The Convergence Rate of Neural Networks for Learned Functions of Different Frequencies

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What makes DNs so successful?

Common deep networks seem to defy basic machine learning principles:

How come over-parameterized networks do not overfit?

- Resnet has 60M learnable parameters (VGG has 140M)
- But ImageNet includes only 1.2M training images
Random relabeling

MNIST images

Labels

(Zhang et al., ICLR 2017)
Understanding deep learning requires rethinking generalization

Loss on training (CIFAR10)
Zhang et al., ICLR 2017
Partial random relabeling

MNIST images

Labels
Partial relabeling: training
Partial relabeling: test against true labels
Frequency bias
Frequency bias

Epoch = 50
Frequency bias

Epoch = 50
Epoch = 500
Epoch = 22452
Frequency bias

Can we explain this frequency bias?

How long should it take to learn a single frequency?
Two-layer network
Two-layer network

\[ f(x,w) = \frac{1}{\sqrt{m}} \sum_{r=1}^{m} a_r \sigma(w_r^T x), \quad \sigma(x) = \max(x, 0) \]

MSE Loss: \[ L(w) = \frac{1}{2} \sum_{i=1}^{n} (y_i - f(x_i, w))^2 \]
Network predictions as a “linear” system

Write predictions for training data as a linear operation:

\[
\begin{align*}
    u(t) &= \begin{pmatrix} u_1 = f(x_1, w) \\ \vdots \\ u_n = f(x_n, w) \end{pmatrix} = Z^T w
\end{align*}
\]

where we define \( Z = Z(t) \) as

\[
Z^T = \frac{1}{\sqrt{m}} \begin{pmatrix} a_1 \mathbb{I}_{11} x_1 & \cdots & a_m \mathbb{I}_{m1} x_1 \\ \vdots & \ddots & \vdots \\ a_1 \mathbb{I}_{1n} x_n & \cdots & a_m \mathbb{I}_{mn} x_n \end{pmatrix}
\]

Back-prop minimizes

\[
\frac{1}{2} \sum_{i=1}^{n} (y_i - Z^T(t)w)^2
\]

Eg., Du et al., ICLR 2019
GD for linear systems

Suppose we want to minimize \( \frac{1}{2} \| y - Zw \|^2 \) using gradient descent with \( w^{(0)} = 0 \)

\[
\begin{align*}
  u^{(1)} &= -\eta Z^T Z y \\
  u^{(2)} &= -2\eta Z^T Z y - \eta^2 (Z^T Z)^2 y \\
  u^{(3)} &= -3\eta Z^T Z y - 3\eta^2 (Z^T Z)^2 y - \eta^3 (Z^T Z)^3 y
\end{align*}
\]

...
The kernel

Define

\[ H(t) = Z^T Z \]

Du et al. 2018’s observation:
when the network is massively over-parameterized
\( H(t) \sim H^\infty \), where

\[ H^\infty_{ij} = \mathbb{E}_{w \sim \mathcal{N}(0, \kappa^2)} H_{ij} = \frac{1}{2\pi} x_i^T x_j (\pi - \cos^{-1}(x_i^T x_j)) \]
What are the eigenvectors?

If the training data is distributed uniformly on the hyper-sphere then $H^\infty$ represents a convolution

$$K \ast f(u) = \int_{S^d} K(u^T v)f(v)dv$$

Therefore, eigenvectors are spherical harmonics

Recall that

$$H^\infty_{ij} = K(x_i, x_j) = \frac{1}{2\pi} x_i^T x_j(\pi - \cos^{-1}(x_i^T x_j))$$

(See also Xie et al., 2017)
Eigenvalues (d=1)

Eigenvectors are the Fourier series

\[ a_k = \begin{cases} 
\frac{2}{\pi} & k = 0 \\
\frac{\pi}{4} & k = 1 \\
\frac{2(k^2+1)}{\pi(k^2-1)^2} & k \geq 2, \text{even} \\
0 & k \geq 2, \text{odd}
\end{cases} \]

