Generalizaiton and Regularizaiton

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Outline

- Statistical Learning Theory
- 2 Regularization
- 3 Hyperparameter Tune
- Overparameterization

- MLPs are parameterized function f_{θ} , where $\theta = \{ \mathbf{W}^{\ell}, \mathbf{b}^{\ell} \}$
- ullet The learning problem involves solving an **optimization** problem to iteratively update the $oldsymbol{ heta}$

$$\min_{\boldsymbol{\theta}} \quad \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Hyperparameter Tune

where ℓ is a loss function and $\mathcal{S} := \{x_i, y_i\}_{i=1}^{\ell}$ is a training set.

• This optimization problem can be solved using gradient-based methods such as (stochastic) gradient descent (SGD), gradient descent with momentum, RMSProp, Adam, etc:

$$\boldsymbol{\theta}^+ = \boldsymbol{\theta} - \boldsymbol{\eta} \cdot \boldsymbol{v}^+,$$

where $\eta > 0$ is a **learning rate** and v is a **search direction**.

The training process involves several key hyperparameters:

- Loss Function $\ell(\cdot,\cdot)$: Square loss, cross-entropy loss, hinge loss
- Activation Function $\phi(\cdot)$: Step, sigmoid, ReLU, tanh, GELU
- Optimizer: SGD, Momentum, RMSProp, Adam
- Learning Rate (η) , Batch Size (b), Epochs
- Network Type: MLPs, CNNs, RNNs, Transformers, GNNs
- Width and Depth
- Layers: Normalization, pooling, dropout, softmax
- Otherwise: Initialization (Xavier, He), \(\ell_2\)-regularization, gradient clipping, early stop

Key Difference: Hyperparameters vs. Trainable Parameters

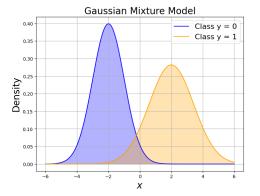
- Hyperparameters are not trainable. Unlike weights and biases, they need to be tuned manually.
- Proper tuning is essential for faster convergence during training and achieving good generalization performance.

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Gaussian Mixture Model

- Assume the output y follows a discrete uniform distribution over $\{0,1\}$, meaning $y \sim \mathcal{U}\{0,1\}$.
- \bullet For each value of y, the input x follows a Gaussian distribution:
 - When y = 0, x follows $x|y = 0 \sim \mathcal{N}(\mu_1, \sigma_1^2)$.
 - When y=1, x follows $x|y=1 \sim \mathcal{N}(\mu_2, \sigma_2^{\overline{2}})$.



- This setup defines a (binary) Gaussian Mixture Model (GMM).
- Both x and y are random variables, with a joint distribution denoted as \mathcal{D} , i.e., $(x,y) \sim \mathcal{D}$.

- Assume the data (x,y) is drawn from an underlying joint distribution \mathcal{D} , i.e., $(x,y) \sim \mathcal{D}$.
- The goal of learning is to find a (parameterized) function f such that:

$$f(x) \approx y$$

for "most" (x, y) pairs in a probabilistic sense.

• The **expected risk** of f is defined as:

$$R(f) := \mathbb{E}_{(x,y) \sim \mathcal{D}} [f(x) - y]^2,$$

where we use the squared loss to measure the difference between f(x) and y.

- In practice, the distribution \mathcal{D} is **unknown**.
- Instead, we collect a random training sample $S := \{(x_i, y_i)\}_{i=1}^n$ and compute the empirical risk or training error:

$$R_S(f) := \frac{1}{n} \sum_{i=1}^{n} [f(x_i) - y_i]^2.$$

• By the law of large numbers, we have:

$$R_S(f) \longrightarrow R(f)$$
 as $n \to \infty$.



