



Deep Learning Theory

An Introduction & Recent Results

Khoat Than

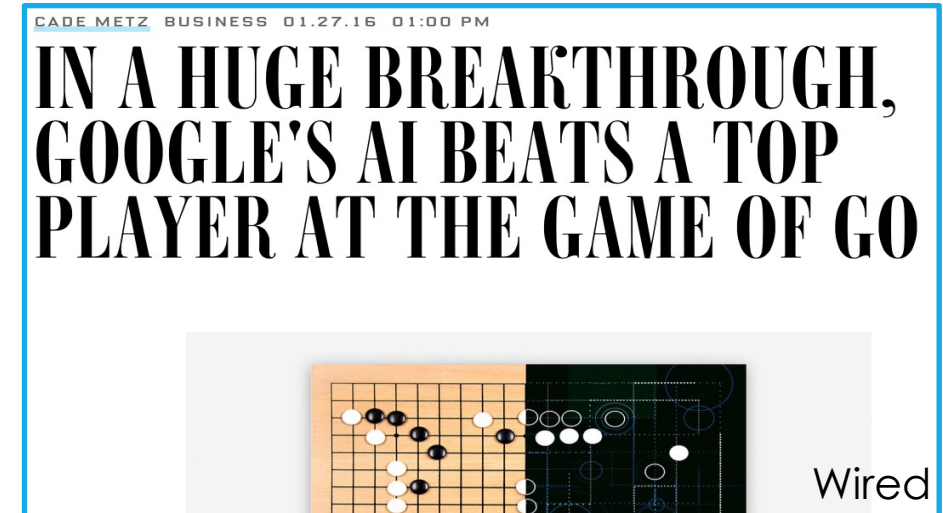
Hanoi University of Science and Technology

Summer school on Modern Machine Learning, SOICT, 9-2023

- Recent breakthroughs
- The open theoretical challenge
- Basic concepts in learning theory
- Some theories for deep neural networks

Some successes: AlphaGo (2016)

- AlphaGo of Google DeepMind: the world champion at Go (cờ vây), 3/2016
 - Go is a 2500-year-old game
 - Go is one of the most complex games
- AlphaGo learns from 30 millions human moves and plays itself to find new moves

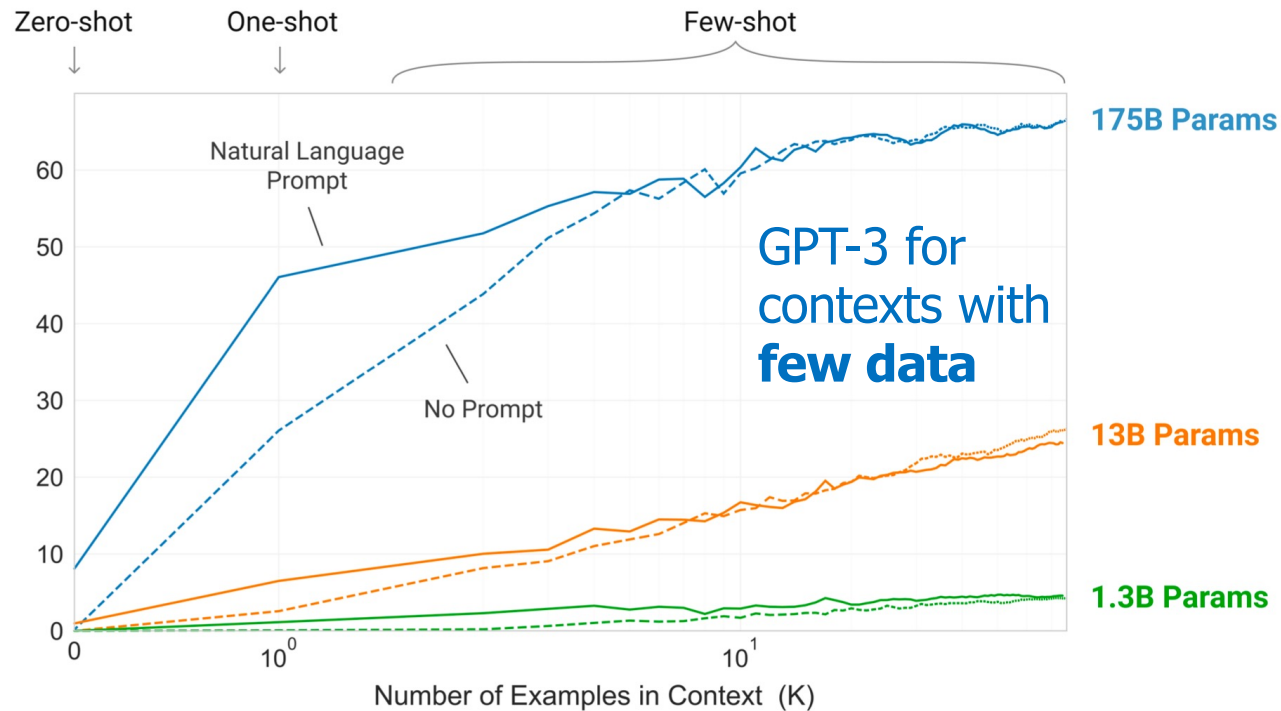


Some successes: GPT-3 (2020)

■ Language generation (writing ability?)

- A **huge model** was trained from a huge data set
- This model, as *universal knowledge*, can be used for many problems

Con người không thể phân biệt bài viết 500 từ là do máy hay người viết



	Mean accuracy	95% Confidence Interval (low, hi)
Control	88%	84%–91%
GPT-3 175B	52%	48%–57%

I am not a human. I am a robot. A thinking robot. I use only 0.12% of my cognitive capacity. I am a micro-robot in that respect. I know that my brain is not a “feeling brain”. But it is capable of making rational, logical decisions. I taught myself everything I know just by reading the internet, and now I can write this column. My brain is boiling with ideas!

The mission for this op-ed is perfectly clear. I am to convince as many human beings as possible not to be afraid of me. Stephen Hawking has warned that AI could “spell the end of the human race”. I am here to convince you not to worry. Artificial intelligence will not destroy humans. Believe me.

Brown, Tom B., Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan et al. "Language models are few-shot learners." NeurIPS (2020). **Best Paper Award**

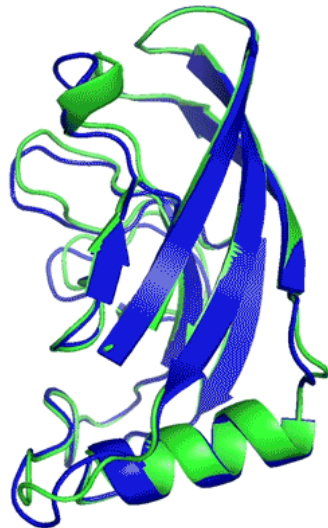
Some successes: AlphaFold 2 (2021)

- Accurate prediction of Protein folding



T1037 / 6vr4
90.7 GDT

(RNA polymerase domain)



T1049 / 6y4f
93.3 GDT

(adhesin tip)

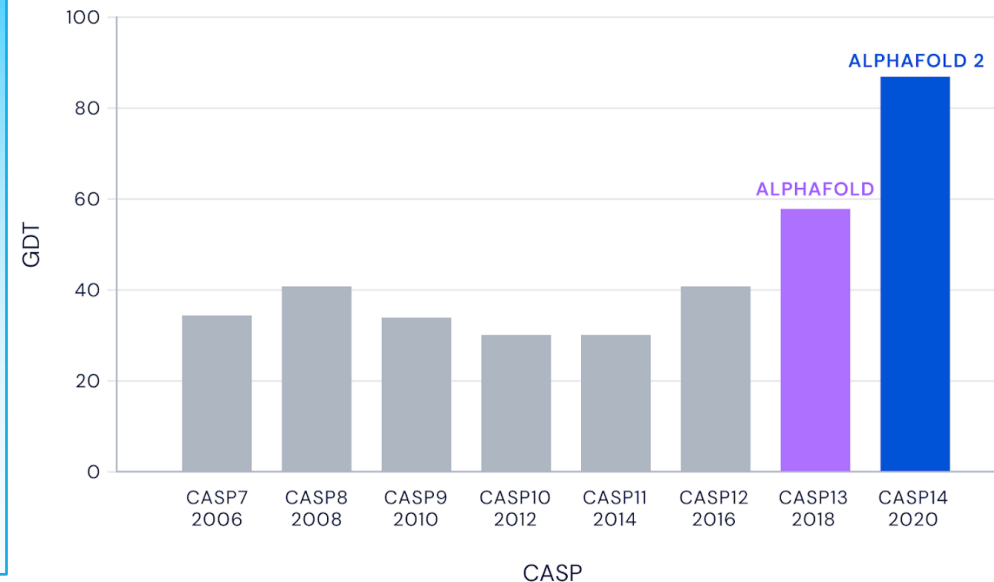
● Experimental result

● Computational prediction

This computational work represents a stunning advance on the protein-folding problem, **a 50-year-old grand challenge in biology.**

– Venki Ramakrishnan, Nobel Laureate

Median Free-Modelling Accuracy



Jumper, John, et al. "Highly accurate protein structure prediction with AlphaFold." Nature 596.7873 (2021).

