Introductions of Approximation Optimization and Generalization Errors

Shijun Zhang[*]

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In this note, we introduce approximation, optimization, and generalization errors in order to measure the discrepancy between the target function and the final network attained by a numerical training/optimization method.

Let $\phi(\boldsymbol{x};\boldsymbol{\theta})$ denote a function computed by a (fully-connected) network with $\boldsymbol{\theta}$ as the set of parameters. See Figure 1 for an example of a σ-activated network with width 5 and depth 2.

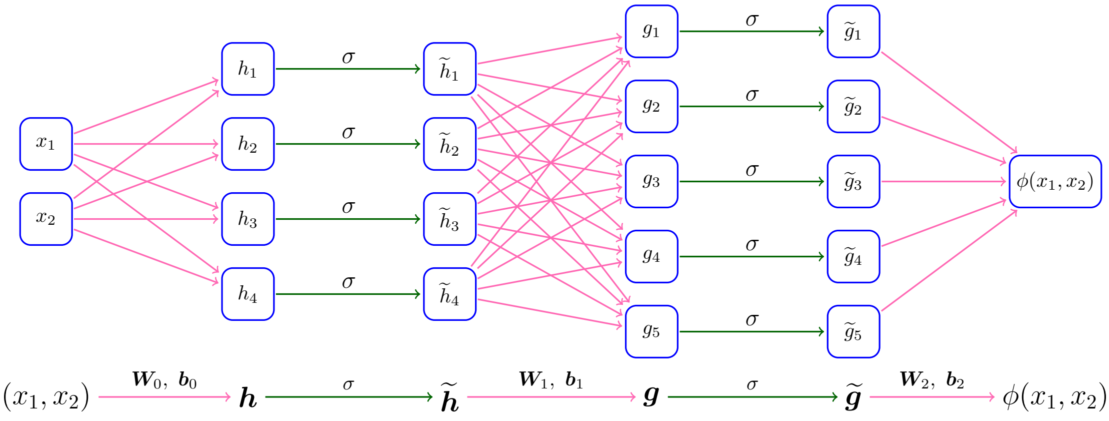

x_1
x_2
h_1
h_2
h_3
h_4
σ
$\widetilde{h}_1$
$\widetilde{h}_2$
$\widetilde{h}_3$
$\widetilde{h}_4$
g_1
g_2
g_3
g_4
g_5
$\widetilde{g}_1$
$\widetilde{g}_2$
$\widetilde{g}_3$
$\widetilde{g}_4$
$\widetilde{g}_5$
$\phi(x_1,x_2)$
$(x_1,x_2) \xrightarrow{\boldsymbol{W}_0,\ \boldsymbol{b}_0} \boldsymbol{h} \xrightarrow{\sigma} \widetilde{\boldsymbol{h}} \xrightarrow{\boldsymbol{W}_1,\ \boldsymbol{b}_1} \boldsymbol{g} \xrightarrow{\sigma} \widetilde{\boldsymbol{g}} \xrightarrow{\boldsymbol{W}_2,\ \boldsymbol{b}_2} \phi(x_1,x_2)$

Figure 1: An example of a σ-activated network with width 5 and depth 2. In this example, $\boldsymbol{\theta}$ is a vector consisting of all parameters in $\boldsymbol{W}_0, \boldsymbol{b}_0, \boldsymbol{W}_1, \boldsymbol{b}_1, \boldsymbol{W}_2, \boldsymbol{b}_2$.

Given a target function f, consider the expected error/risk of $\phi(\boldsymbol{x};\boldsymbol{\theta})$

$$R_{\mathcal{D}}(\boldsymbol{\theta}) \coloneqq \mathbb{E}_{\boldsymbol{x}\sim U(\mathcal{X})}\left[\ell(\phi(\boldsymbol{x};\boldsymbol{\theta}), f(\boldsymbol{x}))\right]$$

with a loss function typically taken as $\ell(y,y') = \frac{1}{2}|y-y'|^2$, where $U(\mathcal{X})$ is an unknown data distribution over $\mathcal{X}$. For example, when $\ell(y,y') = \frac{1}{2}|y-y'|^2$ and U is a uniform distribution over $\mathcal{X} = [0,1]^d$,

$$R_{\mathcal{D}}(\boldsymbol{\theta}) = \int_{[0,1]^d} \tfrac{1}{2}|\phi(\boldsymbol{x};\boldsymbol{\theta}) - f(\boldsymbol{x})|^2 d\boldsymbol{x}.$$

[*] Department of Mathematics, National University of Singapore (zhangshijun@u.nus.edu).