Suppose (x, y) follows GMM, and the function $f(x) = \theta x$.

ullet The expected risk R(f) is given by

$$R(f) = \mathbb{E}_{(x,y) \sim \mathcal{D}} \ell(f(x), y)$$

$$= \int [f(x) - y]^2 p(x, y) dx dy = \int [f(x) - y]^2 p(x|y) p(y) dx dy$$

$$= \frac{1}{2} \int [f(x)]^2 p(x|y = 0) dx + \frac{1}{2} \int [f(x) - 1]^2 p(x|y = 1) dx$$

$$= \frac{1}{2} \int [\theta x]^2 \cdot \mathcal{N}(x; \mu_1, \sigma_1^2) dx + \frac{1}{2} \int [\theta x - 1]^2 \cdot \mathcal{N}(x; \mu_2, \sigma_1^2) dx$$

$$\triangleq R(\theta),$$

where p(x,y) is the joint density, and $\mathcal{N}(x;\mu,\sigma^2)$ is the Gaussian density defined by

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sigma \sqrt{2\pi}} e^{-(x-\mu)^2/2\sigma^2}.$$

ullet The empirical risk $R_S(f)$ over a training sample is given by

$$R_S(f) = \frac{1}{n} \sum_{i=1}^n [\theta x_i - y_i]^2 \triangleq R_S(\theta).$$



Hypothesis Class

In practice, we cannot evaluate all possible functions f. Instead, we restrict our search to a family of functions called a **hypothesis class** \mathcal{H} . Each function $h \in \mathcal{H}$ is called a **hypothesis**.

• The collection of all linear models or the collection of all two-layer neural networks:

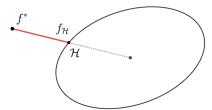
$$\mathcal{H}_1 = \{ h : h(\mathbf{x}) = \mathbf{w}^\top \mathbf{x} \}$$

$$\mathcal{H}_2 = \{ h : h(\mathbf{x}) = \mathbf{v}^\top \phi(\mathbf{W}\mathbf{x}) \}.$$

ullet A learning algorithm aims to find the best hypothesis $h \in \mathcal{H}$ that minimizes the expected risk:

$$f_{\mathcal{H}} := \operatorname*{argmin}_{f \in \mathcal{H}} R(f).$$

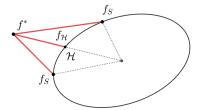
- The difference $||f^* f_{\mathcal{H}}||$ is called the **approximation error**, where f^* is the ground true function.
- The Universal Approximation Theorem (UAT) implies $||f^* f_{\mathcal{H}}|| \approx 0$ if $f_{\mathcal{H}} \in \mathcal{H}_2$.



• Given a learned hypothesis f_S from a sample S, the expected risk of f_S can be decomposed as:

$$R(f_S) = \underbrace{R_S(f_S)}_{\text{Training Error}} + \underbrace{\left[R(f_S) - R_S(f_S)\right]}_{\text{Generalization Error}}.$$

The generalization error is the difference between the expected risk and the empirical risk.



• In practice, the generalization error is estimated using the test error on an independent test set.

• The generalization error can be upper bounded by the **complexity** of the hypothesis class:

$$\sup_{h\in\mathcal{H}}|R(h)-R_S(h)|\leq \text{Complexity Term},$$

where the "Complexity Term" quantifies how flexible or complex the hypothesis class $\mathcal H$ is.

One commonly used complexity measure is the (empirical) Rademacher complexity:

$$\mathfrak{R}_S(\mathcal{H}) := \mathbb{E}_{\sigma} \left[\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^n \ell(h(x_i), \sigma_i) \right],$$

where $\ell(h(x), \sigma) = \sigma h(x)$ and $\sigma_i \in \{-1, 1\}$ are i.i.d. Rademacher random variables (uniformly distributed), i.e., $\sigma \sim \mathcal{U}\{-1,1\}$, and the expectation is taken over these random labels.

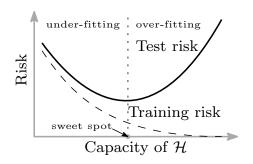
- Rademacher complexity measures the ability of the hypothesis class to fit random noise (i.e., how well the hypothesis class can fit random labels).
- Using model complexity, we can derive the following generalization bound:

$$R(f_S) \le R_S(f_S) + \mathfrak{R}_S(\mathcal{H}) + \tilde{\mathcal{O}}(n^{-1}),$$

where the expected risk is upper bounded by the training error and the complexity of the model.

The expected risk $R(f_S)$ is upper bounded by the training error and the model complexity:

$$R(f_S) \le R_S(f_S) + \mathfrak{R}_S(\mathcal{H}) + \tilde{\mathcal{O}}(n^{-1}).$$



Key Insights on Generalization Bound

- If the model is too simple, it may fail to fit the training data well. This is known as underfitting.
- Conversely, if the model is highly flexible, it may achieve low training error, but perform poorly on unseen data.
 This is known as overfitting.
- The goal is to find a "sweet spot" balancing underfitting and overfitting to minimize the overall expected risk.

