Friedrich-Alexander-Universität
Naturwissenschaftliche Fakultät

Breaking the curse of dimensionality
with Barron Spaces

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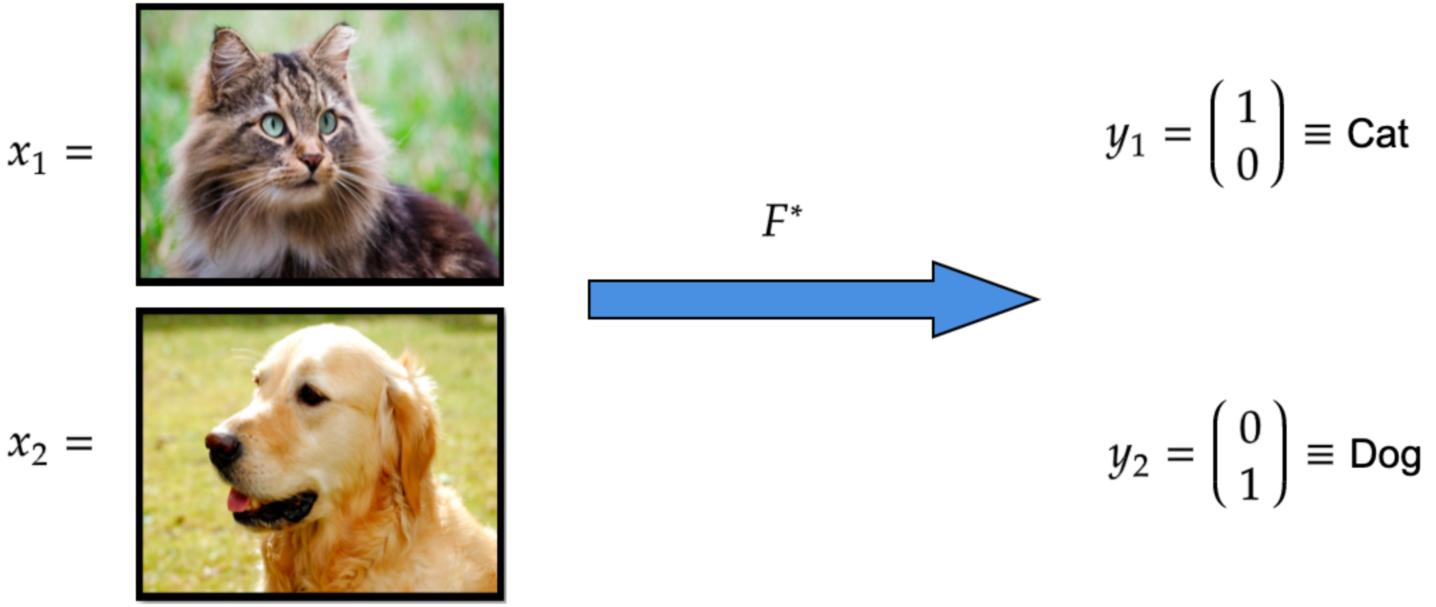
Supervised Learning

Problem statement

- *Input space* $X \subset \mathbb{R}^d$, *output space* $Y \subset \mathbb{R}^m$.
- Given dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N \subset X \times Y$,

Goal

Approximating an ideal unknown *target function* F^* that can label any input $x \in X$ to its corresponding label $y \in Y$, using only the information contained in the dataset $\mathcal{D}$, which verifies $y_i = F^*(x_i)$ for $i = 1, \dots N$.



Supervised Learning

Learning procedure

- We construct, using $\mathcal{D}$, a predictive model $\hat{F}$ from a chosen parametric class of functions that we call the *hypothesis space* $\mathcal{H}$.
- The best possible predictor in $\mathcal{H}$ would be ideally obtained through *population risk minimization*:

$$\arg\min_{F \in \mathcal{H}} \mathbb{E}_{(x,y)\sim\mu^*} L(F(x), y),$$

where μ^* is the unknown input-output distribution and $L(\cdot, \cdot)$ is a suitable *loss function*.

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- In practice, the predictor $\hat{F}$ constructed is obtained through *empirical risk minimization*:

$$\hat{F} = \arg\min_{F\in\mathcal{H}} \frac{1}{N}\sum_{i=1}^{N} L(F(x_i), \underbrace{y_i}_{=F^*(x_i)}),$$

