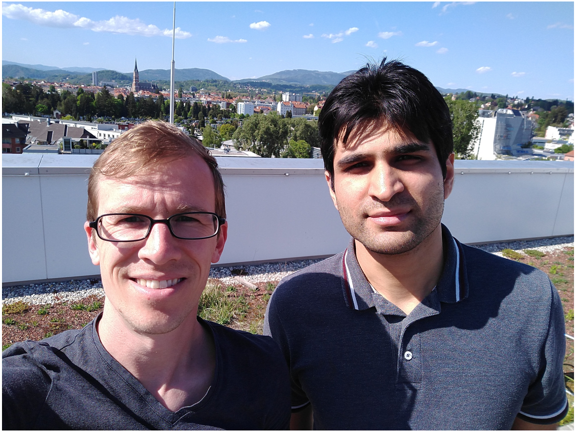
AUSTRIA'S LEADING RESEARCH CENTER
FOR DATA-DRIVEN BUSINESS AND BIG DATA ANALYTICS

Understanding Neural Networks with Information Theory

Bernhard C. Geiger
Joint Work with Rana Ali Amjad and Kairen Liu

Who are we?



FWF
Der Wissenschaftsfonds.

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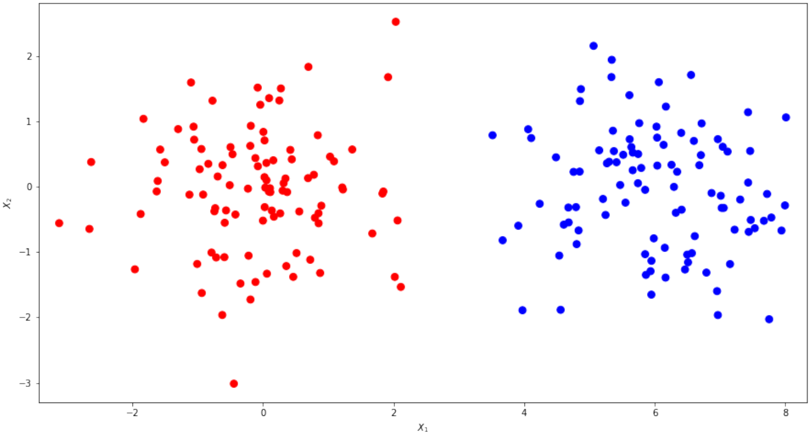
Overview

Binary Classification Task



Logistic Regression

- learn *class label* (red, blue) from *features* X_1 and X_2

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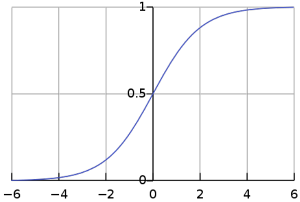
- logistic regression is a linear model
- logistic regression yields class probabilities:

  If $X_1 = x$ and $X_2 = x'$, then the probability that Y is red is p.

Logistic Regression (cont'd)

$$\mathbb{P}[Y = \text{red}] = \sigma(w_1 \cdot X_1 + w_2 \cdot X_2 + w_0)$$



Public Domain by Qef.

- $w_1 \cdot X_1 + w_2 \cdot X_2 + w_0 < 0$, then Y is more likely to be blue
- w_1, w_2, and w_0 define *decision boundary*
- **Task:** Learn w_1, w_2, and w_0 from data
- (typically: cross-entropy loss + L_2 regularization)

Logistic Regression (cont'd)

