Deep Learning Generalization
Measure of Generalization

**Generalization:** difference in performance on train vs. test.

\[
\frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim \mathcal{D}}[\ell(f(x), y)]
\]

**Assumption**

\((x_i, y_i) \text{ i.i.d. } \sim \mathcal{D}\)
Problems with the theoretical idealization

Data is not identically distributed:

- Images (Imagenet) are scraped in slightly different ways
- Data has systematic bias (e.g., patients are tested based on symptoms they exhibit)
- Data is result of interaction (reinforcement learning)
- Domain / distribution shift
Meta Theorem of Generalization

**Meta theorem of generalization:** with probability $1 - \delta$ over the choice of a training set of size $n$, we have

$$
\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim D} [\ell(f(x), y)] \right| = O \left( \sqrt{\frac{\text{Complexity}(\mathcal{F}) + \log(1/\delta)}{n}} \right)
$$

**Some measures of complexity:**

- (Log) number of elements
- VC (Vapnik-Chervonenkis) dimension
- Rademacher complexity
- PAC-Bayes
- …
Classical view of generalization

Decoupled view of generalization and optimization:

- Optimization: find a global minimum: \[
  \min_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{m} \ell(f(x_i), y_i)
\]
- Generalization: how well does the global optimizer generalize

Practical implications: to have a good generalization, make sure \( \mathcal{F} \) is not too “complex”.

Strategies:
- **Direct capacity control**: bound the size of the network / amount of connections, clip the weights, etc.
- **Regularization**: add a penalty term for “complex” predictors: weight decay (\( \ell_2 \) norm), dropout, etc.
Techniques for Improving Generalization
Weight Decay

L2 regularization: \[ \frac{\lambda}{2} \| \theta \|_2^2 \]

Implementation: \[ \theta \leftarrow (1 - \eta \lambda) \theta - \eta \nabla f(\theta) \]
**Dropout**

**Intuition:** randomly cut off some connections and neurons.

**Training:** for each input, at each iteration, randomly “turn off” each neuron with a probability $1 - \alpha$
- Change a neuron to 0 by sampling a Bernoulli variable.
- Gradient only propagated from non-zero neurons.
Dropout changes the scale of the output neuron:

- $y = \text{Dropout}(\sigma(WX))$
- $\mathbb{E}[y] = \alpha \mathbb{E}[\sigma(Wx)]$

**Test time:** $y = \alpha \sigma(Wx)$ to match the scale
Understanding Dropout

- Dropout forces the neural network to learn redundant patterns.
- Dropout can be viewed as an implicit L2 regularizer (Wager, Wang, Liang ’13).
Early Stopping

- Continue training may lead to overfitting.
- Track performance on a held-out validation set.
- Theory: for linear models, equivalent to L2 regularization.
Data Augmentation

Depend on data types.

Computer vision: rotation, stretching, flipping, etc
Mixup data augmentation

- $\hat{x} = \lambda x_i + (1 - \lambda)x_j$
- $\hat{y} = \lambda y_i + (1 - \lambda)y_j$
- $\lambda \sim \text{Beta}(0.2)$
Data Augmentation

Depend on data types.

Natural language processing:

- Synonym replacement
  - This article will focus on summarizing data augmentation in NLP.
  - This write-up will focus on summarizing data augmentation in NLP.

- Back translation: translate the text data to some language and then translate back
  - I have no time. -> 我没有时间. -> I do not have time.
Learning rate scheduling

Start with large learning rate. After some epochs, use small learning rate.
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Theory:
- Linear model / Kernel: large learning rate first learns eigenvectors with large eigenvalues (Nakkiran, ’20).
- Representation learning (Li et al., ‘19)
Normalizations

- Batch normalization (Ioffe & Szegedy, ’15)
- Layer normalization (Ba, Kiros, Hinton, ’16)
- Weight normalization (Salimans, Kingma, ’16)
- Instant normalization (Ulyanov, Vedaldi, Lempitsky, ’16)
- Group normalization (Wu & He, ’18)
- …
Generalization Theory for Deep Learning
**Basic version: finite hypothesis class**

**Finite hypothesis class:** with probability $1 - \delta$ over the choice of a training set of size $n$, for a bounded loss $\ell$, we have

$$\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim D} [\ell(f(x), y)] \right| = O \left( \sqrt{\frac{\log |\mathcal{F}| + \log 1/\delta}{n}} \right)$$
**VC-Dimension**

**Motivation:** Do we need to consider *every* classifier in $\mathcal{F}$?

Intuitively, **pattern of classifications** on the training set should suffice. (Two predictors that predict identically on the training set should generalize similarly).