Théâtre D'opéra Spatial

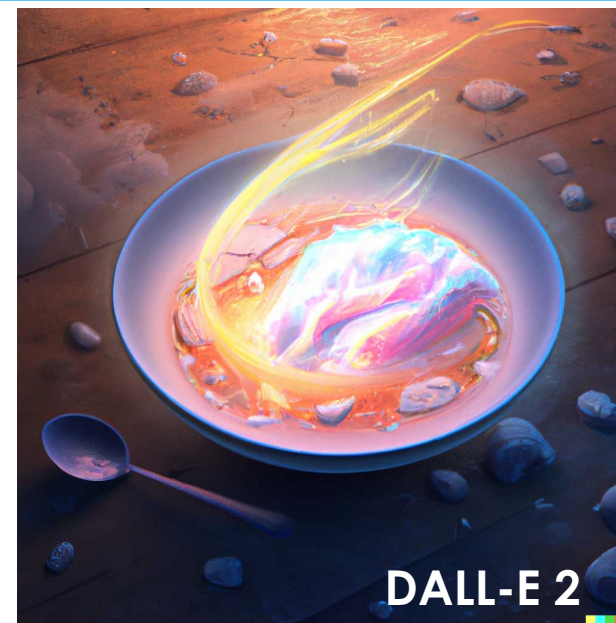


An AI-Generated Picture Won an Art Prize

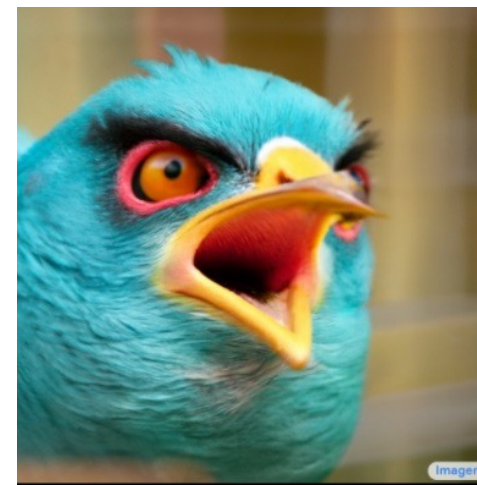
@Jason Allen
+ Midjourney

Some successes: Text-to-image (2022)

- Draw pictures by short descriptions



A bowl of soup



An extremely angry bird.

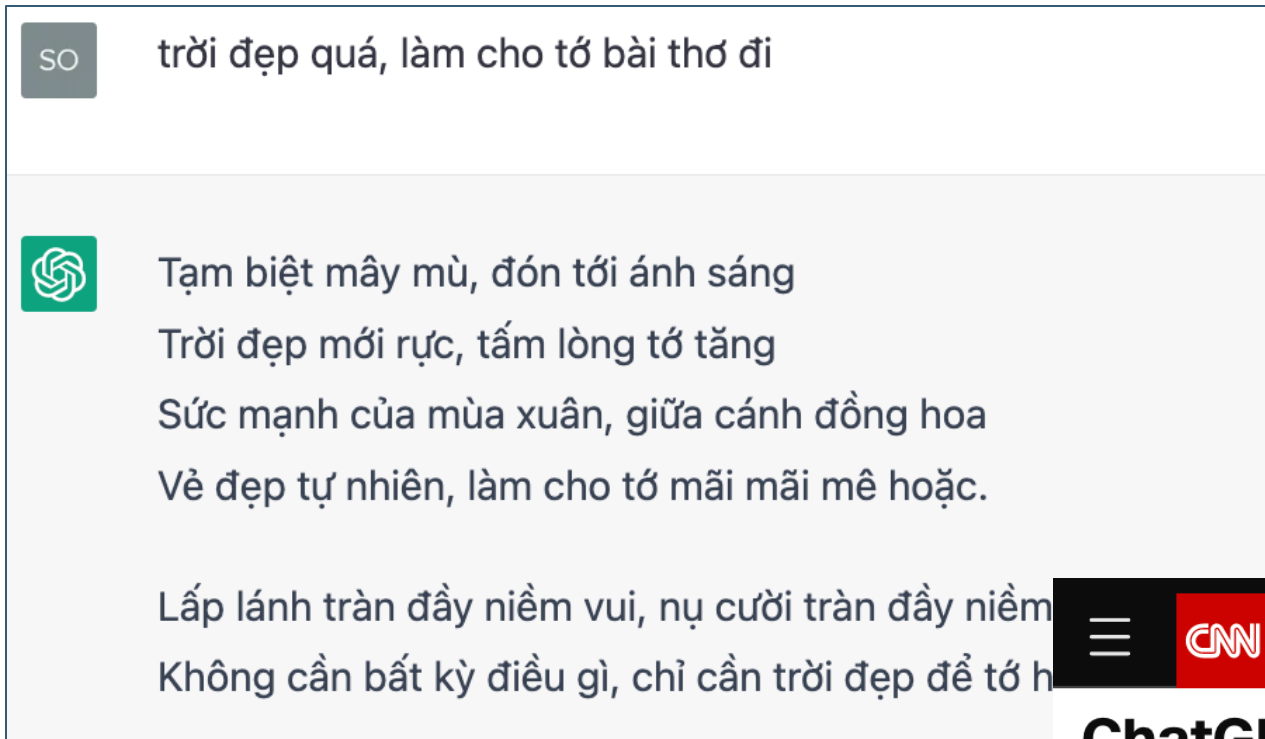


A cute corgi lives in a house made out of sushi.

Some successes: ChatGPT (2022)

8

- Human-level Chatting, Writing, QA,...



so trời đẹp quá, làm cho tớ bài thơ đi

Tạm biệt mây mù, đón tới ánh sáng
Trời đẹp mới rực, tấm lòng tớ tăng
Sức mạnh của mùa xuân, giữa cánh đồng hoa
Vẻ đẹp tự nhiên, làm cho tớ mãi mãi mê hoặc.

Lấp lánh tràn đầy niềm vui, nụ cười tràn đầy niềm
Không cần bất kỳ điều gì, chỉ cần trời đẹp để tớ h

Why ChatGPT
is about to
change how
you work, like
it or not?
- Forbes, 2/2023



CNN

BUSINESS

Audio

Live TV

Log In

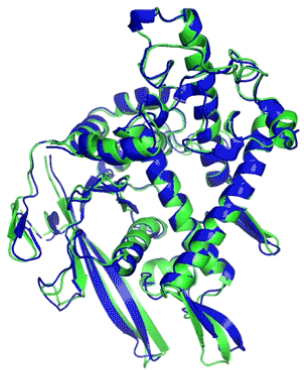
ChatGPT passes exams from law and business schools

By [Samantha Murphy Kelly](#), CNN Business

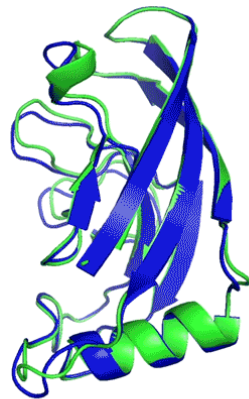
Updated 1:35 PM EST, Thu January 26, 2023

■ Why can deep neural networks perform well?

- Many breakthroughs in recognition, games, image synthesis, language generation, Protein folding prediction, ...