Claim: $f^*(x) = \mathbb{E}[y|x]$ is the **optimal hypothesis** that minimizes the expected risk.

Proof.

For any function f, we can decompose the expected risk as follows:

$$R(f) = \mathbb{E}(f - y)^{2} = \mathbb{E}(f - f^{*} + f^{*} - y)^{2}$$

$$= \mathbb{E}(f - f^{*})^{2} + 2\mathbb{E}(f - f^{*})(f^{*} - y) + \mathbb{E}(f^{*} - y)^{2}$$

$$= \mathbb{E}(f - f^{*})^{2} + \mathbb{E}(f^{*} - y)^{2}$$

$$\geq \mathbb{E}(f^{*} - y)^{2}$$

$$= R(f^{*})$$

where the cross term $\mathbb{E}(f - f^*)(f^* - y) = 0$, because $f^*(x) = \mathbb{E}[y|x]$.

- This is another existence result.
- The optimal hypothesis f^* is not directly accessible unless we know the joint distribution \mathcal{D} .
- Generally, we may have $R(f^*) \neq 0$. For example, consider $y = \theta x + \varepsilon$, where $\varepsilon \sim \mathcal{N}(0, \sigma^2)$

$$\begin{split} f^*(x) = & \mathbb{E}[y|x] = \mathbb{E}[\theta x + \varepsilon|x] = \theta x \\ & R(f^*) = & \mathbb{E}_x[f^*(x) - y]^2 = \mathbb{E}_x[\theta x - (\theta x + \varepsilon)]^2 = \sigma^2 \quad \Longrightarrow \quad \text{irreducible error.} \end{split}$$

- ullet The learned function f_S depends on the random sample S, making f_S a random variable.
- ullet Hence, the expected risk $R(f_S)$ is also **random**, and it varies across different random samples S.
- To capture this variability, we consider the expectation of the $R(f_S)$ over all possible samples S, i.e., $\mathbb{E}_S[R(f_S)]$.
- Let $\bar{f} := \mathbb{E}_S[f_S]$, the average hypothesis over all random samples S.
- Using \bar{f} , we can decompose $\mathbb{E}_S[R(f_S)]$ as follows:

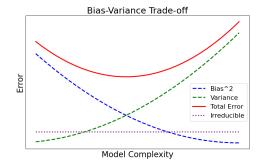
$$\begin{split} \mathbb{E}_{S}[R(f_{S})] = & \mathbb{E}_{S}\mathbb{E}_{(x,y)\sim\mathcal{D}}[f_{S}(x)-y]^{2} \\ = & \mathbb{E}_{S}\mathbb{E}_{\mathcal{D}}[f_{S}-f^{*})]^{2} + R(f^{*}) \\ = & \mathbb{E}_{S}\mathbb{E}_{\mathcal{D}}\left[f_{S}-\bar{f}+\bar{f}-f^{*}\right]^{2} + R(f^{*}) \\ = & \mathbb{E}_{S}\mathbb{E}_{\mathcal{D}}\left[(f_{S}-\bar{f})^{2}+(\bar{f}-f^{*})^{2}\right] + R(f^{*}) \\ = & \mathbb{E}_{S}(f_{S}-\bar{f})^{2} + \mathbb{E}_{\mathcal{D}}(\bar{f}-f^{*})^{2} + R(f^{*}) \end{split}$$

where the cross term $\mathbb{E}_{S,\mathcal{D}}(f_S - \mathbb{E}_S[f_S])(\mathbb{E}_S(f_S) - f^*) = 0$ cancels out.

Bias-Variance Trade-Off

The expected risk $\mathbb{E}_S[R(f_S)]$ can be broken down into three parts:

- Squared Bias: $\mathbb{E}_{\mathcal{D}}[(f^* \mathbb{E}_S(f_S))^2]$ measures the error from approximating the optimal function f^* with the learned model f_S . It reflects the error caused by using a simple model that cannot capture all the data patterns.
- Variance: $Var(f_S) = \mathbb{E}_S[(f_S \mathbb{E}_S(f_S))^2]$ measures how much the learned function f_S varies with different training samples. It represents the error due to the model's sensitivity to fluctuations in the random training sample S.
- Irreducible Error: $R(f^*)$ represents the inherent noise in the data, which no model can eliminate. It is the error we cannot reduce.



