Machine Learning Theory 2024
Lecture 7

Tim van Erven

- Complexity of classification vs regression
- Neural networks
- Bias-variance trade-off and double descent
- Towards an explanation

Binary Classification

- Sample complexity of agnostic PAC-learnability **determined by VC-dimension**:

$$m_{\mathcal{H}}(\epsilon, \delta) \approx \frac{\mathrm{VCdim}(\mathcal{H}) + \ln(1/\delta)}{\epsilon^2}$$

- For some (not all!) hypothesis classes, $\mathrm{VCdim}(\mathcal{H}) =$ **nr. of parameters**:
  - **Linear predictors**: $\mathcal{H} = \{h_{\boldsymbol{w}}(\boldsymbol{X}) = \mathrm{sign}(\langle \boldsymbol{w}, \boldsymbol{X} \rangle) : \boldsymbol{w} \in \mathbb{R}^d\}$
  - Axis-aligned rectangles
  - ...

Regression

$$\mathcal{H}_1^B = \{h_{\boldsymbol{w}}(\boldsymbol{X}) = \langle \boldsymbol{w}, \boldsymbol{X} \rangle : \boldsymbol{w} \in \mathbb{R}^d, \|\boldsymbol{w}\|_1 \leq B\}.$$

Theorem (Lasso Estimator)

Consider linear regression with $\ell(h, \boldsymbol{X}, Y) = \frac{1}{2}(Y - \langle \boldsymbol{w}, \boldsymbol{X} \rangle)^2$ *for* $\boldsymbol{X} \in [-1, +1]^d$, $Y \in [-1, +1]$.
Then $\mathcal{H}_1^B$ *is agnostically PAC-learnable by ERM with sample complexity*

$$m(\epsilon, \delta) \leq c_B \frac{\ln(2d) + \ln(2/\delta)}{\epsilon^2}$$

for some constant $c_B > 0$ *that depends only on* B*.*

General pattern for regression tasks:

- **Complexity** of hypothesis class **depends on bound** B on norm $\|\boldsymbol{w}\|$ of parameters
- (and sometimes weakly on number of parameters d)

Difference between Linear Regression and Linear Classification

Linear Classification:

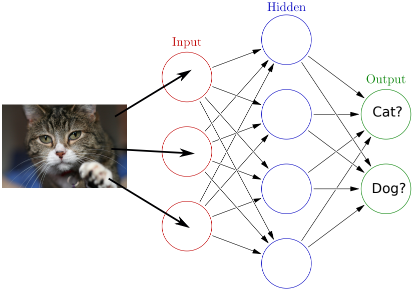
- **Not Lipschitz in w**: tiny change in $\boldsymbol{w}$ can flip prediction $h_{\boldsymbol{w}}(\boldsymbol{X})$
- Measure of complexity: **number of parameters** d

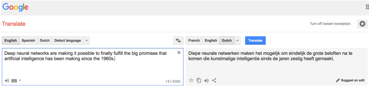
Linear Regression:

- **Lipschitz in w**: tiny change in $\boldsymbol{w}$ implies tiny change in $h_{\boldsymbol{w}}(\boldsymbol{X})$
- Main measure of complexity: **norm constraint** B

Deep Learning / Neural Networks

(Deep) Neural Networks





Deep neural networks are making it possible to finally fulfill the big promises that artificial intelligence has been making since the 1960s.

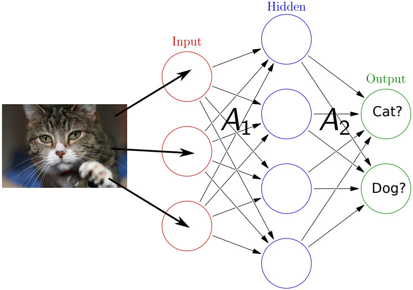
Diepe neurale netwerken maken het mogelijk om eindelijk de grote beloften na te komen die kunstmatige intelligentie sinds de jaren zestig heeft gemaakt.

