DNN: Final Presentation

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Outline

1. Deep Learning/Neural Networks Fundamentals
2. Universal Approximation Results with Neural Nets
3. Piecewise Linear Networks
4. On Expressivity vs. Learnability
Source: Jay Alammar, How GPT3 Works  
Source: European Go Federation
General idea of a Feedforward network

- $z^{(l)} = W^{(l)} a^{(l-1)} + b^{(l)}$
- $a^{(l)} = ReLU(z^{(l)})$
DL Fundamentals

- Activation function
- Cost function
- Minimize cost function through backpropogation
  - Gradient Descent
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- Cost function
- Minimize cost function through backpropogation
  - Gradient Descent
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    \frac{\partial C_0}{\partial w^{(l)}} = \frac{\partial C_0}{\partial a^{(l)}} \cdot \frac{\partial a^{(l)}}{\partial z^{(l)}} \cdot \frac{\partial z^{(l)}}{\partial w^{(l)}}
    \]
    \[
    \frac{\partial C_0}{\partial b^{(l)}} = \frac{\partial C_0}{\partial a^{(l)}} \cdot \frac{\partial a^{(l)}}{\partial z^{(l)}} \cdot \frac{\partial z^{(l)}}{\partial b^{(l)}}
    \]
  - Stochastic Gradient Descent
Motivation: computational issues with feedforward networks

For image recognition problems, on which CNNs are largely applied:

**Figure**: Source: missinglink.ai
Convolutional Networks

- Motivation: computational issues with feedforward networks

![Diagram of Convolutional Networks](source: missinglink.ai)

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![Convolutional Networks Diagram](missinglink.ai)

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  - Finishes with fully connected layers
SVD classification model

- Initial model from linear algebraic techniques as a baseline
- MNIST dataset: handwritten digit classification for digits 0 to 9
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- Classification objective: $\arg\min_{c=0,1,...,9} ||x - U_c (U_c^T x)||_2$

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Results from SVD Classification Algorithm

Accuracy based on ratio of train to test images

Accuracy

Percent of Train Images
Results from SVD Classification Algorithm

Accuracy over rank

Accuracy over number of test images

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Neural networks for MNIST

- Feedforward neural networks: different architectures
  - Best performance, 1 hidden layer, with 128 units over 12 EPOCHS, 97.8% accuracy
- Convolutional neural network: two convolutional layers (convolution + max pooling) and three fully connected layers (one of them being output)
- CNN was the best model, achieving 98.35 percent accuracy after 3 epochs (nearing 99 percent accuracy after roughly 10 epochs)
Accuracy over the number of Trainable Parameters

Test Accuracy vs. Trainable Parameters
Motivating questions in NN approximation theory

- What class of functions can be approximated/expressed by a standard feedforward neural network of depth $k$?

- How do we think about the shift to rectified activations from sigmoidal functions, which perform well in practice?

- What subset of all functions that are provably approximable by neural networks are actually learnable in practice?
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- What subset of all functions that are provably approximable by neural networks are actually learnable in practice?
Definition: let $\epsilon$-approximation of a function $f(x)$ by another function $F(x)$ with a shared domain $X$ denote that for arbitrary $\epsilon > 0$,

$$\sup_{x \in X} |f(x) - F(x)| < \epsilon$$
Classical Results: Shallow Neural Networks as Universal Approximators

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- **Cybenko (1989):** Shallow neural networks (one hidden layer) with continuous sigmoidal activations are universal approximators, i.e. capable of $\epsilon$-approximating any continuous function defined on the unit hypercube.
Loosening of restrictions on activation function that still yield notion of $\epsilon$-approximation:

- Hornik (1990): extension to any continuous and bounded activation functions, support extends to more than just the unit hypercube
- Leshno (1993): extension to nonpolynomial activation functions
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  - Leshno (1993): extension to nonpolynomial activation functions
- By extension, deeper neural networks of depth $k$ also enjoy the same theoretical guarantees.
Let $k$ denote the depth of a network. The following results are due to Rolnick and Tegmark (2018).
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- Let $f(x)$ be a multivariate polynomial function of finite degree $d$, and $N(x)$ be a network with nonlinear activation having nonzero Taylor coefficients up to degree $d$. Then there exists a number of neurons $m_k(f)$ that can $\varepsilon$-approximate $f(x)$, where $m_k$ is independent of $\varepsilon$. 

$$m_1(f) = \sum_{i=1}^{n} (r_i + 1)^{m_k(f)} \leq \sum_{i=1}^{n} 7^d \log_2 (r_i) e + 4$$
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- Let $f(x) = x_1^{r_1}x_2^{r_2} \ldots x_n^{r_n}$ be a monomial function of finite terms, network $N(x)$ has nonlinear activation having nonzero Taylor coefficients up to degree $2d$, and $m_k(f)$ defined as above. Then $m_1(f)$ is exponential, but linear in a log-depth network.

$$m_1(f) = \prod_{i=1}^{n}(r_i + 1)$$

$$m(f) \leq \sum_{i=1}^{n}7[\log_2(r_i)] + 4$$
ReLU Networks as Partitioning Input Space

A ReLU activation function - used between affine transformations to introduce nonlinearities in the learned function.
Known theorems:

ReLU networks are bijective to the appropriate class of piecewise linear functions (up to isomorphism of network).