- High bias, low variance: Simple models (e.g., linear models) have low variance since they are less sensitive to training data, but have high bias because they are too simple to capture all patterns in the data.
- Low bias, high variance: Complex models (e.g., polynomial model) have low bias as they can model complex relations, but high variance due to overfitting to the training data.

• The goal is to find a hypothesis f within a hypothesis class \mathcal{H} that minimizes the expected risk:

$$R(f) = \mathbb{E}_{(x,y)\sim\mathcal{D}}\left[(f(x) - y)^2\right].$$

• Since the underlying distribution \mathcal{D} is **unknown**, we approximate f by minimizing the **empirical risk** based on a **random** training sample S:

$$R_S(f) = \frac{1}{n} \sum_{i=1}^{n} (f(x_i) - y_i)^2.$$

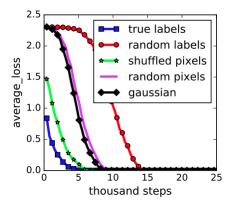
• Using model complexity $\mathfrak{R}_S(\mathcal{H})$, the expected risk is upper bound as:

$$R(f_S) \le R_S(f_S) + \mathfrak{R}_S(\mathcal{H}) + \tilde{\mathcal{O}}(n^{-1}),$$

- By considering variations across different random training samples S, the expected risk $\mathbb{E}_S[R(f_S)]$ can be decomposed into three components: bias, variance, and irreducible error:
 - High bias, low variance: Simple models underfit and miss important patterns in the data.
 - Low bias, high variance: Complex models overfit and perform poorly on unseen data.
- Find the "sweet spot" between underfitting and overfitting to minimize the overall expected risk.



- Statistical Learning Theory
- Regularization
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- Overparameterization



- Label corruption: Replace true label with random label
- Shuffled pixels: The pixels of each image are rearranged using a fixed random permutation
- Random pixels: Each image has a *unique* random arrangement of pixels).
- **Gaussian**: The pixels in images are replaced with random Gaussian *noise*.
- Average loss: Training error using the cross-entropy loss

Key Observation

DNNs can perfectly fit random labels or data, achieving **zero training error** even on completely unstructured inputs.

Statistical Learning Theory

Regularization typically involves adding an extra term, called the regularizer, to the training loss:

$$\mathcal{L}_{\lambda}(oldsymbol{ heta}) := \mathcal{L}(oldsymbol{ heta}) + rac{\lambda}{2} \|oldsymbol{ heta}\|^2,$$

where $\lambda > 0$ is the **regularization hyperparameter**, and $\|\cdot\|$ is the Euclidean norm.

 In deep learning, this regularization is known as weight decay because gradient descent on the regularized loss automatically shrinks (or decays) parameter θ by the factor $(1 - \eta \lambda)$:

$$\begin{split} \boldsymbol{\theta}^+ = & \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\lambda}(\boldsymbol{\theta}) = \boldsymbol{\theta} - \eta \left[\nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) + \lambda \boldsymbol{\theta} \right] \\ = \underbrace{\left(1 - \eta \lambda \right)}_{\text{decaying weights}} & \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}). \end{split}$$

• However, θ does **not** shrink to zero, as it must maintain a certain value to minimize the cost $\mathcal{L}(\theta)$.

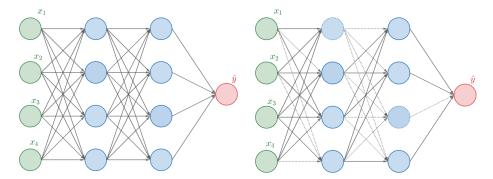
Interpretation: Sparsity

• The regularized optimization can be reformulated as:

$$\min_{\boldsymbol{\theta}} \ \mathcal{L}(\boldsymbol{\theta}), \quad \text{s.t.} \quad \|\boldsymbol{\theta}\| \leq C_{\lambda},$$

where $C_{\lambda} > 0$ is a constant that depends on λ .