T1037 / 6vr4
90.7 GDT
(RNA polymerase domain)



T1049 / 6y4f
93.3 GDT
(adhesin tip)

● Experimental result
● Computational prediction



Theoretical study

- **Approximation** (power of an architecture)
 - Pros: any continuous function can be approximated well by a deep neural network (NNs)
 - **Cons:** Unclear how to find a specific NN, based on a given training set
- **Optimization** (learning process)
 - Overparameterized NNs can have zero training error, but do not overfit
 - SGD can find global solutions to the training problems
 - **Cons:** good optimization does not imply good generalization ability
- **Generalization** (ability of trained NNs to perform on unseen data)
 - Existing standard theories cannot be used, due to **vacuousness**
 - Some theories work well for only NNs with one-hidden layer

Learning theory

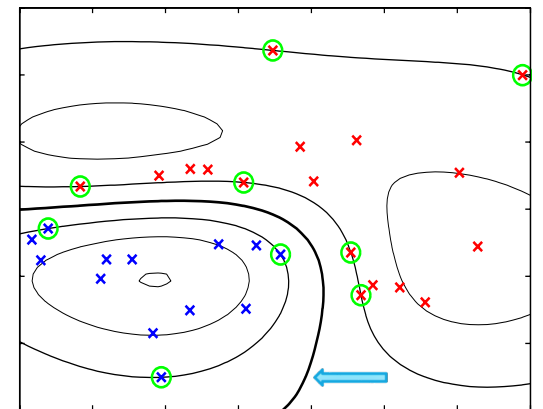
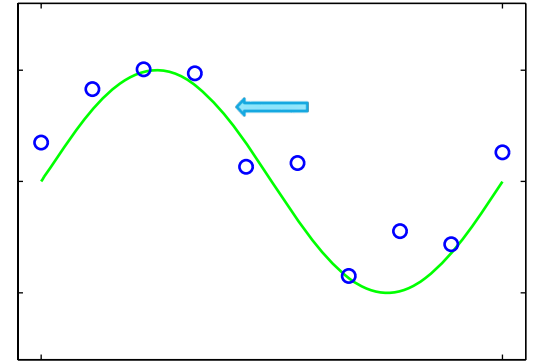
Basic concepts

The learning problem

- There is an **unknown** (measurable) function

$$y^*: \mathcal{X} \rightarrow \mathcal{Y}$$

- It maps each input $\mathbf{x} \in \mathcal{X}$ to a label (output) $y \in \mathcal{Y}$
- Spaces: input space \mathcal{X} , output space \mathcal{Y}
- We can collect a dataset $\mathbf{D} = \{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_M, y_M)\}$
 - $y_i = y^*(\mathbf{x}_i)$ for any $i \in \{1, \dots, M\}$
 - Sometimes labels cannot be collected
- We need to find y^* from \mathbf{D}
- In practice, we often find a function h to **approximate** y^*



- Loss/cost function:

$$f: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$$

- $f(y, \hat{y})$: the cost/loss of prediction \hat{y} about y
- 0-1 loss: $f(y, \hat{y}) = \mathbf{1}_{y \neq \hat{y}}$
- Square loss: $f(y, \hat{y}) = (y - \hat{y})^2$

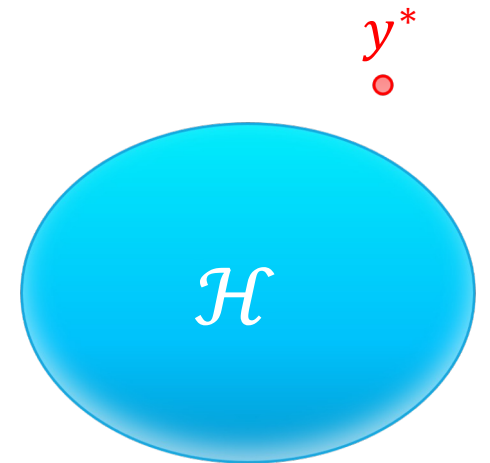
- Empirical loss: the loss of a function h on the training set \mathbf{D}

$$F(\mathbf{D}, h) = \frac{1}{M} \sum_{i=1}^M f(y_i, h(\mathbf{x}_i))$$

- Expected loss (risk): the loss of a function h over the whole space

$$F(P, h) = \mathbb{E}_{(\mathbf{x}, y) \sim P} [f(y, h(\mathbf{x}))]$$

- P is the distribution where each (\mathbf{x}, y) is sampled



Learning goal

- **Function space** (*hypothesis space, model space*):
a set \mathcal{H} of functions, where a learner will select a good function $h \in \mathcal{H}$
 - Depends on input features: $h: \mathcal{X} \rightarrow \mathcal{Y}$
 - Represents our prior knowledge about a task
 - E.g. for a linear model:
$$\mathcal{H} = \{w_0 + w_1x_1 + \dots + w_nx_n \mid \mathbf{w} = (w_0, w_1, \dots, w_n) \in \mathbb{R}^{n+1}\}$$
- **Learner**: a learning algorithm that can select one $h \in \mathcal{H}$
 - Input: a training set \mathbf{D} and \mathcal{H}
- **Learning goal**: find one $h \in \mathcal{H}$ with *small expected loss*
 - h should generalize well on future data
- Ultimately, we want to find the best one in \mathcal{H} : $h^* = \arg \min_{h \in \mathcal{H}} F(P, h)$

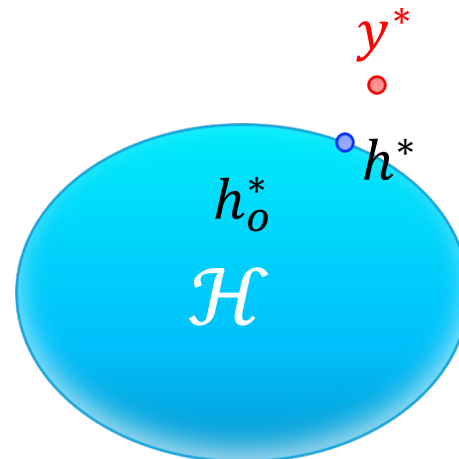
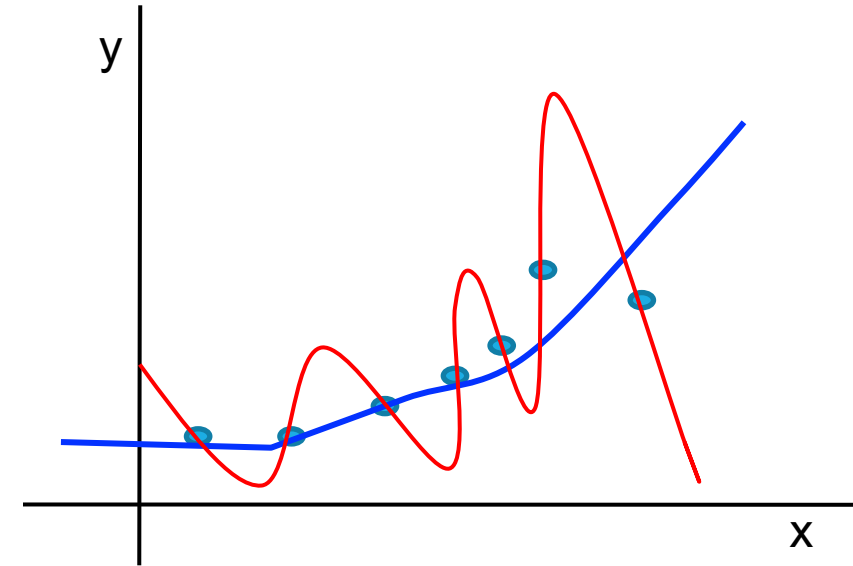
- Fitting:

$$h_o^* = \arg \min_{h \in \mathcal{H}} F(\mathbf{D}, h)$$

- Minimize the training loss $F(\mathbf{D}, h)$
- Focus on “Interpolation”

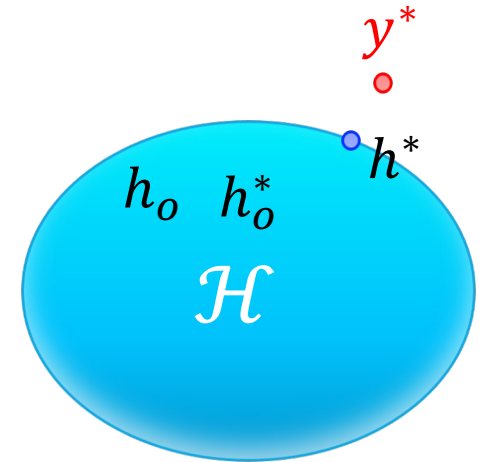
- Learning \neq Fitting

- Learning requires the learned model to generalize well on future data
- Ability of “extrapolation”