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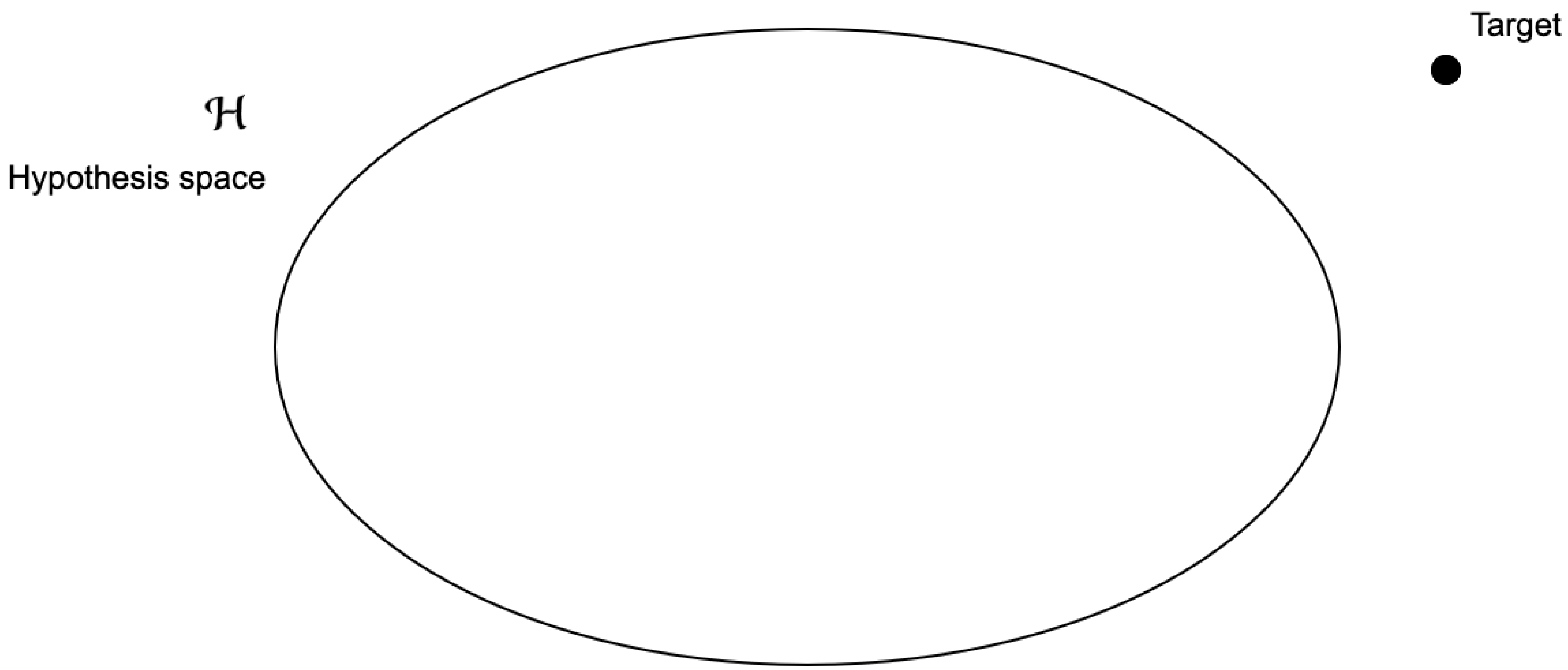
- Main paradigms:
  - **Approximation**: How close is our hypothesis space $\mathcal{H}$ of any target function F^*?
  - **Optimization**: How can we find or get close to the best possible approximation $\hat{F} \in \mathcal{H}$ of F^*?
  - **Generalization**: Can the constructed predictor $\hat{F}$ generalize well to unseen examples?

Supervised Learning

Main paradigms



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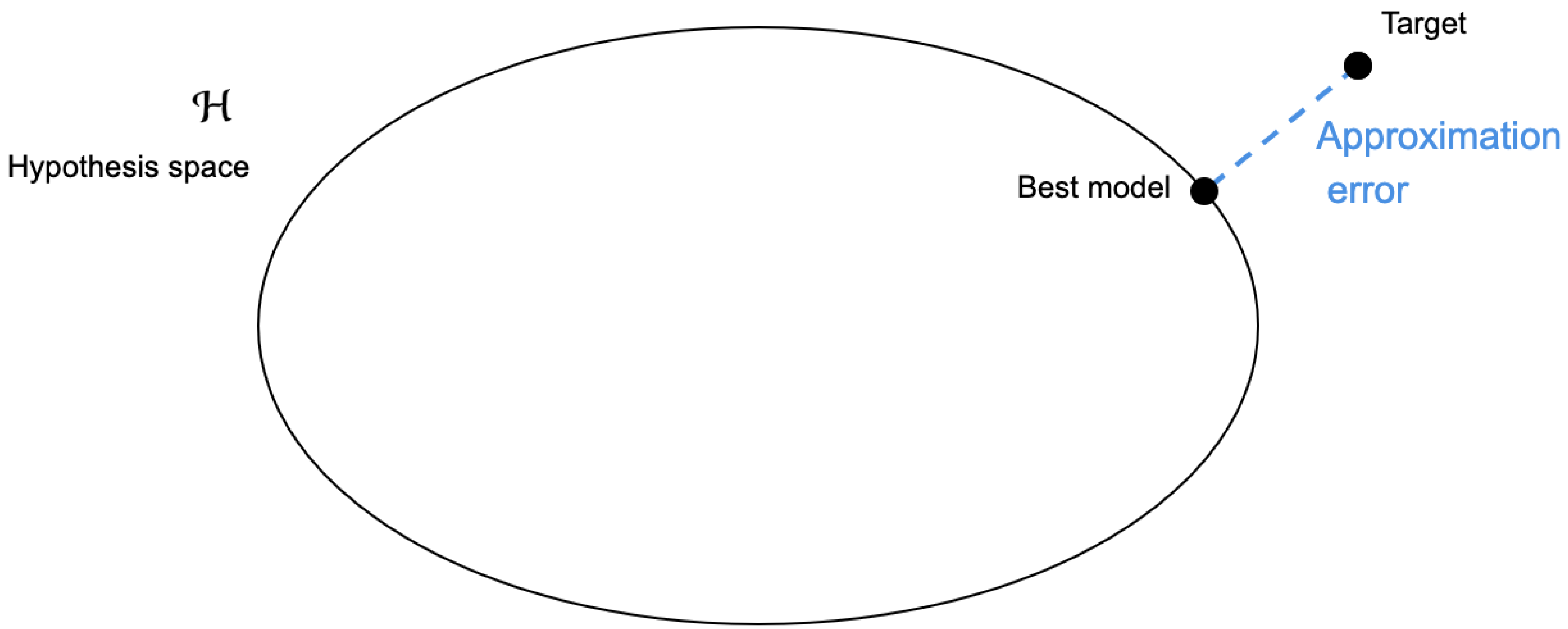