- In deep learning, θ is called **sparse** if most parameters are zero or close to zero (i.e., $\theta_i \approx 0$).
- Sparse θ reduces the flexibility and complexity of the DNN, leading to a simpler model.

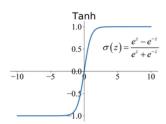


Interpretation: Linearity

Consider a simple two-layer neural network:

$$f_{\boldsymbol{\theta}}(x) = \sum_{i=1}^{n} v_i \phi(w_i x),$$

where $x \in \mathbb{R}$ is a scalar and $\phi(\cdot)$ is tanh.



• When $w_i \approx 0$, then $w_i x \approx 0$, and the network operates near the linear region of tanh:

$$v_i\phi(w_ix)\approx v_i(w_ix)\approx (v_iw_i)x=u_ix \quad \Longrightarrow \quad \text{a linear model},$$
 where $u_i:=v_iw_i.$

• If $v_i \approx 0$, then

$$v_i\phi(w_ix)\approx 0,$$

indicating fewer neurons are used.

Interpretation: Stability

A learning algorithm is stable if small changes to its input do not result in large changes to its output.

Consider the same two-layer neural network:

$$f_{\theta}(x) = \sum_{i=1}^{n} v_i \phi(w_i x).$$

• The derivative of f_{θ} with respect to the **input** x is:

$$\nabla_x f_{\boldsymbol{\theta}}(x) = \sum_{i=1}^n v_i \phi'(w_i x) w_i.$$

- If either v_i or w_i is small, then $\nabla_x f_{\theta}(x)$ is small.
- Hence, DNNs with sparse parameters are generally more stable than those with dense parameters.

Dropout Regularization

Statistical Learning Theory

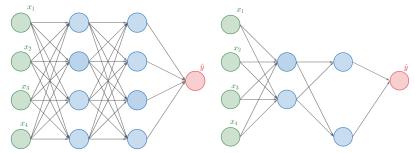
Recall the forward propagation:

$$oldsymbol{z}^\ell = oldsymbol{W}^\ell oldsymbol{x}^{\ell-1}, \quad oldsymbol{x}^\ell = \phi(oldsymbol{z}^\ell).$$

• During training, each neuron is randomly dropped with probability p (a hyperparameter):

$$\hat{oldsymbol{x}}^{\ell-1} = oldsymbol{r}^{\ell} \odot oldsymbol{x}^{\ell-1}, \quad oldsymbol{z}^{\ell} = oldsymbol{W}^{\ell} \hat{oldsymbol{x}}^{\ell-1}$$

where $r_i^{\ell} \sim \text{Bernoulli}(p)$.



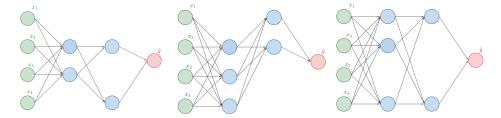
- The gradient update applies only to a **thinned subbnet** of the network.
- At test time, dropout is turned off, and weights are scaled by p to respect the dropout probability:

$$\boldsymbol{z}^{\ell} = p \boldsymbol{W}^{\ell} \boldsymbol{x}^{\ell-1}.$$



Interpretation: Implicit Ensemble Learning

- By randomly dropping units, a different **thinned subnet** is trained at each gradient descent step.
- ullet With n neurons in the full network, we are effectively training 2^n different subnets simultaneously that all **share** the same weights.
- At test time, the output is an **ensemble** prediction, aggregating the contributions of all subnets.



Key Insight

Dropout ensures that **no** single neuron or small group of neurons can dominate the prediction. By **spreading** the responsibility across all units, it improves model robustness to the input change and prevents overfitting.

Summary

- DNNs can fit random labels and data, achieving zero training error.
- Weight decay controls large weights, promoting sparsity, linearity, and stability.
- During training, dropout randomly drops units, effectively training an exponential number of thinned subnets simultaneously.
- At test time, the output is an ensemble prediction, aggregating contributions from all subnets.

- Statistical Learning Theory
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- 3 Hyperparameter Tune

Validation Set

- Split the dataset into three parts: training set, validation set, and test set.
- Build the model using the training set.
- Optimize or tune hyperparameters on the validation set.
- After tuning, evaluate the final model on the test set.
- Suggested split ratios:
 - For datasets between 100 and 1,000,000 samples: 60/20/20.
 - For datasets larger than 1,000,000 samples: 98/1/1.
- Ensure the validation and test sets come from the same distribution
 - Example: Training and validation images from the web, but test images from user cell phones can cause a mismatch.