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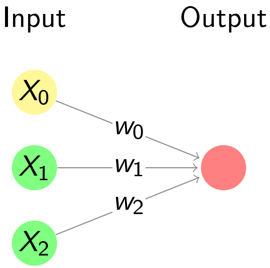
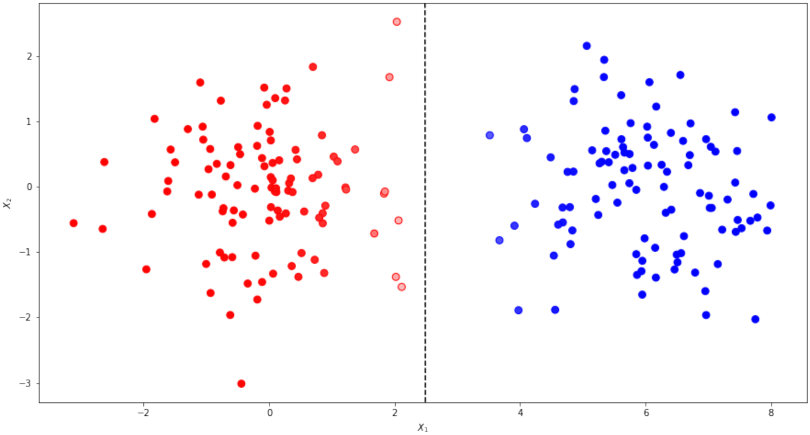
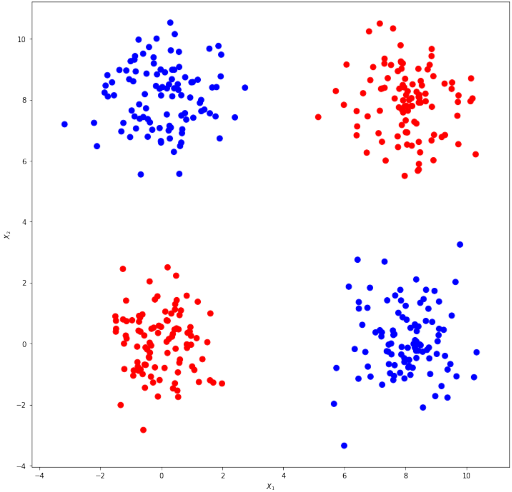


Binary Classification using Logistic Regression



Binary Classification (slightly more complicated)



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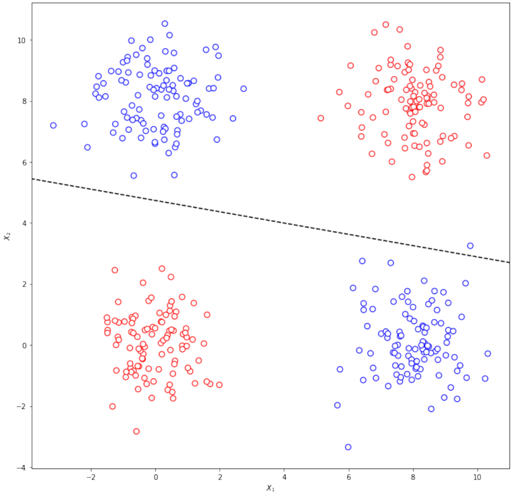

Logistic Regression Fails. . .

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Idea: Stack multiple linear regression models on top of each other!

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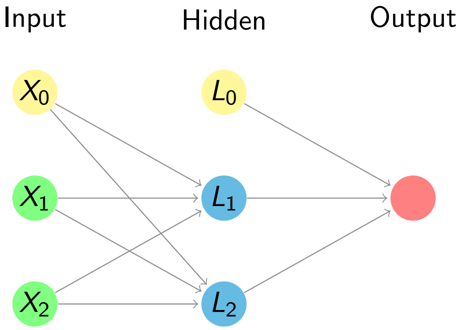
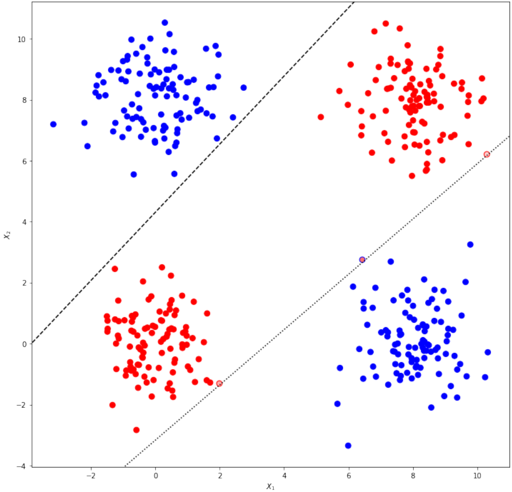