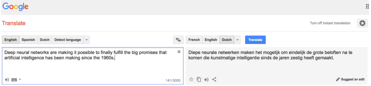
Machine translation

Speech recognition

Self-driving cars

(Deep) Neural Networks





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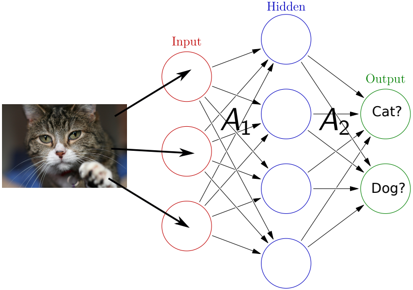
Class of **non-convex** functions parametrized by matrices $\boldsymbol{w} = (A_1, \ldots, A_m)$:

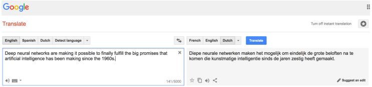
Fully connected network: $\mathcal{H} = \{h_{\boldsymbol{w}}(\boldsymbol{X}) = A_m \sigma A_{m-1} \cdots \sigma A_1 \boldsymbol{X} : \boldsymbol{w} \in \mathcal{W}\}$,

with **activation function** $\sigma(z)$ applied component-wise to vectors. E.g.

- Rectified linear unit (ReLU): $\sigma(z) = \max\{0, z\}$
- Sigmoid: $\sigma(z) = 1/(1 + e^{-z})$

(Deep) Neural Networks





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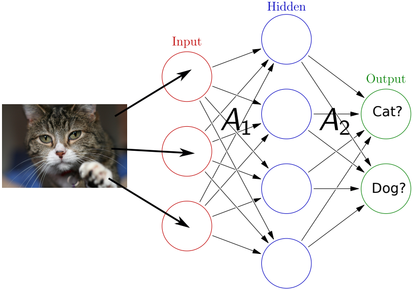

VC-dimension dependence on nr. of parameters d:

ReLU:	$\tilde{\Theta}(d)$	[Bartlett et al., 2017]
Sigmoid:	$\Theta(d^2)$	[Anthony and Bartlett, 1999]

Conclusion: need sample size $m \gg$ **nr. of parameters** to learn

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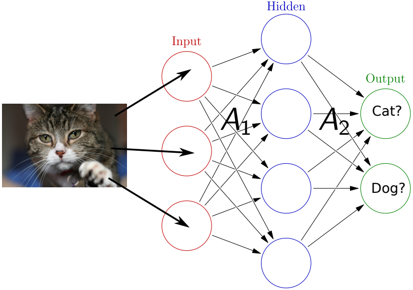

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Fully c … $: \boldsymbol{w} \in \mathbb{R}^d\}$,

with **a** … E.g.

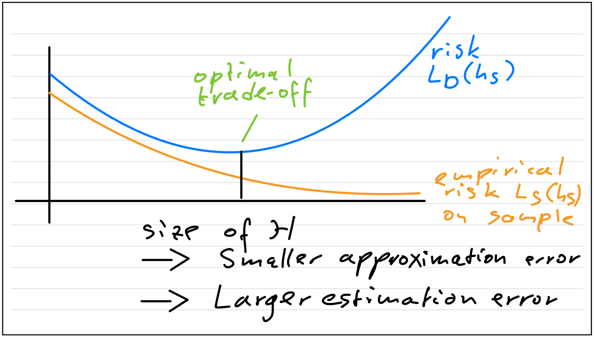
- R…
- Sigmoid: $\sigma(z) = 1/(1 + e^{-z})$

A First Glimpse of a Mystery:

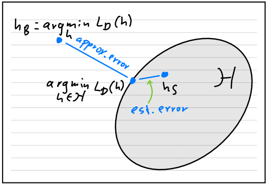
- In theory: need sample size $m \gg$ nr. parameters d
- In practise: sample size $m \ll$ nr. parameters d

