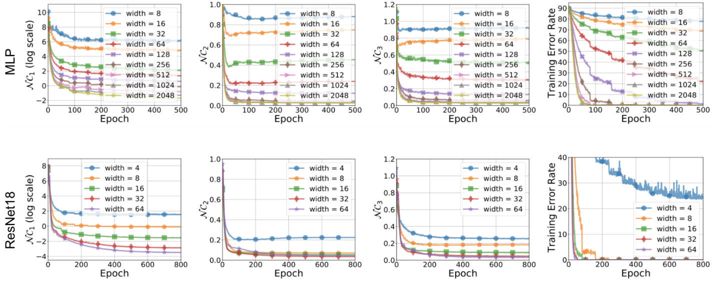
If each of the 4 previous metrics $\to 0$, the network is considered **collapsed**.

Do We Even Want This? – Data Independence

Here's what the metric convergence plots look like, with *random labels*.



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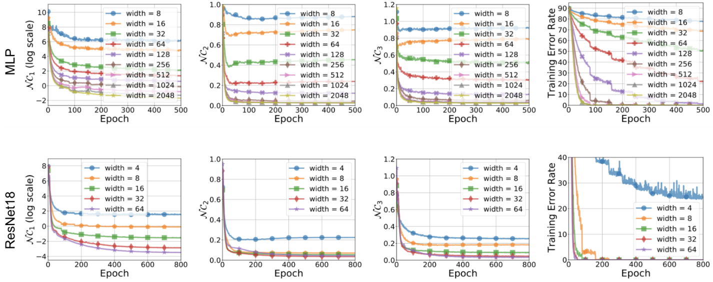

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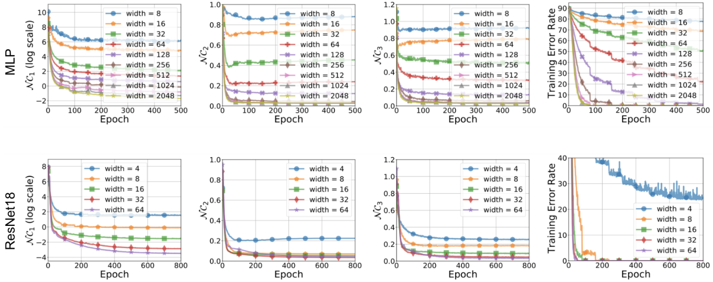

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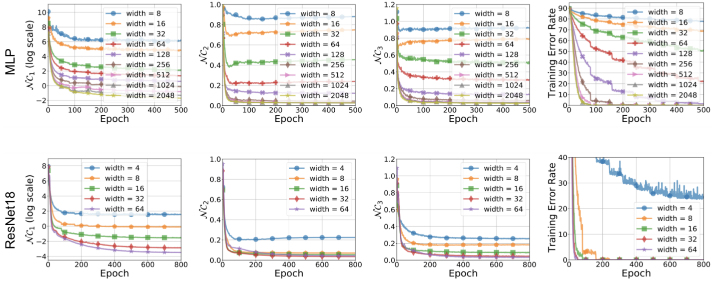

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2. **Forced ETF**: The final layer can be a fixed as a simplex!

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Given dataset $X \in \mathbb{R}^{d_0 \times N} \sim \mathcal{D}^n$, $f : \mathbb{R}^{d_0 \times 1} \to \mathbb{R}^{K \times 1}$, we define AGOP:

$$\mathrm{AGOP}(f, X) := \underbrace{\frac{1}{N} \sum_{c=1}^{K} \sum_{i=1}^{N}}_{\text{average}} \underbrace{\underbrace{\frac{\partial f(x_{ci})}{\partial x_{ci}}}_{\text{gradient}} \frac{\partial f(x_{ci})}{\partial x_{ci}}^{T}}_{\text{outer product}} \tag{20}$$

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Why is this useful?

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Why is this useful? $\mathrm{AGOP}(\hat{f}, X) \approx \mathrm{EGOP}(f^*, \mathcal{D})$:

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EGOP contains useful information like low-rank structure, that can improves predictions.

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Bonus: This makes AGOP backpropogation-free.

Features Identified by AGOP

So, what *exactly* does AGOP find?

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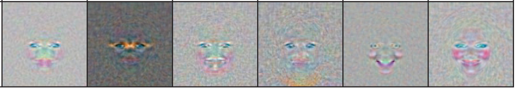
So, what *exactly* does AGOP find? **A lot**.

A Features captured by AGOP of Laplace kernel trained on CelebA prediction tasks

Task	Lipstick	Glasses	5 o'clock shadow	Necktie	Smiling	Rosy Cheeks
AGOP of Laplace Kernel (Top Eigenvector)						

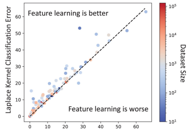
B

	Classification Tasks (Test Accuracy)							Regression Tasks (Test R^2)	
	CelebA Lipstick	CelebA Glasses	CelebA 5 o'clock shadow	CelebA Necktie	CelebA Smiling	CelebA Rosy Cheeks	SVHN	Low Rank Polynomial (Vyas et al. 2022)	Low Rank Polynomial (Damian et al. 2022)
Laplace Kernel + AGOP	**91.62%**	**94.06%**	**88.18%**	**90.39%**	**91.24%**	**88.72%**	**83.25%**	**0.997**	**0.941**
Laplace Kernel	90.89%	90.19%	84.90%	88.92%	90.00%	86.52%	74.83%	0.495	0.481