Binary Classification with a Neural Network



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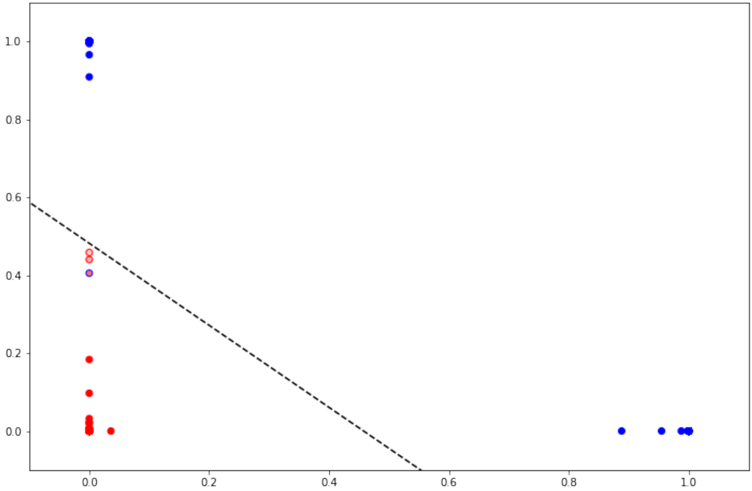
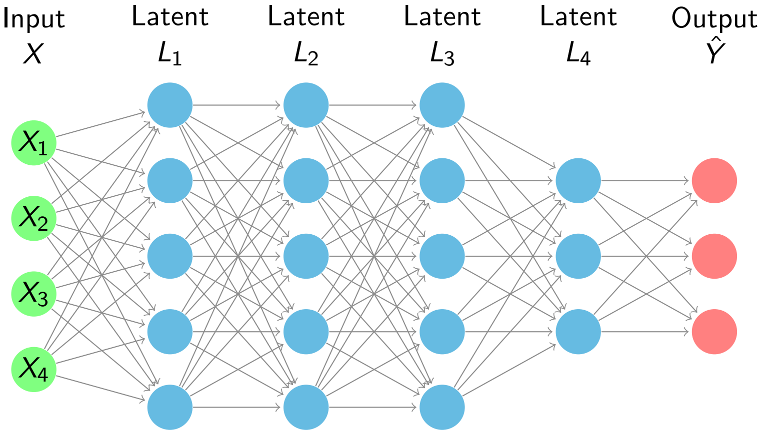


Binary Classification with Neural Networks



Binary Classification with Neural Networks

- Still easy to understand with two input features, hidden layers of width two (2D scatter plot)
- What happens for higher-dimensional input?
  - MNIST: input has 784 dimensions
  - CIFAR-10: input has 3×1024 dimensions
  - ...
- What happens for wider layers?
  - e.g., a $100-100$ MLP trained on MNIST?
  - ...

Two Approaches to Understand NNs

- Explainable/Interpretable AI:
  - What input features led to the decision?[1]
  - What training data was most influential for this decision?[2]
  - Simplified decision boundaries[3], extract decision procedure, etc.
  - ...
- How do NNs work internally?
  - Behavior during training
  - Why do NNs generalize so well?[4]
  - Importance of individual ("cat") neurons
  - ...

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[1] Montavon, Samek, and Müller, "Methods for interpreting and understanding deep neural networks", 2018

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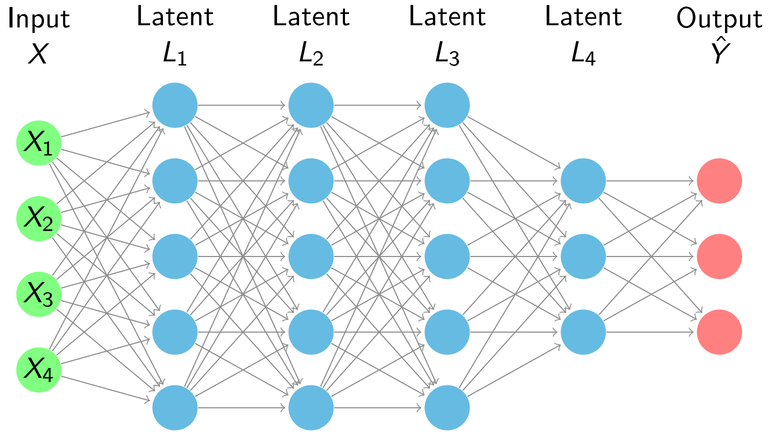
Prerequisite: Mutual Information

$$I(U;V)$$

- is defined for general random variables
- measures statistical dependence between U and V
- generalizes (linear) correlation
- is zero if and only if U and V are independent
- is invariant under invertible maps
- (can be difficult to estimate)

Information Plane Analyses



Information Plane Analyses (cont'd)

Intermediate representation L (NN layer) should

P1 contain sufficient info for classification

- e.g., L should suffice to determine whether X is a cat or a dog

P2 ...but not more info than necessary (compression)

- e.g., L should not contain information about the color of the fur, length of ears, etc.