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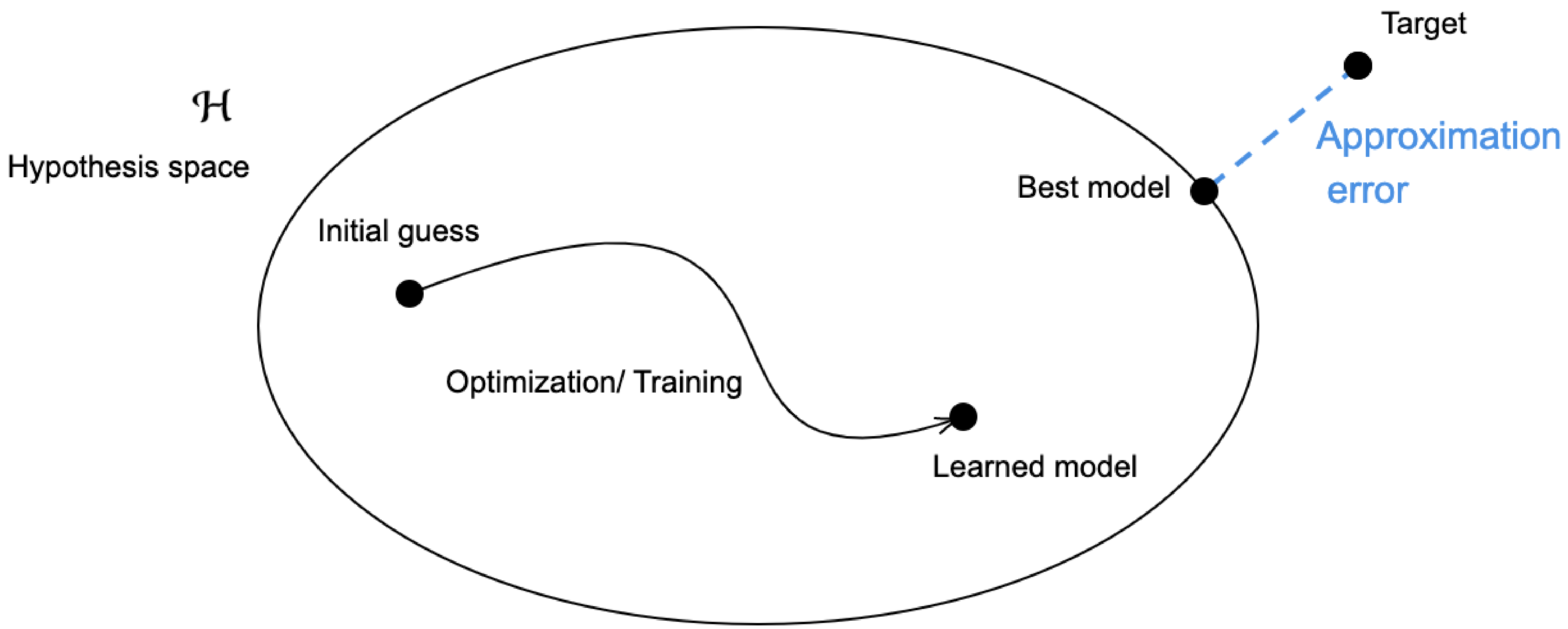