Bias-Variance Trade-off and the Double Descent Phenomenon

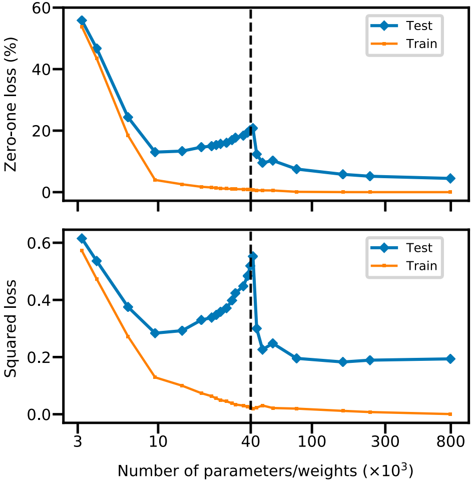
Classical Bias-Variance Trade-off



- Approximation error (bias): $\inf_{h\in\mathcal{H}} L_{\mathcal{D}}(h) - \inf_h L_{\mathcal{D}}(h)$
- Estimation error (variance): $L_{\mathcal{D}}(h_S) - \inf_{h\in\mathcal{H}} L_{\mathcal{D}}(h)$


$h_B := \arg\min_h L_D(h)$
approx. error
$\arg\min_{h\in\mathcal{H}} L_D(h)$
h_S
$\mathcal{H}$
est. error

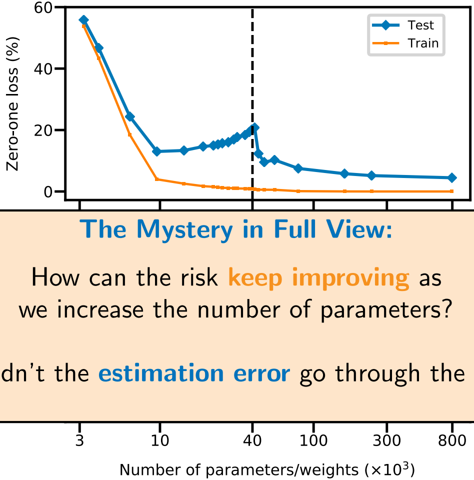
Double Descent Phenomenon



[Belkin, Hsu, Ma, Mandal, 2019]

- Varying the number of hidden units in a two-layer neural network
- Classification: MNIST hand-written digits data with 10 classes

Double Descent Phenomenon



The Mystery in Full View:

How can the risk **keep improving** as
we increase the number of parameters?

Shouldn't the **estimation error** go through the roof?

[Belkin, Hsu, Ma, Mandal, 2019]

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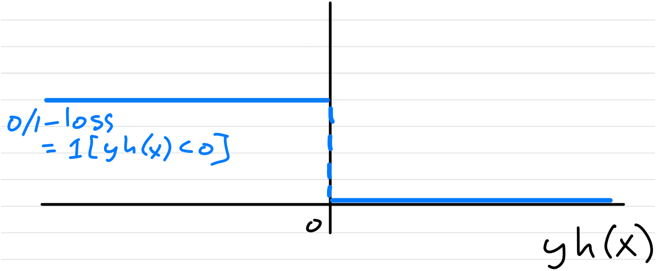
Towards an Explanation

1. **Large margins turn classification into regression**
2. Explaining double descent

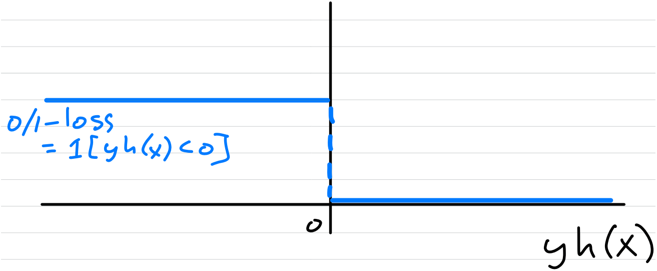
Classifiers as Real-valued Functions



NB Real-valued classifiers. E.g. $h_{\boldsymbol{w}}(\boldsymbol{X}) = \langle \boldsymbol{w}, \boldsymbol{X} \rangle$.
Prediction is sign$(h(\boldsymbol{X}))$