Let $\mathcal{F} = \{ f : \mathbb{R}^d \to \{+1, -1\} \}$ be a class of binary classifiers.

The **growth function** $\Pi_{\mathcal{F}} : \mathbb{N} \to \mathbb{F}$ is defined as:

$$\Pi_{\mathcal{F}}(m) = \max_{(x_1, x_2, \ldots, x_m)} \left\{ (f(x_1), f(x_2), \ldots, f(x_m)) \mid f \in \mathcal{F} \right\}.$$

The **VC dimension** of $\mathcal{F}$ is defined as:

$$\text{VCdim}(\mathcal{F}) = \max\{ m : \Pi_{\mathcal{F}}(m) = 2^m \}.$$
Theorem (Vapnik-Chervonenkis): with probability $1 - \delta$ over the choice of a training set, for a bounded loss $\ell$, we have

$$\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim D} [\ell(f(x), y)] \right| = O \left( \sqrt{\frac{\text{VCdim}(\mathcal{F}) \log n + \log 1/\delta}{n}} \right)$$

Examples:
- Linear functions: VC-dim = $O(\text{dimension})$
- Neural network: VC-dimension of fully-connected net with width $W$ and $H$ layers is $\Theta(WH)$ (Bartlett et al., ’17).
Problems with VC-dimension bound

1. In over-parameterized regime, bound $>> 1$.
2. Cannot explain the random noise phenomenon:
   • Neural networks that fit random labels and that fit true labels have the same VC-dimension.

Practice: gradient descent

$$\theta(t + 1) \leftarrow \theta(t) - \eta \frac{\partial L(\theta(t))}{\partial \theta(t)}$$

Optimization error $\to 0$ for both true labels and random labels!
PAC Bayesian Generalization Bounds

Setup: Let $P$ be a prior over function in class $\mathcal{F}$, let $Q$ be the posterior (after algorithm’s training).

Theorem: with probability $1 - \delta$ over the choice of a training set, for a bounded loss $\ell$, we have

$$
\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim D} [\ell(f(x), y)] \right| = O \left( \sqrt{\frac{KL(Q \mid \mid P) + \log 1/\delta}{n}} \right)
$$
Rademacher Complexity

**Intuition:** how well can a classifier class fit random noise?

**(Empirical) Rademacher complexity:** For a training set $S = \{x_1, x_2, \ldots, x_n\}$, and a class $\mathcal{F}$, denote:

$$\hat{R}_n(S) = \mathbb{E}_\sigma \sup_{f \in \mathcal{F}} \sum_{i=1}^{n} \sigma_i f(x_i).$$

where $\sigma_i \sim \text{Unif}\{+1, -1\}$ (Rademacher R.V.).

**(Population) Rademacher complexity:**

$$R_n = \mathbb{E}_S \left[\hat{R}_n(S)\right].$$
Rademacher Complexity Generalization Bound

**Theorem:** with probability $1 - \delta$ over the choice of a training set, for a bounded loss $\ell$, we have

$$\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim D} [\ell(f(x), y)] \right| = O \left( \frac{\hat{R}_n}{n} + \frac{\log 1/\delta}{n} \right)$$

and

$$\sup_{f \in \mathcal{F}} \left| \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i) - \mathbb{E}_{(x,y) \sim D} [\ell(f(x), y)] \right| = O \left( \frac{R_n}{n} + \frac{\log 1/\delta}{n} \right)$$
Kernel generalization bound