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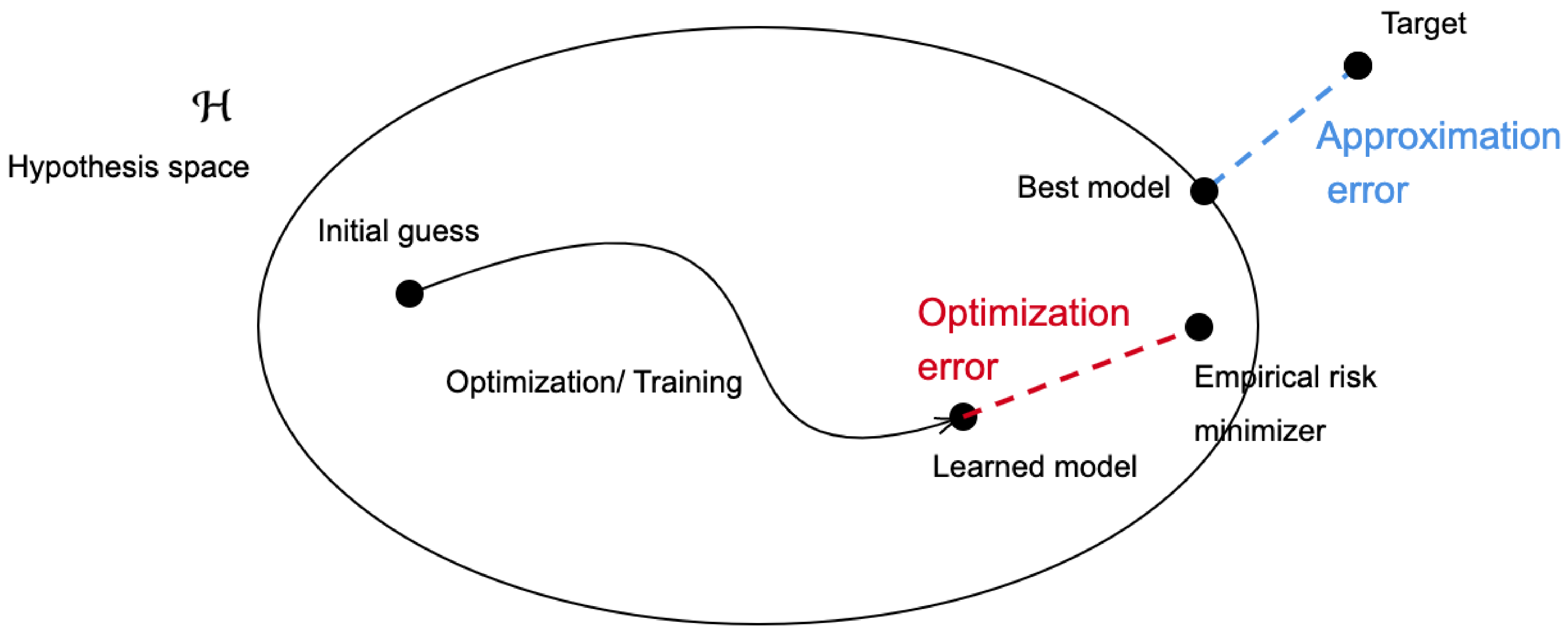

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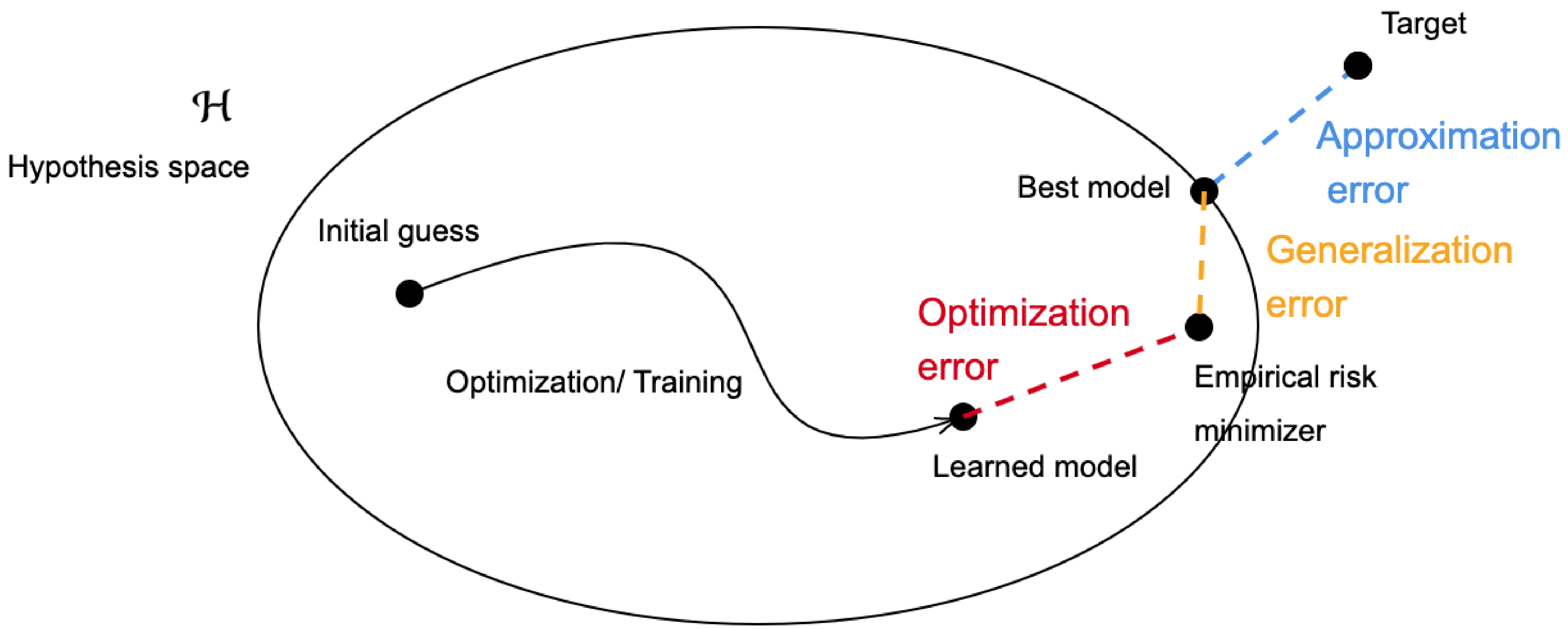