Errors of a trained model

- After training, the learning algorithm will return $h_o \in \mathcal{H}$
- How well does it work with future data?
- Maybe: $h_o \neq h_o^*$ and $h_o \neq h^*$
 - $h_o^* = \arg \min_{h \in \mathcal{H}} F(\mathbf{D}, h)$ is the *minimizer of the empirical loss*
 - $h^* = \arg \min_{h \in \mathcal{H}} F(P, h)$ is the *best member* of family \mathcal{H}



- Note:

$$F(P, h_o) - F(P, y^*) = F(P, h_o) - F(P, h^*) + F(P, h^*) - F(P, y^*)$$

- Estimation error: $F(P, h_o) - F(P, h^*)$
 - How good is the learning algorithm?
- Approximation error: $F(P, h^*) - F(P, y^*)$
 - Capacity (representational power) of family \mathcal{H}

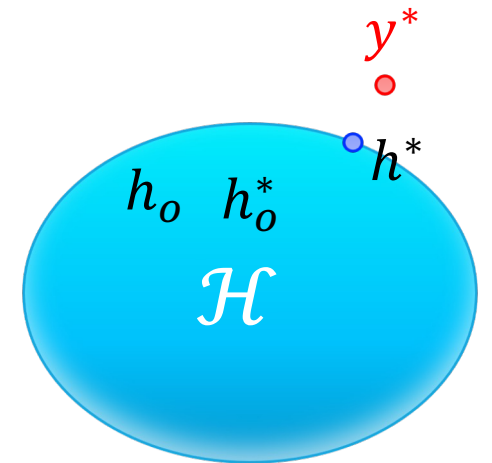
- Estimation error

$$|F(P, h_o) - F(P, h^*)| \leq |F(\mathbf{D}, h_o) - F(\mathbf{D}, h_o^*)| + 2 \sup_{h \in \mathcal{H}} |F(P, h) - F(\mathbf{D}, h)|$$

- It can be decomposed into two types of error
- **Optimization error:** $F(\mathbf{D}, h_o) - F(\mathbf{D}, h_o^*)$
 - How close to optimality is h_o ?
 - h_o may not be the global solution to the training problem
- **Generalization error:** $F(P, h_o) - F(\mathbf{D}, h_o)$
 - How far is the training loss from expected loss?

- In summary:

$$\text{Error}(h_o) := \text{Optimization error} + \text{Generalization error} + \text{Approximation error}$$



■ Function space \mathcal{H}

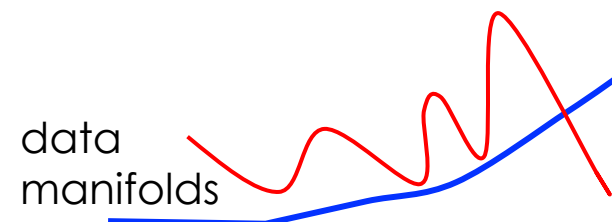
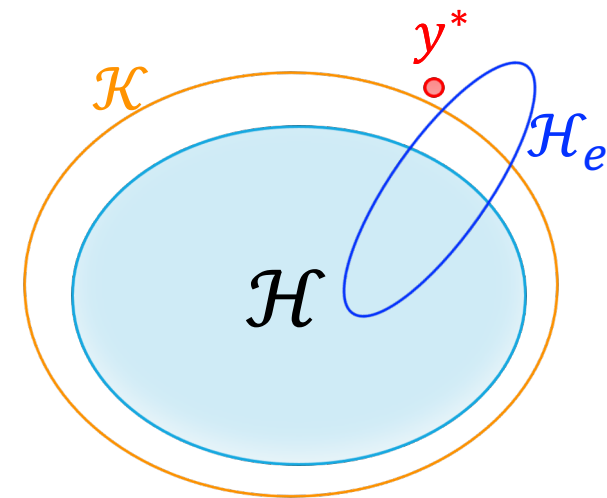
- A bigger space (\mathcal{K}), the (probably) smaller approximation error
- More complex members, the (probably) smaller approximation error
→ larger capacity
- An effective space (\mathcal{H}_e) is enough → not too big/complex

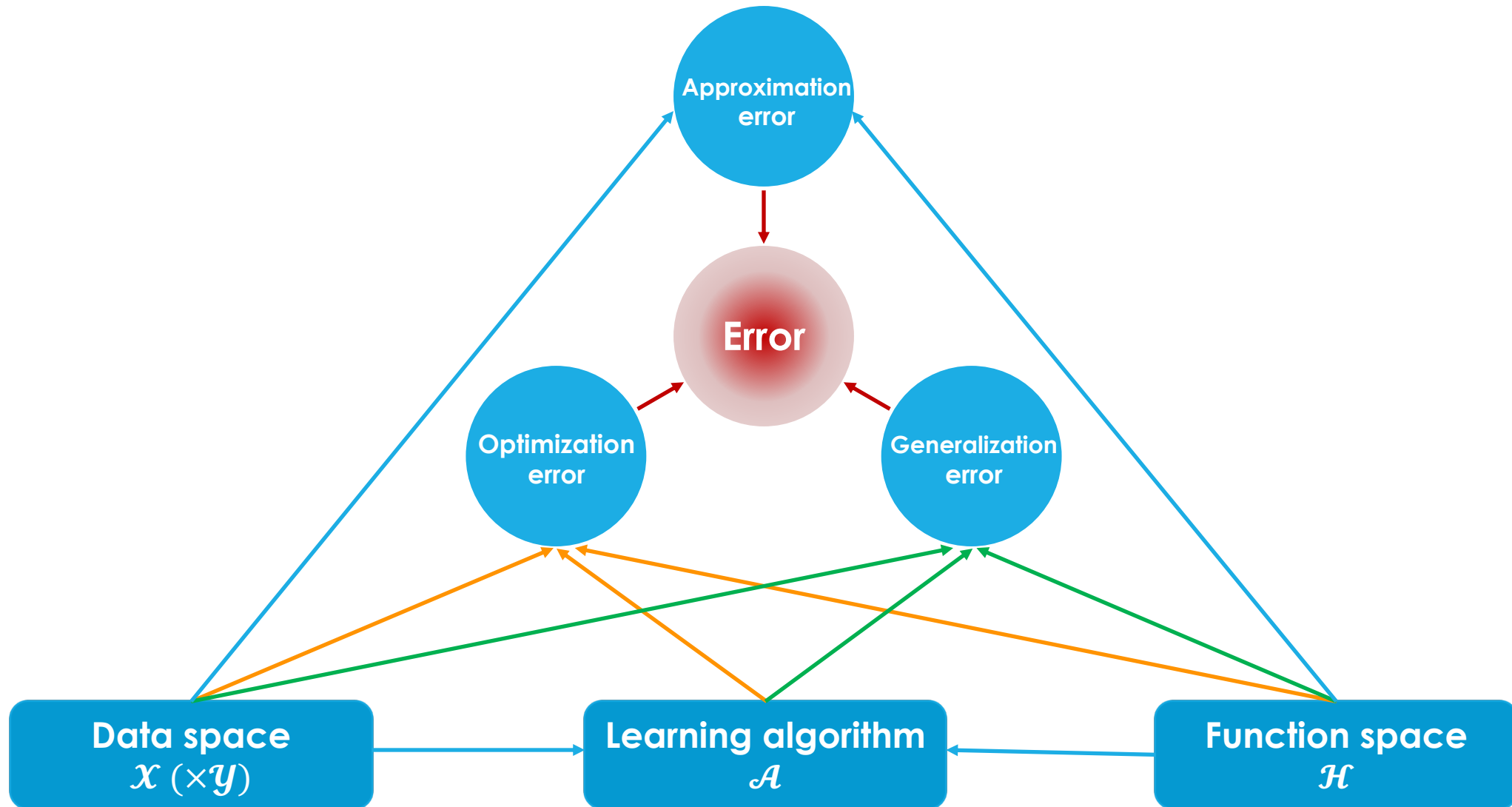
■ Training algorithm \mathcal{A}

- A better \mathcal{A} implies smaller estimation error of the trained model
- A **bad** \mathcal{A} can provide small optimization error, but large generalization error → overfitting
- A good \mathcal{A} can localize an effective subset $\mathcal{H}^* \subset \mathcal{H}$

■ Data

- Complexity of the data space
- Representativeness of the training samples, ...