[5] Alemi et al., "Deep Variational Information Bottleneck", 2017

[6] Kolchinsky, Tracey, and Wolpert, "Nonlinear Information Bottleneck", 2019

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Idea has been successfully applied in NN training[5,6,7]

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[6] Kolchinsky, Tracey, and Wolpert, "Nonlinear Information Bottleneck", 2019

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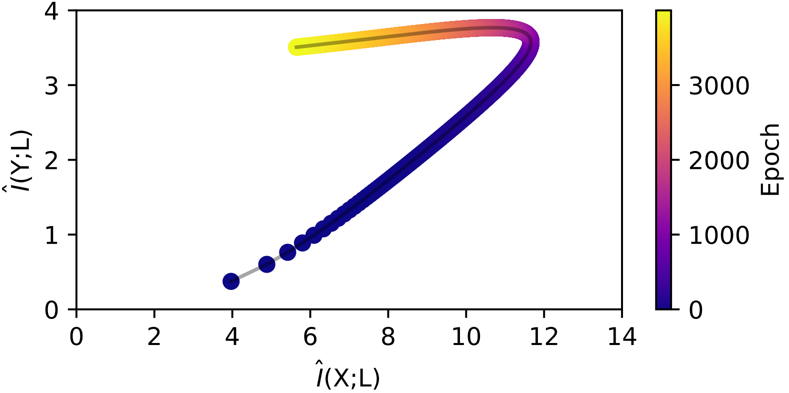
Information Plane Analyses (cont'd)

Estimate how $I(X;L)$ and $I(Y;L)$ evolve during NN training[8]:



[8]Shwartz-Ziv and Tishby, *Opening the Black Box of Deep Neural Networks via Information*, 2017

Information Plane Analyses (cont'd)

Hot Topic, but many open questions:

- requires estimating mutual information, which is problematic[9]
- connection to generalization not fully clear, e.g.[10]
- information plane appears to show geometric picture (clustering)[11]
- current results in the literature are inconsistent (is there a compression phase?, etc.)[12]
- ongoing debate

[9] Amjad and Geiger, "Learning Representations for Neural Network-Based Classification Using the Information Bottleneck Principle", 2020

[10] Saxe et al., "On the Information Bottleneck Theory of Deep Learning", 2018

[11] Goldfeld et al., "Estimating Information Flow in Deep Neural Networks", 2019

[12] Geiger, *On Information Plane Analyses of Neural Network Classifiers – A Review*, 2020

Bounds on Generalization Gap

i.e., difference between expected and estimated loss as a function of size m of dataset $\mathcal{D} = \{D_1, \dots, D_m\}$

[13] Vera, Piantanida, and Vega, “The Role of the Information Bottleneck in Representation Learning”, 2018

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- $\propto \sqrt{I(X;L)}\frac{\log m}{\sqrt{m}}$, see[13]
- $\left(2^{I(X;L)} + \log(2/\delta)\right)/(2m)$ with probability $1-\delta$, see[14]

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- extensions to SGD-type training[17]

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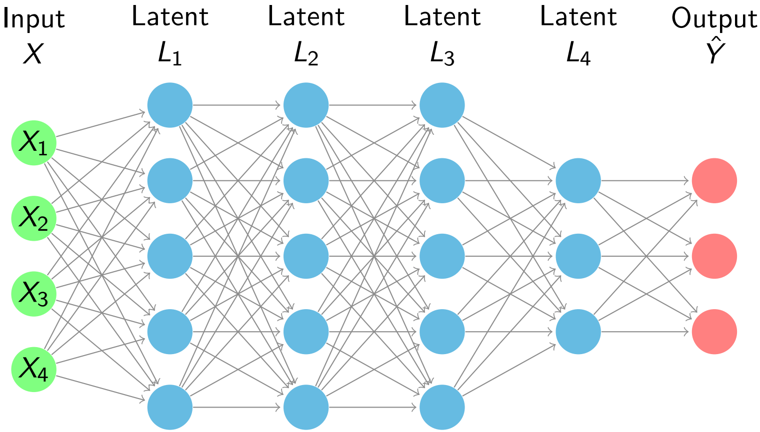
What about Individual Neurons?



What about Individual Neurons? (cont'd)

How important is the ℓ-th neuron in the i-th layer?