Supervised Learning

Examples of hypothesis spaces

- *Linear models*: $\mathcal{H} = \left\{ F : \mathbb{R}^d \to \mathbb{R} \;\middle|\; F(\mathbf{x}) = \sum_{i=0}^{M-1} w_i \phi_i(\mathbf{x}), w_i \in \mathbb{R} \right\}$, where $\phi_i : \mathbb{R}^d \to \mathbb{R}$ are a prefixed set of *basis functions* or *feature maps*:

$$\phi_j(\mathbf{x}) = \mathbf{x}^j, \qquad \phi_j(\mathbf{x}) = \exp\left(-\frac{(\mathbf{x}-\mathbf{m_j})^2}{2d^2}\right), \qquad \phi_j(\mathbf{x}) = \text{sigm}\left(\frac{\mathbf{x}-\mathbf{m_j}}{d}\right), \text{ with } \text{sigm}(b) = \frac{1}{1+e^{-b}}.$$

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- *Shallow Neural Networks (SNNs)*: $\mathcal{H} = \left\{ F_M : F_M(\mathbf{x}) = \sum_{i=1}^{M} w_i \sigma(\mathbf{a_i}^T \cdot \mathbf{x} + b_i),\; w_i \in \mathbb{R}, \mathbf{a_i} \in \mathbb{R}^d, b_i \in \mathbb{R}, M \in \mathbb{N} \right\}$.
  - σ is the *activation function*.

$$\text{ReLU: } \sigma(z) = \max(0, z), \qquad \sigma(z) = \tanh(z), \qquad \sigma(z) = \text{sigm}(z), \ldots$$

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  - M is the *width*, which controls the complexity of the model.
- *Deep Neural Networks* (DNNs):
  - *Multilayer Perceptron* (MLP) of *depth* K: $\mathcal{H}_K = \left\{ F_K : F_K(\mathbf{x}) = \mathbf{w^T x}(K),\; \mathbf{w} \in \mathbb{R}^{d_K} \right\}$, with
    - $\mathbf{x}(k+1) = \mathbf{w}(k)\sigma\left(\mathbf{a}(k)^T \mathbf{x}(k) + b(k)\right), \qquad \mathbf{w}(k) \in \mathbb{R}^{d_{k+1}}, \qquad \mathbf{a}(k) \in \mathbb{R}^{d_k}, \qquad b(k) \in \mathbb{R}, \qquad k = 0, \ldots, K-1.$
    - $d_k \in \mathbb{N}$ for all k, and $d_0 = d$, $\mathbf{x}(0) = \mathbf{x}$.
  - *Residual Networks* (ResNets): take MLP redefining $\mathbf{x}(k+1) = \mathbf{x}(k) + \mathbf{w}(\mathbf{k})\sigma\left(\mathbf{a}(k)^T \mathbf{x}(k) + b(k)\right)$.

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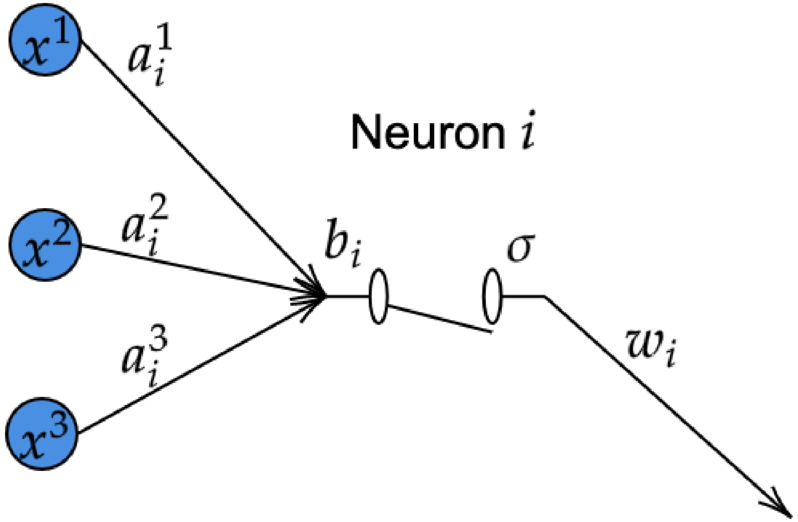
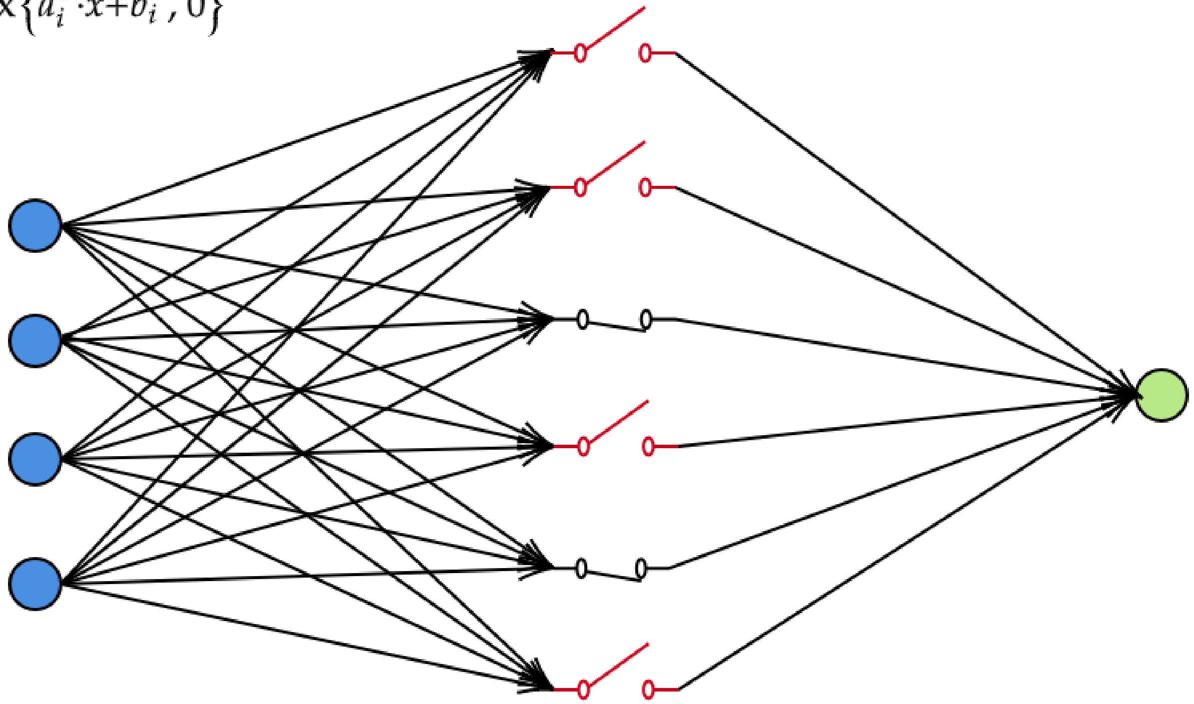
Shallow Neural Networks