The goal of supervised learning is to find the expected risk minimizer

$$\boldsymbol{\theta}_{\mathcal{D}} \coloneqq \arg\min_{\boldsymbol{\theta}} R_{\mathcal{D}}(\boldsymbol{\theta}),$$

which is unachievable in practice since f and $U(\mathcal{X})$ are not available.

In practice, for given samples $\{(\boldsymbol{x}_i, f(\boldsymbol{x}_i))\}_{i=1}^{n}$, we use the empirical risk

$$R_{\mathcal{S}}(\boldsymbol{\theta}) \coloneqq \frac{1}{n}\sum_{i=1}^{n} \ell\big(\phi(\boldsymbol{x}_i;\boldsymbol{\theta}), f(\boldsymbol{x}_i)\big).$$

to approximate/model the expected risk $R_{\mathcal{D}}(\boldsymbol{\theta})$. Our goal is to identify the empirical risk minimizer

$$\boldsymbol{\theta}_{\mathcal{S}} \coloneqq \arg\min_{\boldsymbol{\theta}} R_{\mathcal{S}}(\boldsymbol{\theta}). \tag{1}$$

When a numerical optimization method is applied to solve (1), it may result in a numerical solution (denoted as $\boldsymbol{\theta}_{\mathcal{N}}$), which is generally not a global minimizer. Hence, the actually learned function generated by a neural network is $\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}})$. And the discrepancy between the target function f and the actually learned function $\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}})$ is measured by an inference error

$$R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) = \mathbb{E}_{\boldsymbol{x}\sim U(\mathcal{X})}\left[\ell(\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}}), f(\boldsymbol{x}))\right] \overset{e.g.}{=} \int_{[0,1]^d} \tfrac{1}{2}|\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}}) - f(\boldsymbol{x})|^2 d\boldsymbol{x},$$

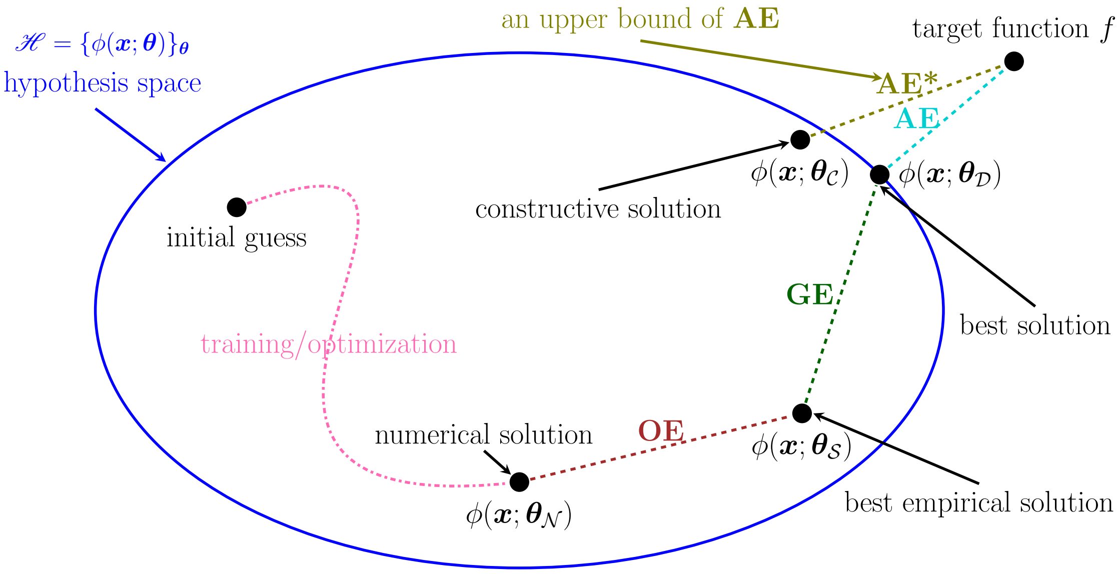
where the second equality holds when $\ell(y,y') = \frac{1}{2}|y-y'|^2$ and U is a uniform distribution over $\mathcal{X} = [0,1]^d$,