C Performance across 121 classification tasks from Fernández-Delgado et al. 2014

Classifier	Avg. Test Accuracy
Laplace Kernel + AGOP	**85.39%**
Laplace Kernel	83.76%

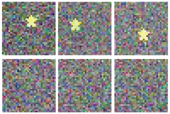
Laplace Kernel vs. Laplace Kernel + AGOP



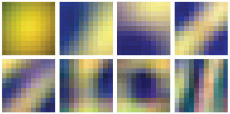
D Data Samples

Class 1

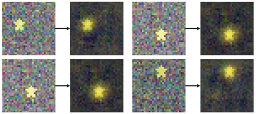
Class 0



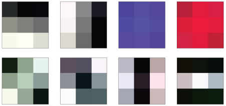
E Top 8 Eigenvectors of CNTK AGOP



F Transforming data samples with CNTK AGOP

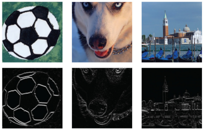


G Eigenvectors of CNTK AGOP (SVHN)



H ImageNet Images

+CNTK AGOP



I Performance Comparison

Dataset	CNTK Test Acc. (%)	CNTK +AGOP Test Acc. (%)
Stars in Noise	80.20	**99.70**
MNIST in Noise	72.55	**79.03**
SVHN	81.38	**85.02**
CIFAR-10	67.74	**67.97**
CIFAR-100	**37.64**	**37.64**
GTSRB	91.76	**93.02**
EMNIST	86.01	**86.73**

Outline

1. Background & Intuition
2. Deep Neural Collapse (DNC)
3. Average Gradient Outer Product (AGOP)
4. AGOP As a Mechanism for DNC

AGOP As a Mechanism for DNC (1/2)

Observation: *within*-class variability collapse occurs predominantly through multiplication by right singular-structure of weights (NFMs).

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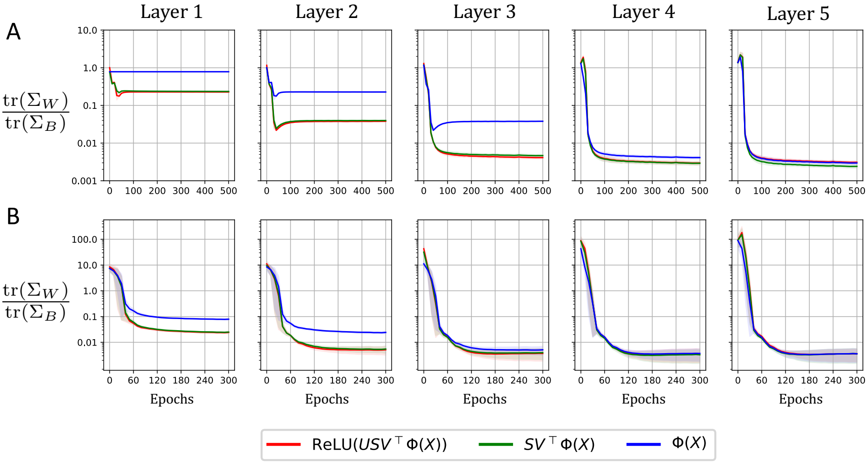
We see that computing $NC1(S_l {V_l}^T) \equiv NC1(W_l)$:

$$\begin{aligned} &\frac{1}{K} \operatorname{Tr}\left(\operatorname{Cov}_W(W_l) \operatorname{Cov}_B^{\dagger}(W_l)\right) \\ \equiv\ &\frac{1}{K} \operatorname{Tr}\left(\operatorname{Cov}_W(U_l S_l {V_l}^T U_l^T) \operatorname{Cov}_B^{\dagger}(U_l S_l {V_l}^T U_l^T)\right) \\ \equiv\ &\frac{1}{K} \operatorname{Tr}\left(\operatorname{Cov}_W(S_l {V_l}^T) \operatorname{Cov}_B^{\dagger}(S_l {V_l}^T)\right) \end{aligned} \tag{25}$$

AGOP As a Mechanism for DNC (2/2)

We can identify the collapse occurs by the right-singular structure:



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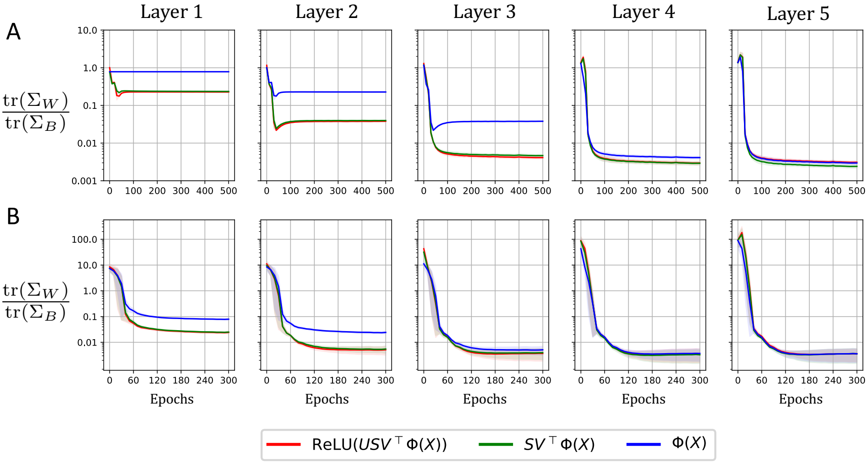

Additionally, $NC2$ (Simplex ETF) was observed, but only in the last layer.

Thank you!

Have an awesome rest of your day!

Slides: `https://cs.purdue.edu/homes/jsetpal/slides/dnc_by_agop.pdf`