Structure

$$\sigma \equiv ReLU: \quad x \in \mathbb{R}^d \quad \mapsto \quad \Big[\underbrace{\sigma\big(a_i^T \cdot x + b_i\big)}_{=\max\left\{a_i^T \cdot x + b_i\,,\, 0\right\}} \Big]_{i=1}^{m} \quad \mapsto \quad F(x) = \sum_{i=1}^{m} w_i \sigma\big(a_i^T \cdot x + b_i\big) \in \mathbb{R}$$





Shallow Neural Networks

Approximation Properties

Universal Approximation Theorem for SNNs [Cyb89]

Let $\Omega \subset \mathbb{R}^d$ be a compact set, and $F^* \in C(\Omega)$. Assume that the activation function σ is continuous and *sigmoidal*, i.e. $\lim_{z\to\infty} \sigma(z) = 1$, $\lim_{z\to-\infty} \sigma(z) = 0$. Then, for every $\epsilon > 0$ there exists $F_M \in \mathcal{H}$ such that

$$\|F_M - F^*\|_{C(K)} = \max_{\mathbf{x}\in K} |F_M(\mathbf{x}) - F^*(\mathbf{x})| < \epsilon. \tag{1}$$

Universal Approximation Theorem for SNNs [Pin99]

Let $\Omega \subset \mathbb{R}^d$ be a compact set and σ a continuous activation function. Then, $\mathcal{H}$ is dense in $C(\Omega)$ in the topology of uniform convergence if and only if σ is non-polynomial.

Also for Deep Neural Networks:

Universal Approximation Theorem for Deep-Narrow NNs [KL20]

Let $\Omega \subset \mathbb{R}^d$ be a compact set and σ a nonaffine continuous activation function. Assume further that σ is continuously differentiable with nonzero derivative at least at one point. Then, $\mathcal{H}_K$ is dense in $C(K; \mathbb{R}^{d_K})$ in the topology of uniform convergence if $K = d + d_K + 2$.

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- No $\rightarrow$ *Curse of dimensionality (CoD)*: Complexity of the models required for better estimates increases exponentially with the dimension of the ambient space

$$\|F_M - F^*\|_{L^p(\Omega)} \leq C \frac{\|F^*\|_{W^{s,p}}}{M^{\alpha(s)/d}}.$$

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- The curse of dimensionality is intrinsic for high dimensional spaces.
- The model works *without* curse of dimensionality when the complexity depends at most polynomially on d for fixed ϵ.
- We can only avoid it by considering a smaller set of problems $\rightarrow$ Find the “right” space of target functions to approximate.

Example

Classical numerical analysis

- Theory of splines and theory of finite element methods approximate functions using piecewise polynomials.
- One starts from a function that lies in a Sobolev/Besov space and proceeds to derive optimal error estimates.
- These estimates depend on the function norm and the regularity encoded in the function space, as well as the approximation scheme.
- Sobolev/Besov spaces are the right ones for these classical theories:
  - Direct and inverse approximation theorems: a function can be approximated by piecewise polynomials with certain convergence rate if and only if the function is in a certain Sobolev/Besov space
  - The functions that we are interested in (e.g. solutions of PDEs) lie on these spaces.