- **Margin** $= Yh(\boldsymbol{X})$, where $Y \in \{-1, +1\}$
- Larger margin > 0: more confident correct classification

Classifiers as Real-valued Functions



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Prediction is $\text{sign}(h(\boldsymbol{X}))$

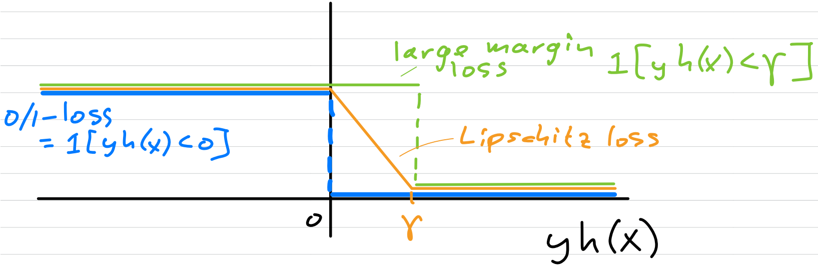
- **Margin** $= Yh(\boldsymbol{X})$, where $Y \in \{-1, +1\}$
- Larger margin > 0: more confident correct classification
- Common loss functions encourage finding large margin solutions:

$$\text{logistic loss: } \ln(1 + e^{-Yh(\boldsymbol{X})})$$

$$\text{squared loss for classification: } (Y - h(\boldsymbol{X}))^2 = (1 - Yh(X))^2$$

Large Margins 1

[Anthony and Bartlett, 1999]



0/1-loss $\leq$ γ-Lipschitz loss $\leq$ γ-large margin loss

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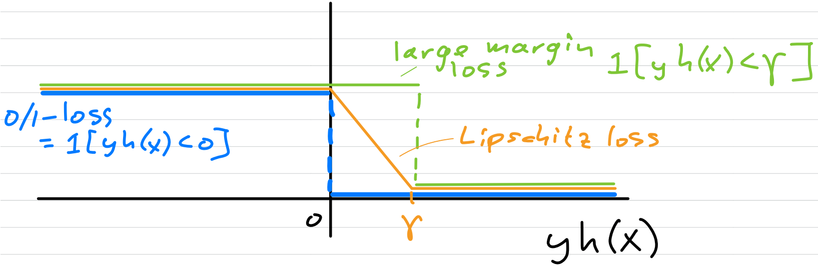

0/1-loss ≤ γ-Lipschitz loss ≤ γ-large margin loss

$$
\begin{aligned}
L_{\mathcal{D}}^{0/1}(h_S) &\leq L_{\mathcal{D}}^{\text{Lipschitz}}(h_S) \\
&\leq L_S^{\text{Lipschitz}}(h_S) + 2\,\mathbb{E}[\mathcal{R}(\ell^{\text{Lipschitz}}, \mathcal{H}, S)] + \sqrt{\frac{\ln(4/\delta)}{2m}} \quad \text{w.p.} \geq 1-\delta \\
&\leq L_S^{\text{large margin}}(h_S) + 2\,\mathbb{E}[\mathcal{R}(\ell^{\text{Lipschitz}}, \mathcal{H}, S)] + \sqrt{\frac{\ln(4/\delta)}{2m}}
\end{aligned}
$$

Large Margins 2 [Anthony and Bartlett, 1999]

Theorem

Let $h_S \in \mathcal{H}$ be the output of a learning algorithm. Then, with probability at least $1 - \delta$,

$$L_{\mathcal{D}}^{\textit{0/1}}(h_S) \leq L_S^{\gamma\textit{-large margin}}(h_S) + 2\,\mathbb{E}[\mathcal{R}(\ell^{\gamma\textit{-Lipschitz}}, \mathcal{H}, S)] + \sqrt{\frac{\ln(4/\delta)}{2m}}.$$

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1. If h_S has **margin** $\geq \gamma$ on (most of) S, then $L_S^{\gamma\text{-large margin}}(h_S)$ is small