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How important is the ℓ-th neuron in the i-th layer?

- compute mutual information $I(Y; L_{i,\ell})$
- much easier to estimate than $I(Y; L_i)$ (whole layer) or $I(X; L_i)$ (X is high-dimensional/continuously distributed)
- **Hypothesis**: Large values indicate that the ℓ-th neuron in the i-th layer is important for the task

Information-Ordered Cumulative Ablation[19]

- **Ablation**: Turning off individual neurons, i.e., set $L_{i,\ell} = 0$

[19] Liu, Amjad, and Geiger, *Understanding Individual Neuron Importance Using Information Theory*, 2018

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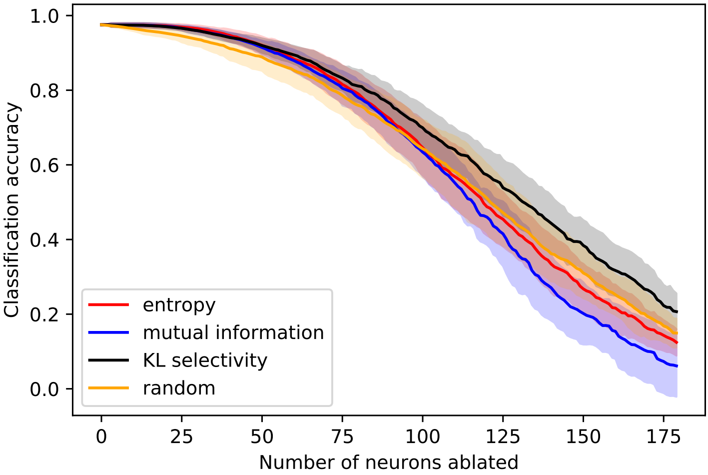
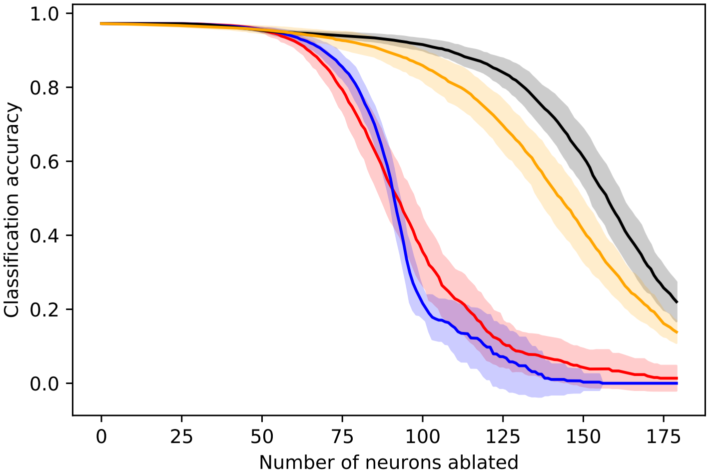
- **Cumulative** Ablation: Turn off more and more neurons and see how, e.g., classification accuracy is affected
- **Information-Ordering**: Turn off the k neurons with lowest (highest) mutual information and compare with turning off neurons randomly

[19] Liu, Amjad, and Geiger, *Understanding Individual Neuron Importance Using Information Theory*, 2018

MNIST $100 - 100$, L_2 regularization



MNIST $100 - 100$, Dropout



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How important is the ℓ-th neuron in the i-th layer?

- it seems as if neurons with *high* mutual information are *not useful/hurting* classification performance
- reproduces results from[20]

[20] Morcos et al., *On the importance of single directions for generalization*, 2018