For one hidden layer neural networks (p-dimensional input, q-dimensional hidden layer): can combinatorially show an upper bound on the number of piecewise linear regions:

\[ r(q, p) = \prod_{i=0}^{p} \binom{q}{i} \]

Montufar et al. (2014): The maximal number of linear regions of the functions computed by a NN with \( n_0 \) input units and \( L \) hidden layers, with \( n_i \) rectifiers at the \( i \)th layer, is lower bounded by

\[
\left( \sum_{i=1}^{L} n_i \right) \left( \sum_{j=0}^{n_0} \binom{n_0}{j} \right)
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Visualizing the hyperplanes to depth $k$
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- First layer: hyperplanes through input space
Visualizing the hyperplanes to depth $k$

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- All proceeding layers: "bent hyperplanes" that bend at the established bent hyperplanes of previous layers

Figure 1 of Raghu et al. (2017)
The following is from the work of Hanin and Rolnick (2019ab), and concerns ReLU networks. The results are stated informally. For any line segment through input space, the average number of regions intersected is linear, and not exponential, in the number of neurons. Both the number of regions and the distance to the nearest region boundary stay roughly constant during training.
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- For any line segment through input space, the average number of regions intersected is linear, and not exponential, in the number of neurons.

- Both the number of regions and the distance to the nearest region boundary stay roughly constant during training.
Expressibility vs. Learnability: Graphs

(a) Over Epochs

(b) Over Test Accuracy

Figure: Normalization by squared number of neurons
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Figure: Normalization by squared number of neurons

- Across different networks, number of piecewise linear regions is \( O(n^2) \), and this doesn’t change with greater depth.
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Upshot: empirical success of depth on certain problems is not because deep nets learn a complex function inaccessible to shallow networks.
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- Are networks that learn an exponential number of linear regions "usable", or are they purely a theoretical guarantee?
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- Are networks that learn an exponential number of linear regions “usable”, or are they purely a theoretical guarantee?
- How can we adjust the traditional deep learning pipeline to allow learning of piecewise linear functions in the exponential regime?
Sawtooth functions/triangular wave functions

Type of function that achieves an exponential number of regions in number of nodes/depth.

Figure: Sawtooth functions
To achieve a feedforward neural network that represents a sawtooth function with $2^n$ affine regions in $2n$ hidden layers:
Sawtooth functions as feedforward neural networks

To achieve a feedforward neural network that represents a sawtooth function with \(2^n\) affine regions in \(2n\) hidden layers:

- **Mirror map**, defined on \([0, 1]\):
  \[
  f(x) = \begin{cases} 
  2x & \text{when } 0 \leq x \leq \frac{1}{2} \\
  2(1 - x) & \text{when } \frac{1}{2} \leq x \leq 1 
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- **As a two-layer neural network**:

  $$f(x) = \text{ReLU}(2\text{ReLU}(x) - 4\text{ReLU}(x - \frac{1}{2}))$$
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- Composing mirror map with itself $n$ times will yield a sawtooth function with $2^n$ equally spaced affine components on $[0, 1]$. 
Questions regarding sawtooth functions

- How robust are sawtooth functions to multiplicative weight perturbation, of the form $w(1 + \epsilon)$? (The perturbations are zero-mean Gaussians, and experiments changed the variance.)
- Can randomly initialized or perturbed networks re-learn the sawtooth function?
Perturbing the parameters

(a) All weights and biases

(b) All weights

(c) All biases

(d) First layer only
Re-learning sawtooth networks from different initializations

(a) Mean squared error

(b) Number of linear regions
Re-learning sawtooth networks from different initializations

(c) Variance = 0.01

(d) Variance = 0.05

(e) Variance = 0.1

(f) Variance = 0.5
"Sawtooth networks" fall apart with mild variance on the weights.

Even when starting from perturbed versions of the original function, the original sawtooth network is not retained, implying that the set of parameters yielding exponential nets in the loss landscape is localized and challenging to learn.
How to adjust the DL framework to encourage feedforward model to learn functions currently in $F_{\text{express}} \setminus F_{\text{learn}}$?

First attempt: adding terms to the objective function to encourage network to learn more complex functions (“anti-regularization”).

For 2D input, two hidden-layer ReLU nets, can think about encouraging all hyperplanes/bent hyperplanes to intersect:

Can think of an inactive ReLU activation function as replacing appropriate column of outer weight vector by zeros:

$$w_2 \text{ReLU}(W_1 x + b_1) + b_2 = w_0 \text{ReLU}(W_1 x + b_1) + b_2$$

For a first-layer activation pattern, this yields a square matrix equation and a collection of inequalities, and one can add “perceptron-like” error terms to the objective function to encourage regions to intersect.
Learning functions in the exponential regime (sketch)

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Conclusion

- Thank you for listening!