Odd frequencies vanish!!
Fitting to pure frequency

$k=4$

$k=3$
Convergence times

Relying on Arora et al., 2019, the number of iterations required to achieve accuracy $\delta$:

$$t_i > \frac{-\log(\delta + \epsilon)}{\eta \lambda_i} = O\left(\frac{1}{\lambda_i}\right)$$

Even frequencies: $t_i \geq \frac{\pi(k^2 - 1)^2}{2(k^2 + 1)} = O(k^2)$

Odd frequencies: $t_i \rightarrow \infty$
Convergence times
Adding bias

Adding bias rectifies the problem

\[
\overline{H}_{ij}^\infty = \frac{1}{4\pi} (\mathbf{x}_i^T \mathbf{x}_j + 1)(\pi - \cos^{-1}(\mathbf{x}_i^T \mathbf{x}_j))
\]

\[
\bar{a}_k = \begin{cases} 
1/\pi + \pi/4 & k = 0 \\ 
1/\pi + \pi/8 & k = 1 \\ 
\frac{2(k^2 + 1)}{\pi(k^2 - 1)^2} & k \geq 2, \text{ even} \\ 
\frac{1}{\pi k^2} & k \geq 2, \text{ odd}
\end{cases}
\]
Convergence times (with bias)
Convergence
(Resnet-10, 1D data embedded in $\mathcal{R}^{30}$)
Higher dimension

Eigenvectors are spherical harmonics

Eigenvalues can be derived using the Gegenbauer polynomials

With no bias odd frequencies $k \geq 2$ vanish

Convergence time for high frequencies increase exponentially in the dimension
Eigenvalues for higher dim.

\[
\bar{a}_k = \begin{cases} 
    \frac{c}{2} \left( \frac{1}{d_2 d+1} \left( \frac{d}{d} \right) + \frac{2^{d-1}}{d^{d-1}} \right) - \frac{1}{2} \sum q=0 (-1)^q \left( \frac{d-2}{2q+1} \right) & k = 0 \\
    \frac{c}{2} \sum_{q=[k/2]}^{k+d-2} b_q \left( \frac{1}{4q+2} + \frac{1}{4q} \left( 1 - \frac{1}{2^{2q}} \left( \frac{2q}{q} \right) \right) \right) & k = 1 \\
    \frac{c}{2} \sum_{q=[k/2]}^{k+d-2} b_q \left( \frac{-1}{4q-2k+2} + \frac{1}{4q-2k+4} \left( 1 - \frac{1}{2^{2q-k+2}} \left( \frac{2q-k+2}{2} \right) \right) \right) & k \geq 2, \text{ even} \\
    \frac{c}{2} \sum_{q=[k/2]}^{k+d-2} b_q \left( \frac{1}{4q-2k+2} \left( 1 - \frac{1}{2^{2q-k+1}} \left( \frac{2q-k+1}{2} \right) \right) \right) & k \geq 2, \text{ odd} 
\end{cases}
\]

\[
c = \frac{(-1)^k 2\pi^{d/2}}{2^k \Gamma(k+d/2) d} \quad \text{and} \quad b_q = (-1)^q \left( k + \frac{d-2}{2} \right) \left( \frac{2q)!}{k!} \right)
\]
2D, no bias
2D, with bias
2D, deep
Higher dimension

\[ g(d) \]

\[ d \]

\[ 95.8 \]

\[ 50 \]

\[ 30 \]

\[ 3 \]

\[ 2 \]

\[ 50 \]

\[ 100 \]
What will the network learn?
What will the network learn?
What will the network learn?
Conclusion

Deep networks show a frequency bias – low frequencies appear to be learned faster than high frequencies.

Our work determines the rate of learning analytically, as a function of frequency, for over-parameterized, two-layer network.

It further points out that two-layer, bias free networks are non-universal, and cannot represent odd frequencies.