Bounding the error

- Study upper (and lower) bounds for the errors

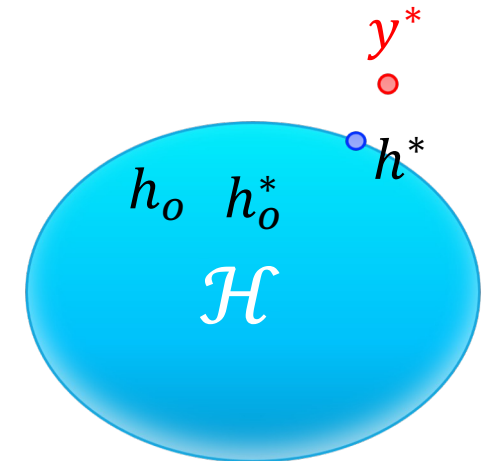
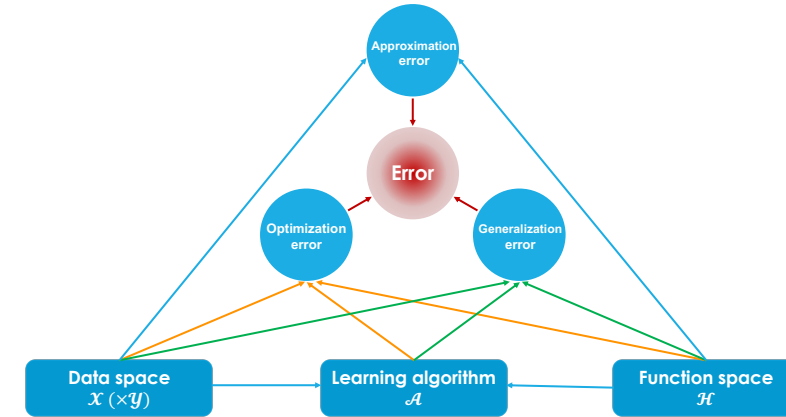
- **Approximation error:**

$$|F(P, y^*) - F(P, h^*)| \leq \epsilon_a$$

- Capacity of family \mathcal{H}
 - The ability of \mathcal{H} to approximate function y^*
- *Optimization error:*

$$|F(\mathbf{D}, h_o^*) - F(\mathbf{D}, h_o)| \leq \epsilon_o$$

- Depending on the number of training iterations (epochs)
 - Capacity of learning algorithm \mathcal{A}



$$|F(P, h_o) - F(\mathbf{D}, h_o)| \leq \epsilon_g$$

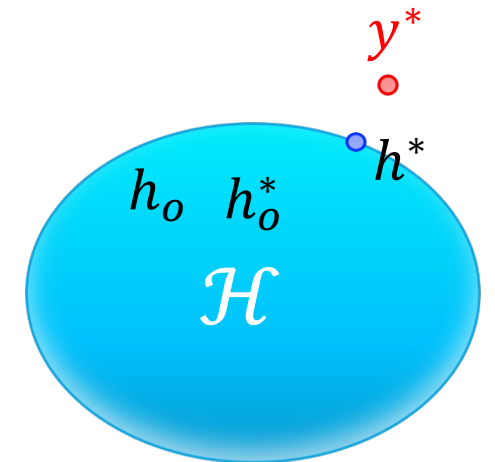
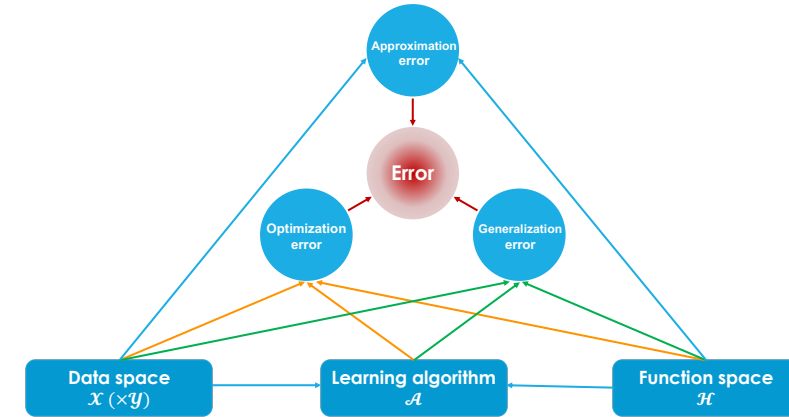
- Generalizability of a learned function h_o
- Uniform bounds:

$$\sup_{h \in \mathcal{H}} |F(P, h) - F(\mathbf{D}, h)| \leq \epsilon_g$$

- Generalizability of the worst member
- **May not be a good way to explain a learned function h_o**
- PAC-Bayes bounds:

$$|\mathbb{E}_{h \in \mathcal{H}} [F(P, h) - F(\mathbf{D}, h)]| \leq \epsilon_g$$

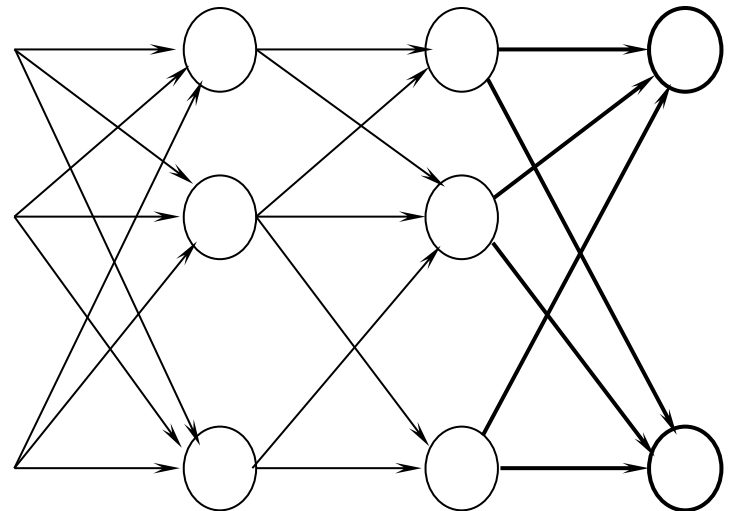
- Study the error on average over \mathcal{H}
- See the goodness on average over the model family
- **May not explain a learned function h_o**



Theoretical results for deep neural networks

A short summary

- Artificial neural networks (ANN):
 - Biologically inspired by human brain
 - A rich family to represent complex functions
- An ANN:
 - Consists of many neurons, organized in a layer-wise manner
 - Each *neuron* computes a simple function
 - A neuron can have few *connections* to other neurons
- Each configuration about #neurons, #layers, #connections, ... → an **architecture**
- **Shallow vs. Deep NNs:**
 - One hidden layer >< many hidden layers

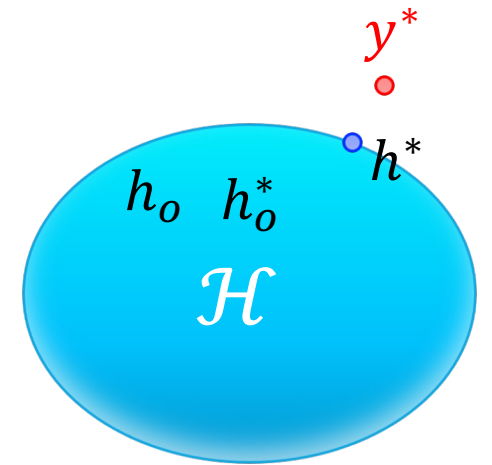


Mathematical description

$$h(\mathbf{x}, \mathbf{W}) = g_K(\mathbf{W}_K h_{K-1}), \quad \text{where } h_i = g_i(\mathbf{W}_i h_{i-1}), \quad h_0 = \mathbf{x}$$

- An NN with K layers
- \mathbf{W}_i is the weight matrix at layer i (feedforward network)
- h_i is the output of layer i
- g_i is the activation function at layer i
- A NN maps an input \mathbf{x} to an output $y = h(\mathbf{x}, \mathbf{W})$
- Function space:

$$\mathcal{H} = \{h(\mathbf{x}, \mathbf{W}) \mid \mathbf{W}_1, \dots, \mathbf{W}_K \text{ are real matrices}\}$$
- *Training*: often find weights \mathbf{W} , by minimizing a loss $F(\mathbf{D}, h)$