Since $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}})$ is the expected inference error over all possible data samples, it can quantify how good the learned function $\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}})$ is. Note that

$$\begin{aligned} R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) &= \underbrace{[R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}})]}_{\text{GE}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}})]}_{\text{OE}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}})]}_{\le 0 \text{ by Eq. (1)}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}}) - R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})]}_{\text{GE}} + \underbrace{R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})}_{\text{AE}} \\ &\le \underbrace{R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})}_{\text{Approximation error (AE)}} + \underbrace{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}})]}_{\text{Optimization error (OE)}} + \underbrace{[R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}})] + [R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}}) - R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})]}_{\text{Generalization error (GE)}}. \end{aligned} \tag{2}$$

Constructive approximation provides an upper bound of the approximation error in terms of the network size, e.g., in terms of the network width and depth, or in terms of the number of parameters. To reduce the optimization error, one only needs to design a good numerical algorithm to make $R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}})$ small, but not $\boldsymbol{\theta}_{\mathcal{N}} - \boldsymbol{\theta}_{\mathcal{S}}$. The study of the third and fourth terms in (2) is referred to as the generalization error analysis of neural networks. See Figure 2 for the intuitions of these three errors.

One of the key targets in the area of deep learning is to develop algorithms to reduce $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}})$. In [1, 2, 3, 4, 5, 6, 7, 8], we provide upper bounds of the approximation error $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})$ for several function spaces, which is crucial to estimate an upper bound of $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}})$. Instead of deriving an approximator to attain the approximation error bound, deep learning algorithms aim to identify a solution $\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}})$ reducing the generalization and optimization errors in (2). Solutions minimizing both generalization and optimization errors will lead to a good solution only if we also have a good upper bound estimate of $R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})$ as shown in (2). Independent of whether our analysis here leads to a good approximator, which is an interesting topic to pursue, the theory in [1, 2, 3, 4, 5, 6, 7, 8] does provide a key ingredient in the error analysis of deep learning algorithms.


an upper bound of **AE**
target function f
$\mathscr{H} = \{\phi(\boldsymbol{x};\boldsymbol{\theta})\}_{\boldsymbol{\theta}}$
hypothesis space
AE*
AE
$\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{C}})$
$\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{D}})$
initial guess
constructive solution
GE
best solution
training/optimization
numerical solution
OE
$\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{S}})$
best empirical solution
$\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}})$

$$R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) \le \underbrace{\overset{\text{theoretical construction}}{R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})}}_{\textbf{AE}} + \underbrace{\overset{\text{models and algorithms}}{[R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{S}})]}}_{\textbf{OE}} + \underbrace{\overset{\text{models, algorithms, and hypothesis space}}{[R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) - R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{N}})] + [R_{\mathcal{S}}(\boldsymbol{\theta}_{\mathcal{D}}) - R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{D}})]}}_{\textbf{GE}}$$

Figure 2: The intuitions of the approximation error (AE), the optimization error (OE), and the generalization error (GE). One needs to control AE, OE, and GE in order to bound the discrepancy between the target function f and the numerical solution $\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}})$ (what we can get in practice), measured by

$$R_{\mathcal{D}}(\boldsymbol{\theta}_{\mathcal{N}}) = \mathbb{E}_{\boldsymbol{x}\sim U(\mathcal{X})}\left[\ell(\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}}), f(\boldsymbol{x}))\right] \overset{e.g.}{=} \int_{[0,1]^d} \tfrac{1}{2}|\phi(\boldsymbol{x};\boldsymbol{\theta}_{\mathcal{N}}) - f(\boldsymbol{x})|^2 d\boldsymbol{x}.$$

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