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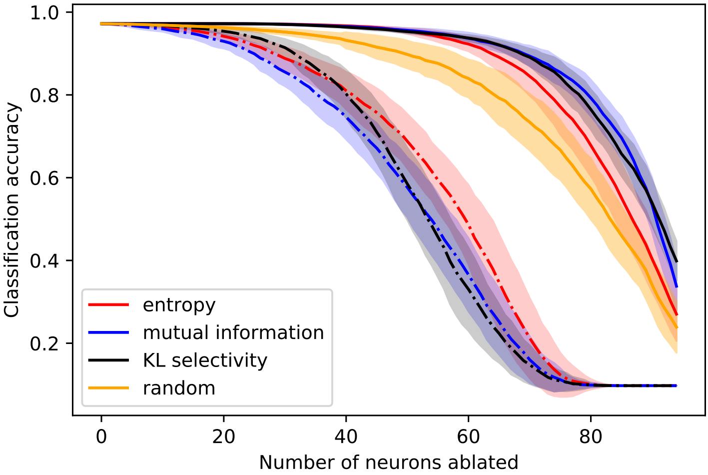
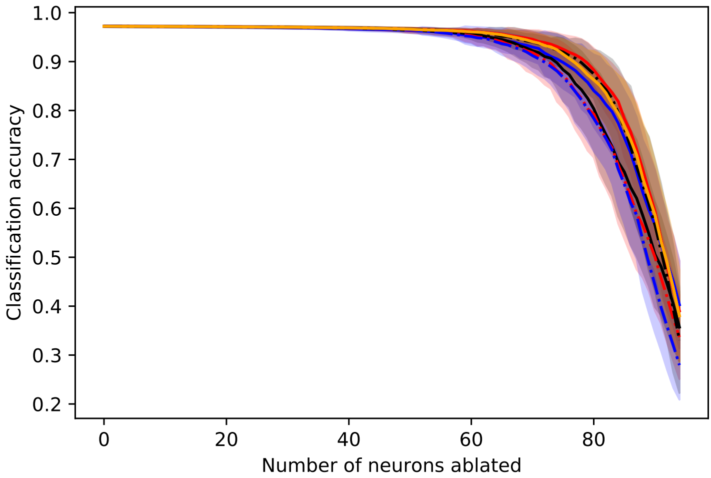
Let's take a closer look!

[20] Morcos et al., *On the importance of single directions for generalization*, 2018

MNIST $100 - 100$, Dropout, Layer 1



MNIST $100 - 100$, Dropout, Layer 2



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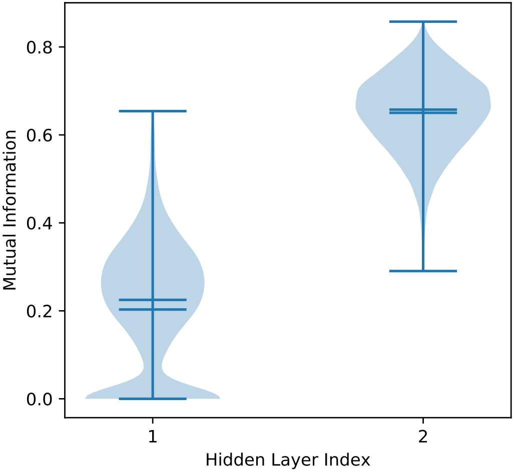


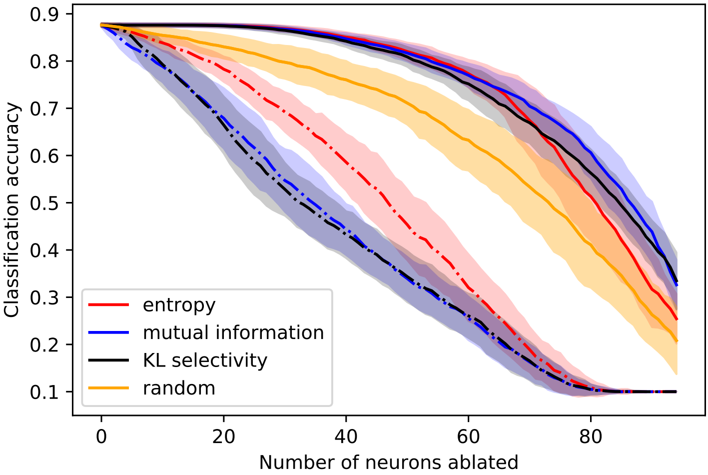
What about Individual Neurons? (cont'd)

How important is the ℓ-th neuron in the i-th layer?