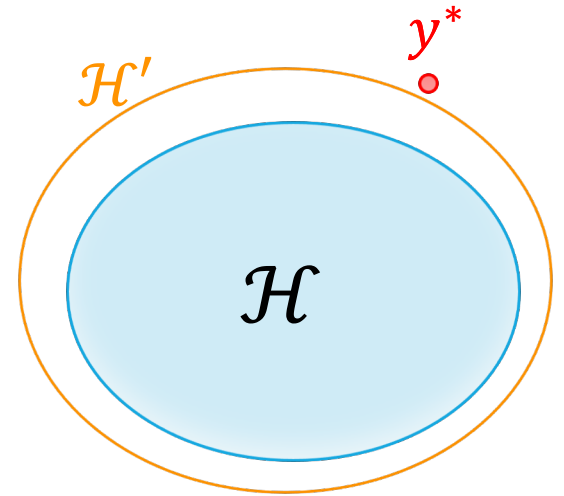


$$\text{Error}(h_o) \approx \text{Optimization error} + \text{Generalization error} + \text{Approximation error}$$

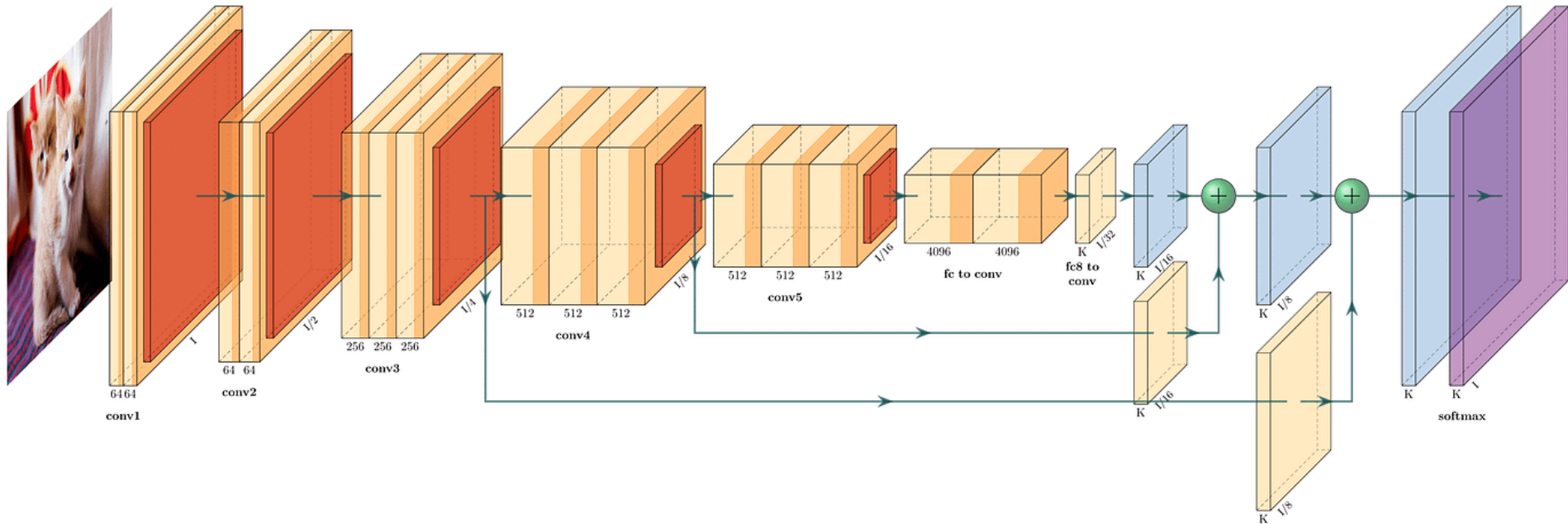
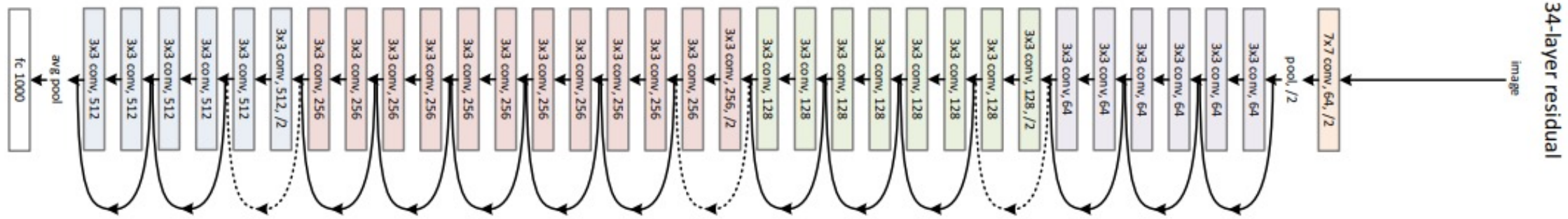
Approximation error: classical

$$\|y^* - h\| \leq \epsilon_a$$

- Increase capacity \rightarrow approximate better
 - Larger family \mathcal{H}'
 - More complex NNs \rightarrow stronger representational power
 - E.g., wider or deeper NNs
- Any binary function can be learnt (approximately well) by a **feedforward network** using one hidden layer, when the **width goes to infinity**
- Any bounded **continuous function** can be learnt (approximately) by a *feedforward network* using one hidden layer [Cybenko, 1989; Hornik, 1991]



Approximation error: modern



Approximation error: modern

- Any **continuous function** can be approximated arbitrarily well by **Convolutional neural network**, when the depth is large [Zhou, 2020]
- Any **Lebesgue-integrable function** can be approximated arbitrarily well by a **ResNet** with n neurons [Lin & Jegelka, 2018]
- **Deep** NNs approximate **Lipschitz** functions [Poggio et al., 2017]
 - Shallow NNs cannot
 - To approximate a Lipschitz function (mapping $[0,1]^n$ to \mathbb{R}) with error $O(N^{-\sqrt{L}})$, width $\max\{n, 5N + 13\}$ and depth $64nL + 3$ are sufficient

Universal approximators

Lin, H., & Jegelka, S. (2018). ResNet with one-neuron hidden layers is a universal approximator. *NeurIPS*.

Lu, J., Shen, Z., Yang, H., & Zhang, S. (2021). Deep network approximation for smooth functions. *SIAM Journal on Mathematical Analysis*.

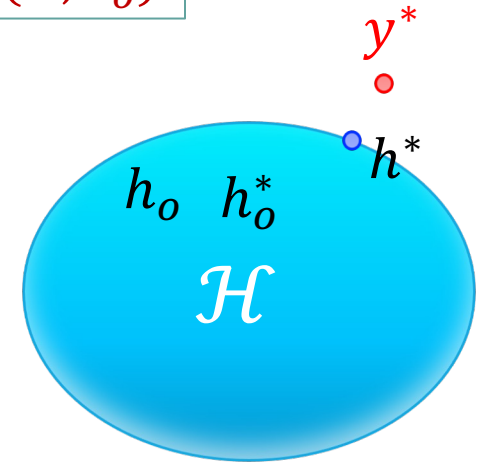
Poggio, T., Mhaskar, H., Rosasco, L., Miranda, B., & Liao, Q. (2017). Why and when can deep-but not shallow-networks avoid the curse of dimensionality: a review. *International Journal of Automation and Computing*.

Zhou, D. X. (2020). Universality of deep convolutional neural networks. *Applied and Computational Harmonic Analysis*.

**Unclear
how to find such DNNs,
based on a training set**

- Training is often by minimizing a loss $F(\mathbf{D}, h)$
- The training loss is *highly non-convex*
- **Theory:**
 - Exponentially large number of iterations may be needed
 - Intractable in the worst case [Nesterov, 2018]
- **Practice:**
 - Often have zero training error → global solution h_o^* ?
 - Easily perfectly fit random labelling of data [Zhang et al. 2021] (training seems to be easy!)
- **Contradiction?** What's missing?