Barron Spaces

Definition

- Let $\Omega \subset \mathbb{R}^d$ be a compact set. We will work with $\sigma \equiv$ ReLU.
- Consider functions $f : \Omega \to \mathbb{R}$ that admit the representation

$$f(\mathbf{x}) = \int_{\Theta} w\sigma(\mathbf{a}^T\mathbf{x} + c)\rho(dw, \mathbf{da}, db) = \mathbb{E}_{\rho}[w\sigma(\mathbf{a}^T\mathbf{x} + b)], \qquad \mathbf{x} \in \Omega, \tag{2}$$

where $\Theta = \mathbb{R} \times \mathbb{R}^d \times \mathbb{R}$ space of parameters and ρ is a probability distribution on $(\Theta, \Sigma_{\Theta})$, being Σ_{Θ} a Borel σ-algebra on Θ.

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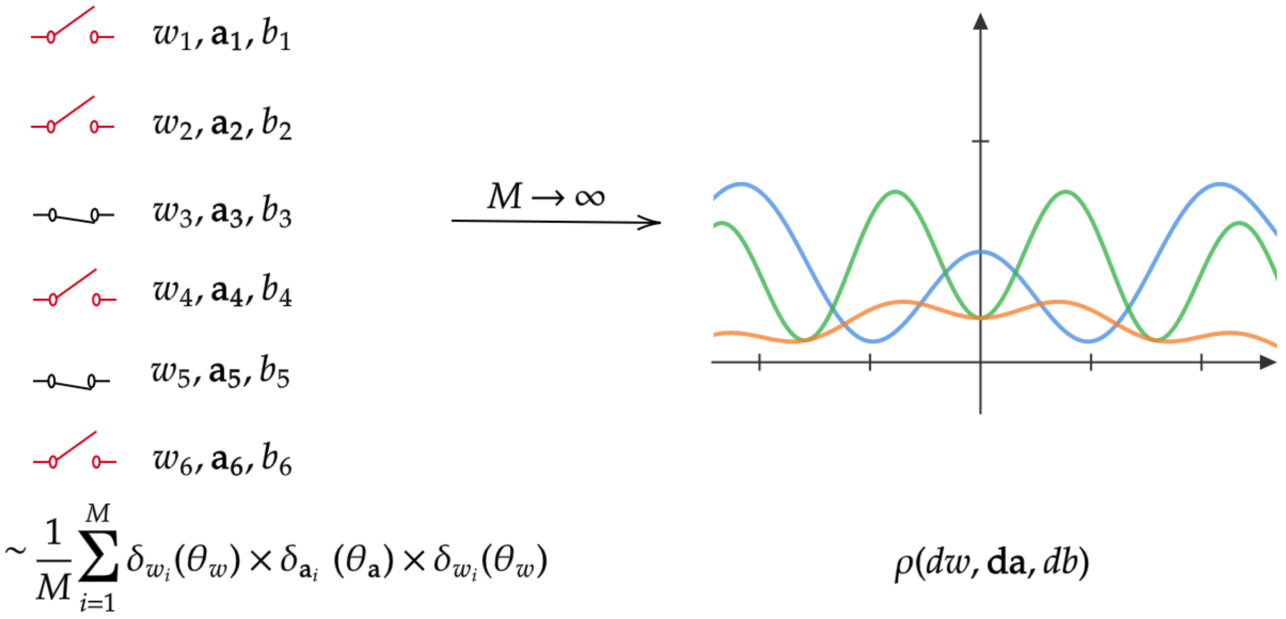

Barron Spaces

Definition

- In general, the ρ's for which (2) holds are not unique. For a function that admits this representation, we define its *Barron norm*
$$\|f\|_{\mathcal{B}_p} = \inf_{\rho} \left(\mathbb{E}_{\rho}[|w|^p(\|\mathbf{a}\|_1 + |b|)^p]\right)^{1/p}, \qquad 1 \leq p \leq \infty, \tag{3}$$
where the infimum is taken over all ρ for which (2) holds for all $\mathbf{x} \in \Omega$.
- Barron spaces $\mathcal{B}_p$ are defined as
$$\{f \in C(\Omega) : f \text{ admits a representation (2)}, \|f\|_{\mathcal{B}_p} < \infty\}.$$

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- By Hölder's inequality, we have

$$\mathcal{B}_\infty \subset \cdots \subset \mathcal{B}_2 \subset \mathcal{B}_1 :$$

- The opposite is also true:

Proposition [MW+22]

For any $f \in \mathcal{B}_1$, we have $f \in \mathcal{B}_\infty$ and

$$\|f\|_{\mathcal{B}_1} = \|f\|_{\mathcal{B}_\infty}.$$

- As a consequence, there is just one Barron space and one Barron norm that we denote by $\mathcal{B}$ and $\|\cdot\|_{\mathcal{B}}$, respectively.

What functions belong to $\mathcal{B}$?