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1. If h_S has **margin $\geq \gamma$** on (most of) S, then $L_S^{\gamma\text{-large margin}}(h_S)$ is small
2. Lipschitz loss is $\frac{1}{\gamma}$-Lipschitz, so can apply **contraction lemma**:

$$\mathcal{R}(\ell^{\text{Lipschitz}}, \mathcal{H}, S) \leq \frac{1}{\gamma}\mathcal{R}\Big(\big\{(h(\boldsymbol{X}_1), \ldots, h(\boldsymbol{X}_m)) : h \in \mathcal{H}\big\}\Big)$$

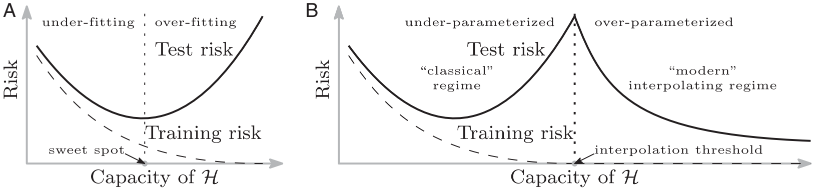
- So small changes in h imply small changes in loss
- We have **turned the classification problem into a regression task**!
- Complexity of $\mathcal{H}$ can be controlled by some norm on h.

Towards an Explanation

1. Large margins turn classification into regression
2. **Explaining double descent**

A Potential Explanation

[Belkin, Hsu, Ma, Mandal, 2019]



[Belkin et al., 2019] Double Descent

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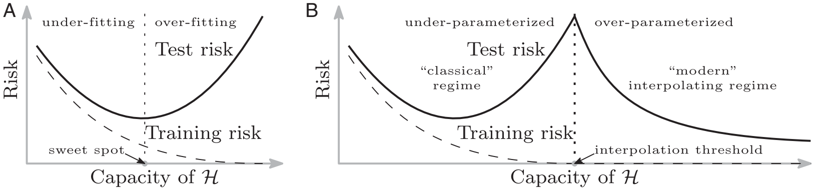

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Proposed explanation: suppose learning alg roughly behaves as

among **ERM solutions** $h_S \in \arg\min_{h \in \mathcal{H}} L_S(h)$

choose solution with **smallest norm** $\|h_S\|_{??}$

Below int. threshold: ERM unique → classical bias-variance trade-off
Above int. threshold: larger $\mathcal{H}$ → more ERM solutions → smaller $\|h_S\|_{??}$

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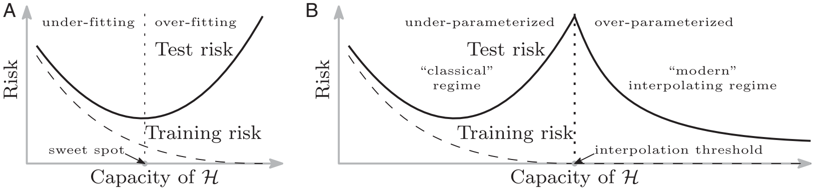

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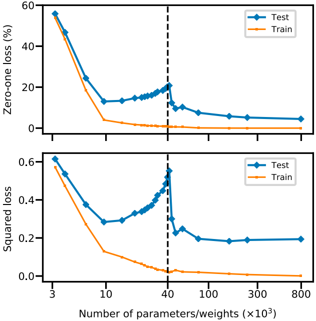
- L_S for e.g. logistic or squared loss (encouraging large margin)
- Different norm depending on manifestation of double descent

Double Descent for Neural Networks Again



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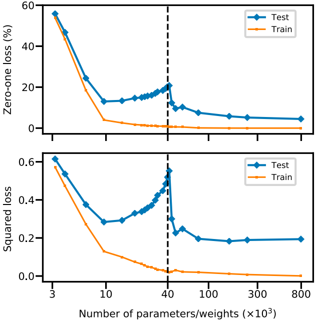
- Classification: CIFAR-10 32x32 images from 10 classes, e.g. airplanes, cats, dogs