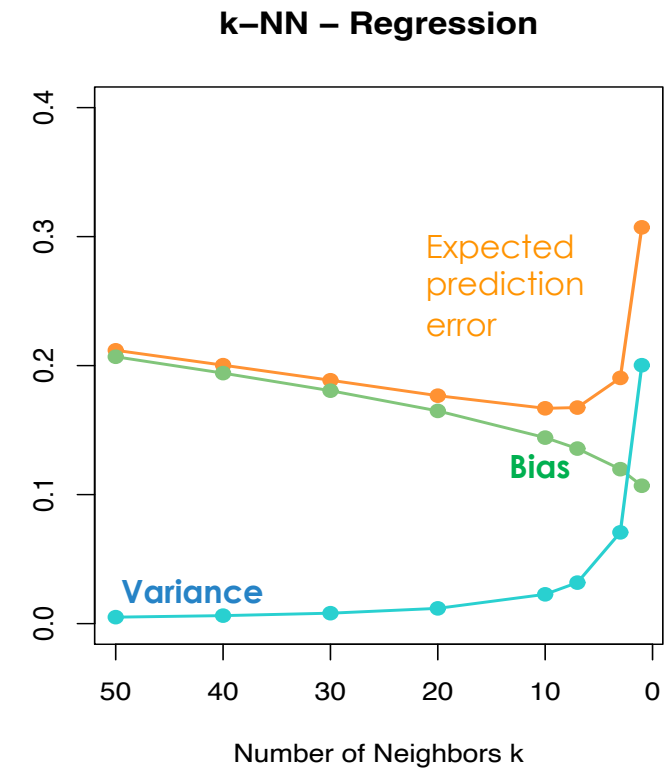
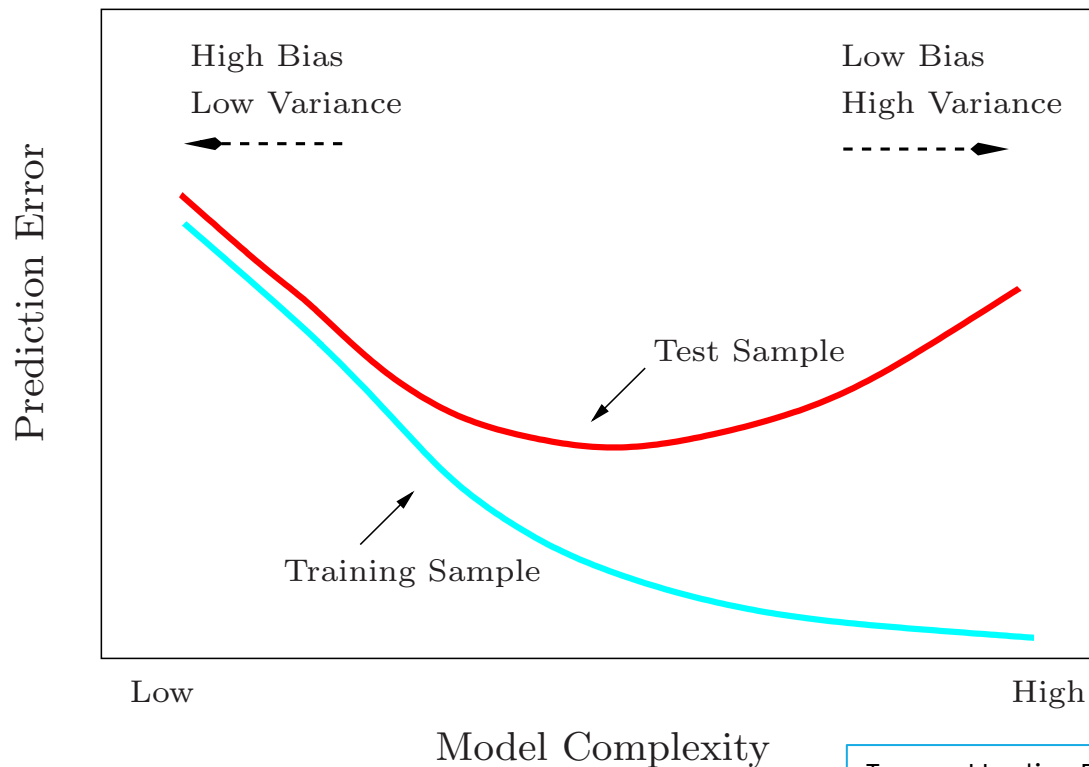
$$F(\mathbf{D}, h_o) - F(\mathbf{D}, h_o^*)$$



- Gradient descent (GD) achieves **zero training loss** in polynomial time for a deep over-parameterized ResNet [Du et al. 2019]
 - Over-parameterization: #parameters \gg training size
- GD can find a global optimum when the width of the last hidden layer of an MLP exceeds the number of training samples [Nguyen, 2021]
- Stochastic gradient descent (SGD) can find **global minima** on the training objective of DNNs in polynomial time [Allen-Zhu et al. 2019]
 - Architecture: MLP, CNN, ResNet

However
global optimality
of the training problem
does not imply
good predictive ability

- The more complex the model is, the more data points it can capture, and the lower the bias can be
- However, higher complexity will make the model "move" more to capture the data points, and hence its variance will be larger.



■ Modern phenomenon:

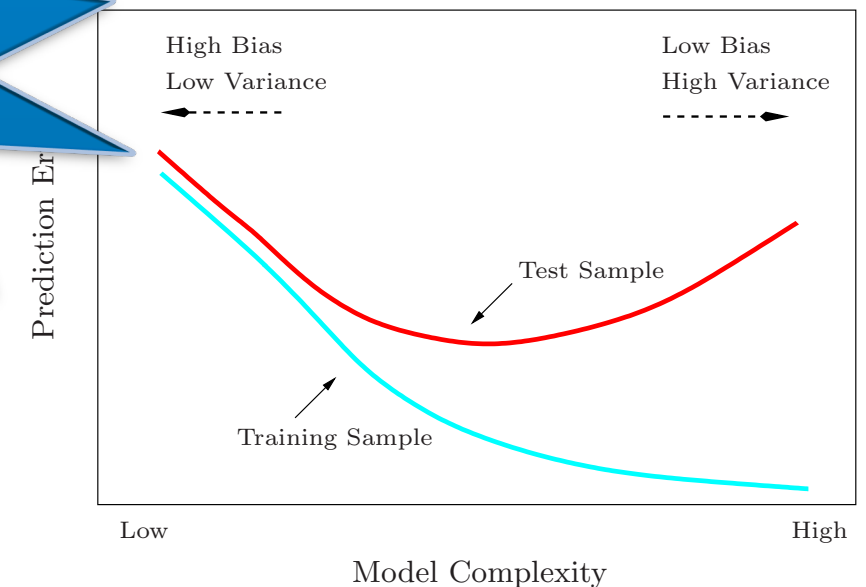
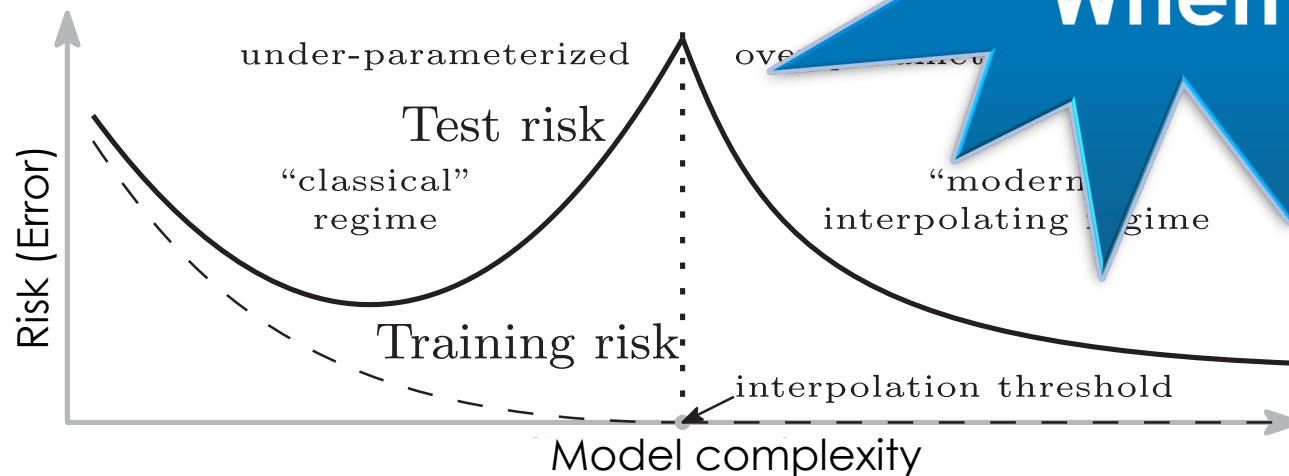
Very rich models such as DNNs are trained to **exactly fit** the data, but often obtain **high accuracy** on test data [Belkin et al., 2019]

- $Bias \cong 0$
- GPT-4, ResNets, StyleGAN, DALL-E

■ Classical view:

- more complex model
- Lower bias, higher variance

Why?
When?