Early study

- Recall:
  - *Fourier transform* of $f : \mathbb{R}^d \to \mathbb{R}$:
  $$\hat{f}(\xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} f(\mathbf{x}) e^{-i\xi\cdot\mathbf{x}} \mathbf{dx}.$$
  - *Fourier inversion formula*:
  $$f(\mathbf{x}) = \int_{\mathbb{R}^d} \hat{f}(\mathbf{x}) e^{i\xi\cdot\mathbf{x}} d\xi.$$
  - $\widehat{Df}(\xi) = i\xi\hat{f}(\xi)$

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Barron's Theorem [Bar93]

For a function $F^* : \Omega \to \mathbb{R}$, let $\hat{F}^*$ be the Fourier transform of any extension of F^* to $\mathbb{R}^d$. Then, if

$$\gamma(F^*) := \inf_{\hat{F}} \int_{\mathbb{R}^d} \|\xi\|_1^2 |\hat{F}^*(\xi)| d\xi = \|\widehat{D^2 F^*}\|_1 < +\infty,$$

for any $M > 0$ there exists a SNN $F_M(\mathbf{x}) = \frac{1}{M}\sum_{i=1}^M w_i \sigma(\mathbf{a_i}^T\mathbf{x} + b_i)$ satisfying

$$\|F_M - F^*\|_{L^2(\Omega)}^2 \leq \frac{3\gamma(F^*)^2}{M},$$

and $\sum_{i=1}^M |w_i|(\|\mathbf{a_i}\|_1 + |b_i|) \leq 2\gamma(F^*)$.

What functions belong to $\mathcal{B}$?

Theorem [Bar93]

Let $F^* \in C(\Omega)$ and assume that F^* satisfies $\gamma(F^*) < \infty$. Then F^* admits an integral representation (2). Moreover,

$$\|F^*\|_{\mathcal{B}} \leq 2\gamma(F^*) + 2\|\nabla F^*(0)\|_1 + 2|F^*(0)|.$$

- To achieve $\gamma(F^*) < \infty$:
  - Necessary condition: All first order partial derivatives are bounded.
  - Sufficient condition: All partial derivatives of order less or equal than s belong to $L^2(\mathbb{R}^d)$, being $s = \lceil 1 + d/2 \rceil$.
- Not enough to generally avoid CoD ($\gamma(F^*)$ involves a $d-$dimensional integral), but there are many examples for which $\gamma(F^*)$ is only moderately large, e.g., $O(d)$ or $O(d^2)$.

Corollary

All **gaussian** functions, **positive definite** functions, **linear** functions and **radial** functions belong to $\mathcal{B}$.

Theorem of direct approximation

- Define the *path norm* as

$$\|\theta\|_{\mathcal{P}} := \frac{1}{M}\sum_{i=1}^{M} |w_i|(\|\mathbf{a_i}\|_1 + |b_i|),$$

where θ denotes a specific set of parameters $\{(w_i, \mathbf{a}_i, b_i)\}_{i=1}^{M}$.

Theorem of direct approximation [MW+22]

For any $F^* \in \mathcal{B}$ and $M > 0$, there exists a SNN $F_M(\mathbf{x}) = \frac{1}{M}\sum_{i=1}^{M} w_i\sigma(\mathbf{a_i}^T\mathbf{x} + b_i)$ satisfying

$$\|F_M(\cdot;\theta) - F^*(\cdot)\|_{L^2(\Omega)}^2 \leq \frac{3\|F^*\|_{\mathcal{B}}^2}{M}.$$

Furthermore, we have $\|\theta\|_{\mathcal{P}} \leq 2\|F^*\|_{\mathcal{B}}$.

- $\mathcal{B}$ can be seen as the closure of $\mathcal{H}$ with respect to the path norm.

Inverse approximation theorem

- Define $\mathcal{N}_Q := \{F_M(\mathbf{x};\theta) : \ \|\theta\|_{\mathcal{P}} \leq Q, m \in \mathbb{N}^+\}$.

Theorem of inverse approximation [MW+22]

Let $F^* \in C(\Omega)$. Assume there exists a constant Q and a sequence of functions $(F_M) \subset \mathcal{N}_Q$ such that

$$\lim_{M\to\infty} F_M(\mathbf{x}) = F^*(\mathbf{x}),$$

for all $\mathbf{x} \in \Omega$. Then $F^* \in \mathcal{B}$ and $\|F^*\|_{\mathcal{B}} \leq Q$.

- Idea of the proof:

  Assume $F_M(\mathbf{x}) = \frac{1}{M}\sum_{i=1}^M w_i^{(M)}\sigma\left(\mathbf{a}_i^{(M)}\mathbf{x} + b_i^{(M)}\right)$. The Theorem's hypothesis implies that the sequence (ρ_M) defined by

$$\rho_M(w,\mathbf{a},b) = \frac{1}{M}\sum_{i=1}^M \delta(w - w_i^{(M)})\delta(\mathbf{a} - \mathbf{a}_i^{(M)})\delta(b - b_i^{(M)})$$

  is tight. By Prokhorov's Theorem, there exists a subsequence (ρ_{M_k}) and a probability measure ρ^* such that ρ_{M_k} converges weakly to ρ^*.

Consequences/Conclusions

- The Barron space catches all the functions that can be approximated by Shallow Neural Networks with bounded path norm, and the approximation error does not suffer from CoD.
- The Barron space is the largest function set which is well approximated by Shallow Neural Networks, and the Barron norm is the natural norm associated with it. Target functions outside $\mathcal{B}$ may be increasingly difficult to approximate by SNNs as dimension increases.

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Open questions

- More specific descriptions of the functions that belong to $\mathcal{B}$.
- Extension to Deep Neural Networks? For ResNets $\Rightarrow$ *Compositional function spaces* [MW+22]

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