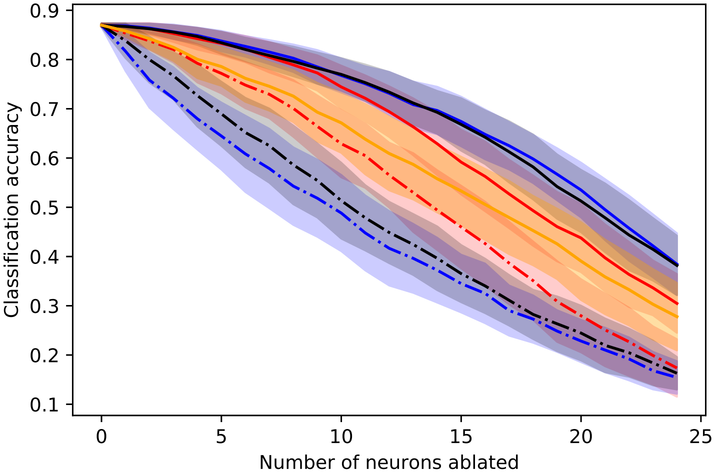
- it seems as if neurons with *high* mutual information are *not useful/hurting* classification performance[21]
- **BUT:** neurons with *high* mutual information are *useful* within a given layer
- layers have different distribution of mutual information values
- $\Rightarrow$ Simpson's paradox

[21] Morcos et al., *On the importance of single directions for generalization*, 2018

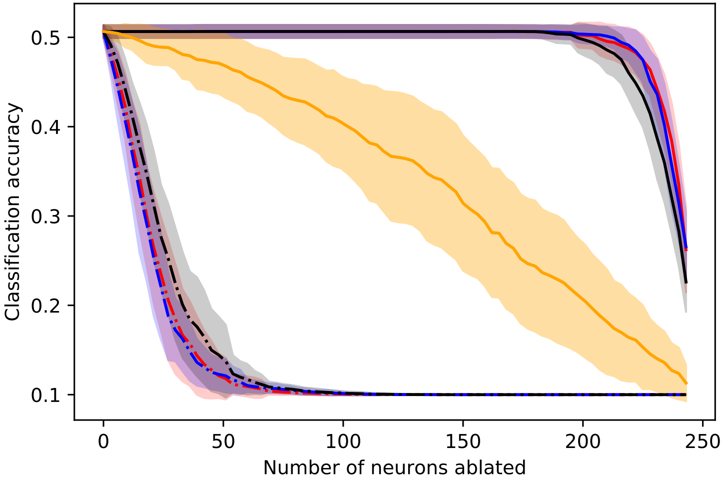
FashionMNIST $100 - 100$, L_2, Layer 1



FashionMNIST $30-30$, L_2, Layer 1



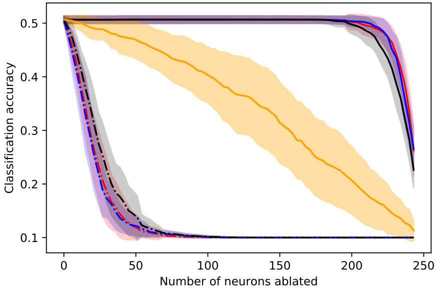
CIFAR-10 $250 - 500 - 250 - 500$, L_2, **Layer 3**



Information-Ordered Cumulative Ablation

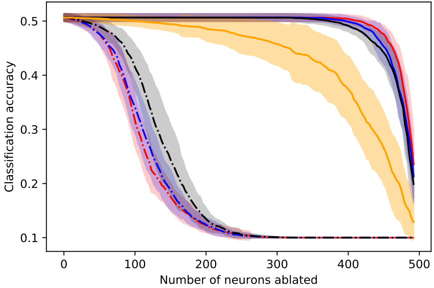
What else can we learn?

CIFAR-10 $250 - 500 - 250 - 500$, L_2, Layer 2



- 40 neurons with highest mutual information suffice
- removing 60 neurons with highest mutual information destroy performance
- $\approx$ 200 neurons are **inactive**

CIFAR-10 $250-500-250-500$, L_2, Layer 4



- 100 neurons with highest mutual information suffice
- removing 250 neurons with highest mutual information destroy performance
- $\approx$ 250 neurons are inactive
- $\approx$ 50-150 neurons are **redundant**

More Insights?

- beyond mutual information
- beyond ReLU activation functions
- beyond L_2 regularization
- effects of quantization
- ...

arXiv:1804.06679v3 [cs.LG]

Conclusion

NNs are difficult to understand, but

information theory is powerful:

- Bounds on the generalization error
- Investigating learning behavior
- Interplay between learning and geometric compression
- Importance of individual neurons via ordered cumulative ablation
  - neurons with large mutual information (**within a layer**) are important for classification
  - mutual information values differ between layers
  - cumulative ablation reveals inactive, redundant, and synergistic neurons

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Thanks for your attention!