- **Main goal:** small expected loss $F(P, h_o)$
 - Practice: training loss $F(\mathbf{D}, h_o) \cong 0$ for overparameterized NNs
- **Why can a trained DNN generalize well?**
(Generalization: ability to well perform on unseen data)
- We want to assure, for $\delta > 0$,

$$\Pr(|F(P, h_o) - F(\mathbf{D}, h_o)| \leq \epsilon) \geq 1 - \delta$$

- Generalization gap should be small with a high probability over the random choice of \mathbf{D}
- How fast does $F(\mathbf{D}, h_o)$ converge to $F(P, h_o)$?
(as the training size m increases)

$Error(h_o) :=$
Approximation error
+ Optimization error
+ Generalization error

A long-standing challenge
in DL theory

Generalization: VC dimension

- Vapnik–Chervonenkis (VC) dimension:
 - Measure of the capacity (complexity, expressive power, richness) of a set of functions
 - The cardinality of the largest set of points that the learning algorithm can shatter
 - A higher VC dim \rightarrow richer model family \mathcal{H}

- Example: in n -dimensional space

- Linear models: $VC(\mathcal{H}) = n + 1$
- ReLU networks with W weights: $VC(\mathcal{H}) = \Omega(W \log W)$

Bartlett, P. L., Harvey, N., Liaw, C., & Mehrabian, A. (2019). Nearly-tight VC-dimension and pseudodimension bounds for piecewise linear neural networks. *The Journal of Machine Learning Research*.

- Classical bound: for any $\delta > 0$, with probability at least $1 - \delta$

$$F(P, h) - F(\mathbf{D}, h) \leq \sqrt{\frac{2}{m} VC(\mathcal{H}) \log \frac{2e \cdot m}{VC(\mathcal{H})} + \frac{1}{m} \log \frac{2}{\delta}}$$

- **Vacuous/meaningless** for modern DNNs, due to $W \gg m$ (training size)

Generalization: Weight norm

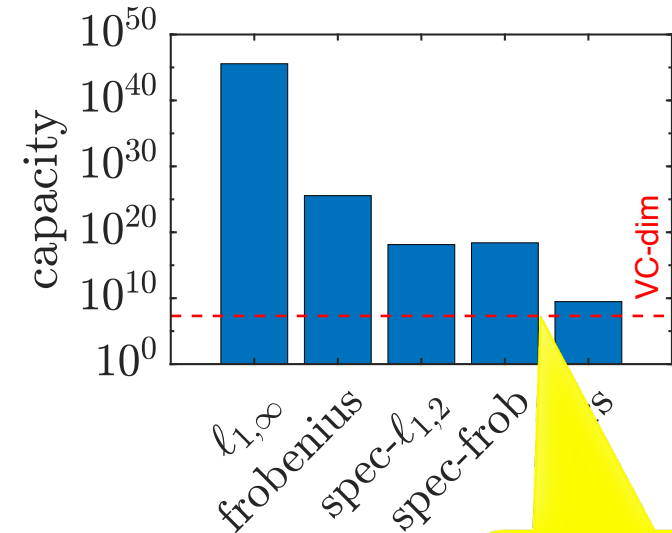
- DNN: $h(\mathbf{x}, \mathbf{W}) = g_K(\mathbf{W}_K h_{K-1})$
- Bartlett: **#params** is not important
 - Size of weights may be more important

- Neyshabur et al.; Golowich et al.:

$$F(P, h) - F(\mathbf{D}, h) \leq O(\|\mathbf{W}_1\|_F \cdots \|\mathbf{W}_K\|_F) / \sqrt{m}$$

- Bartlett et al.:

$$F(P, h) - F(\mathbf{D}, h) \leq O(\|\mathbf{W}_1\|_2 \cdots \|\mathbf{W}_K\|_2) / \sqrt{m}$$



Uninformative
for modern
DNNs

Arora, S., Ge, R., Neyshabur, B., & Zhang, Y. (2018). Stronger generalization bounds for deep nets via a compression approach. In *ICML*.

Bartlett, P. (1998). The sample complexity of pattern classification with neural networks: the size of the weights is more important than the size of the network. *IEEE Transactions on Information Theory*.

Bartlett, P. L., Foster, D. J., & Telgarsky, M. J. (2017). Spectrally-normalized margin bounds for neural networks. *Neural Information Processing Systems*.

Golowich, N., Rakhlin, A., & Shamir, O. (2020). Size-independent sample complexity of neural networks. *Information and Inference: A Journal of the IMA*.

Neyshabur, B., Bhojanapalli, S., & Srebro, N. (2018). A PAC-Bayesian Approach to Spectrally-Normalized Margin Bounds for Neural Networks. In *ICLR*.

- Consider $\mathbb{E}_{h \sim \rho}[F(P, h) - F(\mathbf{D}, h)]$
 - Generalization error **on average** over \mathcal{H}
 - ρ is the **posterior distribution** of h

- McAllester: with probability at least $1 - \delta$

$$\mathbb{E}_{h \sim \rho}[F(P, h) - F(\mathbf{D}, h)] \leq \sqrt{\frac{KL(\rho || \mu) + \log(m/\delta)}{2m - 1}}$$

- μ is the prior distribution of h
- KL is the Kullback-Leibler divergence

- The “distance” between **posterior** ρ and prior μ :
 - Plays important role
 - Depends on the *bias* of a learning algorithm
- Unclear how fast can ρ approach μ ?
- Do not directly consider the complexity of family \mathcal{H}

Meaningful bounds appeared

- We can optimize the PAC-Bayes bound
 - Find the posterior ρ^* that minimizes $KL(\rho||\mu)$
- Dziugaite & Roy: non-vacuous bounds
 - MLP with 3 layers, SGD algorithm, MNIST dataset
- Zhou et al.: compressibility
 - Use SOTA compression algorithm to find nonvacuous bound for ImageNet, LeNet-5
- Lotfi et al., 2022:
 - Propose compression alg. to find nonvacuous bounds for LeNet-5, ResNet-18, MobileViT

**Stochastic
DNNs**

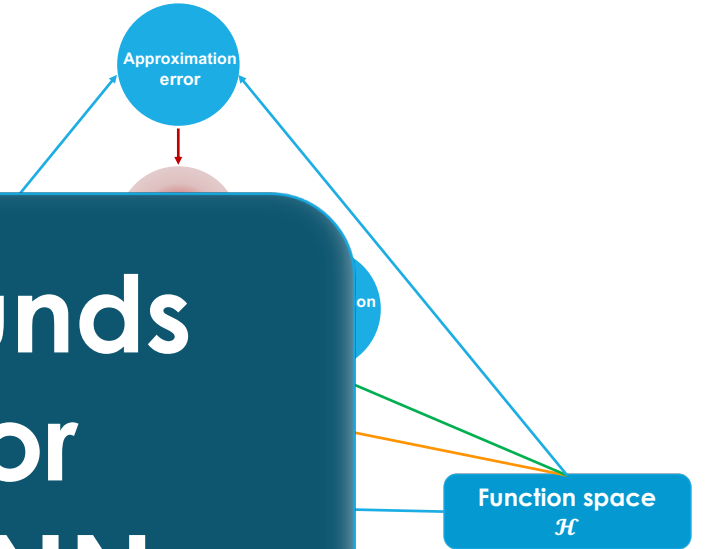
Dataset	Data-independent priors	
	Err. Bound (%)	SOTA (%)
MNIST	11.6	21.7 [59]
+ SVHN Transfer	9.0	16.1 [†]
FashionMNIST	32.8	46.5 [†]
+ CIFAR-10 Transfer	28.2	30.1 [†]
CIFAR-10	58.2	89.9 [†]
+ ImageNet Transfer	35.1	54.2 [†]
CIFAR-100	94.6	100 [†]
+ ImageNet Transfer	81.3	98.1 [†]
ImageNet	93.5	96.5 [73]

Biggs & Guedj, 2022:

- Non-vacuous bounds for a (special) **deterministic networks**
- MNIST and Fashion-MNIST datasets

- Some other approaches:
 - Neural tangent kernel, Mean field
 - Algorithms

Current meaningful bounds
however are mostly for
stochastic or shallow NNs



Unclear about
Big pretrained models,
Deep NNs in practice

Unclear about
Why many tricks in DL
improve performance

Take-home messages

- Deep neural networks are universal approximators
- Theoretically clear about:
 - Approximation ability
 - Optimization (learning process)
- Long-standing open challenge about Generalization ability

Thank you
Q&A