Tuning Process

- Random Search: Randomly sample hyperparameters; more efficient than grid search when some hyperparameters are less important.
- Hyperband/Successive Halving: Dynamically allocate resources and discard poor configurations early, ideal for deep networks with long training times.
- Start with coarse tuning, then refine gradually.
- Use log scale for hyperparameter search when appropriate.
- Leverage parallelization to run multiple experiments simultaneously to accelerate the search.

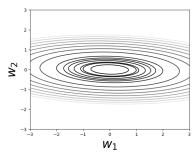
Statistical Learning Theory

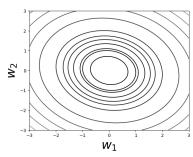
• Normalize the inputs using training set:

$$oldsymbol{\mu} = rac{1}{n}\sum_{i=1}^n oldsymbol{x}_i, \quad ar{oldsymbol{x}}_i = oldsymbol{x}_i - oldsymbol{\mu}, \quad oldsymbol{\sigma}^2 = rac{1}{n}\sum_{i=1}^n ar{oldsymbol{x}}_i^2, \quad \hat{oldsymbol{x}}_i = ar{oldsymbol{x}}_i/oldsymbol{\sigma},$$

where all operations are taken element-wise.

- Consider a binary classification problem using linear model: $f_{\theta}(x) = w_1 x_1 + w_2 x_2$
 - if $x_1 = \mathcal{O}\left(100\right)$ and $x_2 = \mathcal{O}\left(1\right)$, to have output $f_{\theta} = \mathcal{O}\left(1\right)$, we must have $w_1 = \mathcal{O}\left(\frac{1}{100}\right)$ and $w_2 = \mathcal{O}\left(1\right)$.
 - After normalization, $\bar{x}_1 = \mathcal{O}\left(1\right)$ and $\bar{x_2} = \mathcal{O}\left(1\right)$, so we have $w_1 = \mathcal{O}\left(1\right)1$ and $w_2 = \mathcal{O}\left(1\right)$.





ullet At test time, apply μ and σ from **training** to test set.

Learning Rate Decay

- Recall that an epoch k is one pass through all mini-batches in SGD
- Instead of using a fixed learning rate, one can consider using learning rate decay

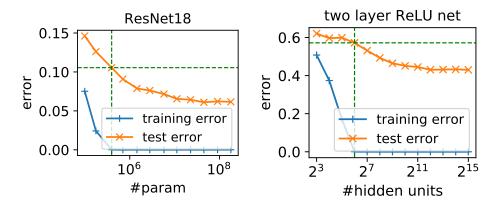
$$\eta_k = \frac{\eta}{k}, \qquad \eta_k = \frac{\eta}{\sqrt{k}}, \qquad \eta_k = (0.95)^k \eta$$

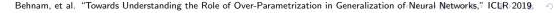
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Overparameterization

Statistical Learning Theory

- A deep neural network (DNN) is said to be overparameterized when the number of neurons or parameters is much larger than the number of training samples.
- This might seem counterintuitive, but it has been found to be surprisingly beneficial in practice.





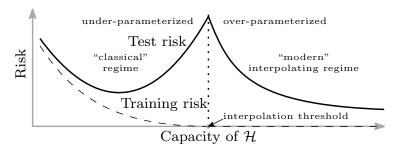
Statistical Learning Theory

Overparameterized neural networks can perfectly fit or interpolate the training data.

ullet Mathematically, there exists a set of parameters ullet such that

$$f_{\boldsymbol{\theta}}(x_i) = y_i, \quad \forall i \in [n].$$
 (1)

- Overparameterization implies there are infinitely many interpolation solutions.
- Some interpolation solutions generalize much better than those in the *underparameterized* regime. This phenomenon is called double descent.



Implicit Regularization

- It is important to understand that different global minima lead to varying test performances.
- A flat minimum typically results in better generalization than a sharp minimum.
- Different optimizers may converge to different minima, each with different generalization outcomes. This is known as implicit regularization.
- Thus, even if your current optimizer achieves low training error, tuning or adjusting it may still be necessary to achieve better test performance.