Double Descent for Neural Networks Again



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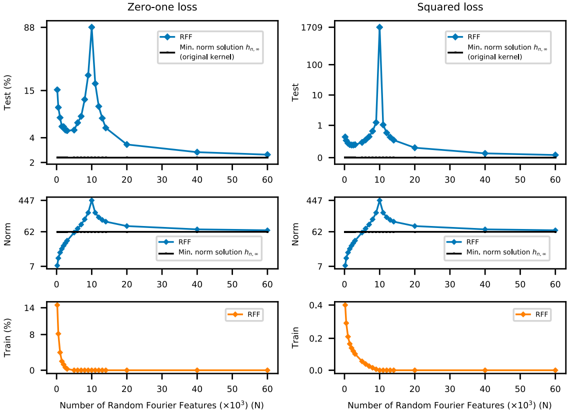
Which norm $\|h_S\|_{??}$?

Implicitly **induced by optimization algorithm!**

- Exist proposals in the literature to characterize norm.
  E.g. using neural tangent kernel [Jacot, Gabriel, Hongler, 2018]

Double Descent: Not Just for Neural Networks

[Belkin et al., 2019] reproduce double descent phenomenon on e.g. MNIST:



Random Fourier features: linear model over N randomly generated basis functions that approximate a certain (reproducing kernel) Hilbert space as $N \to \infty$

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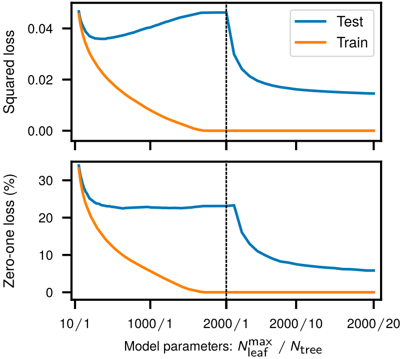


Random forests: ensembles of decision trees

- Complexity controlled by number of leaves per tree and by number of trees

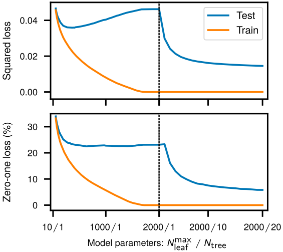
Recent Alternative Explanation [Curth, Jeffares, v.d. Schaar, 2023]: Need More Careful Parameter Counting

In all non-deep learning experiments by [Belkin et al., 2019]:

- Below interpolation threshold *m*: increase model complexity along dimension 1
- Above interpolation threshold *m*: increase model complexity along dimension 2

Examples:

- Random forests: [Belkin et al., 2019] increase depth of single tree up to *m* **(complexity dimension 1)**. Then average additional trees above *m* **(complexity dimension 2)**.



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Examples:

- Random forests: [Belkin et al., 2019] increase depth of single tree up to m **(complexity dimension 1)**. Then average additional trees above m **(complexity dimension 2)**.
- N Random Fourier features: equivalent to least squares on basis with dimension $\min(m, N)$, obtained by unsupervised dimensionality reduction. [Curth, Jeffares, v.d. Schaar, 2023]
  - Nr. of least squares parameters is $\min(m, N)$ **(complexity dimension 1)**.
  - Quality of dimensionality reduction improves with m **(complexity dimension 2)**.

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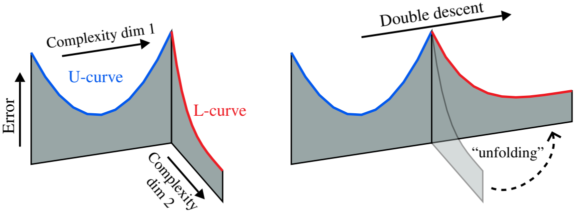

Double descent happens because experiments **stitch together two independent U-curves!**

Conclusion

- Exciting new attempts to understand the **double descent phenomenon** observed in deep learning, random Fourier features, random forests, etc.

- Crucial to understand true model complexity rather than counting parameters.

- Analysis involves tools like **Rademacher complexity** that you have learned in this course.

- Whether proposed explanations can be fully formalized for deep learning remains to be seen...

- In any case, the role of optimization algorithms in determining effective model complexity provides a **fascinating new frontier** for understanding the classical bias-variance trade-off!