Use Rademacher complexity theory, we can obtain a generalization bound $O(\sqrt{y^\top (H^*)^{-1} y/n})$ where $y \in \mathbb{R}^n$ are $n$ labels, and $H^* \in \mathbb{R}^{n \times n}$ is the kernel (e.g., NTK) matrix.
Norm-based Rademacher complexity bound

**Theorem:** If the activation function is $\sigma$ is $\rho$-Lipschitz. Let

$$\mathcal{F} = \{ x \mapsto W_{H+1} \sigma(W_h \sigma(\cdots \sigma(W_1 x)\cdots)), \|W_h^T\|_{1,\infty} \leq B \quad \forall h \in [H] \}$$

then $R_n(\mathcal{S}) \leq \|X^\top\|_{2,\infty}(2\rho B)^{H+1}\sqrt{2 \ln d}$ where

$X = [x_1, \ldots, x_n] \in \mathbb{R}^{d \times n}$ is the input data matrix.
Comments on generalization bounds

• When plugged in real values, the bounds are rarely non-trivial (i.e., smaller than 1)
• “Fantastic Generalization Measures and Where to Find them” by Jiang et al. ’19: large-scale investigation of the correlation of extant generalization measures with true generalization.

Image credits to Andrej Risteski
Comments on generalization bounds

- Uniform convergence may be unable to explain generalization of deep learning [Nagarajan and Kolter, ’19]
  - Uniform convergence: a bound for all $f \in \mathcal{F}$
  - Exists example that 1) can generalize, 2) uniform convergence fails.

- Rates:
  - Most bounds: $1/\sqrt{n}$.
  - Local Rademacher complexity: $1/n$. 
Double descent

- There are cases where the model gets bigger, yet the (test!) loss goes down, sometimes even lower than in the classical “under-parameterized” regime.
- Complexity: number of parameters.

Belkin, Hsu, Ma, Mandal ‘18
Double descent

Widespread phenomenon, across architectures (Nakkiran et al. ’19):

(a) CIFAR-100. There is a peak in test error even with no label noise.

(b) CIFAR-10. There is a “plateau” in test error around the interpolation point with no label noise, which develops into a peak for added label noise.
Double descent

Widespread phenomenon, across architectures (Nakkiran et al. ’19):
Double descent

Widespread phenomenon, also in kernels (can be formally proved in some concrete settings [Mei and Montanari ’20]), random forests, etc.
Double descent

Also in other quantities such as train time, dataset, etc (Nakkiran et al. ’19):

Figure 2: **Left**: Test error as a function of model size and train epochs. The horizontal line corresponds to model-wise double descent—varying model size while training for as long as possible. The vertical line corresponds to epoch-wise double descent, with test error undergoing double-descent as train time increases. **Right** Train error of the corresponding models. All models are Resnet18s trained on CIFAR-10 with 15% label noise, data-augmentation, and Adam for up to 4K epochs.
Double descent

Optimal regularization can mitigate double descent [Nakkiran et al. ’21]:

Effect of Regularization: CNNs on CIFAR-100
Double descent

Optimal regularization can mitigate double descent [Nakkiran et al. ’21]:

(a) Test Classification Error vs. Number of Training Samples.

(b) Test Classification Error vs. Model Size (Number of Random Features).
Implicit Regularization

Different optimization algorithm
  ➡ Different bias in optimum reached
  ➡ Different Inductive bias
  ➡ Different generalization properties
Implicit Bias

Margin:

- Linear predictors:
  - Gradient descent, mirror descent, natural gradient descent, steepest descent, etc maximize margins with respect to different norms.

- Non-linear:
  - Gradient descent maximizes margin for homogeneous neural networks.
  - Low-rank matrix sensing: gradient descent finds a low-rank solution.
Separation between NN and kernel

• For approximation and optimization, neural network has no advantage over kernel. Why NN gives better performance: generalization.

• [Allen-Zhu and Li ’20] Construct a class of functions $\mathcal{F}$ such that $y = f(x)$ for some $f \in \mathcal{F}$:
  • no kernel is sample-efficient;
  • Exists a neural network that is sample-efficient.