Why do overparameterized neural networks generalize?

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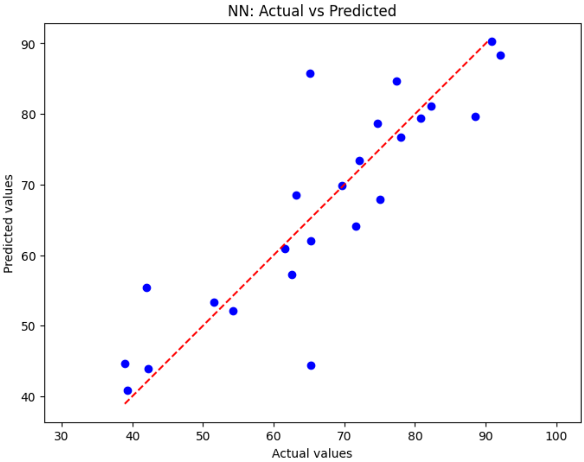
A real-world example



- A very small noisy satellite data with 118 rows and 12 features. The picture shows the performance of a neural network with roughly six million parameters trained on 94 points.

Statistical learning theory

- **Goal:** given i.i.d. samples (measurements) $(x_1, y_1), \dots, (x_N, y_N)$ from an unknown probability distribution μ over $\mathcal{X} \times \mathcal{Y}$, find a predictor $f : \mathcal{X} \to \mathcal{Y}$ from a given set $\mathcal{F}$ for which the risk

$$R(f) := \mathbb{E}_{(x,y)\sim\mu}[\ell(f(x), y)]$$

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Example (Linear regression)

We have $\mathcal{X} = \mathcal{Y} = \mathbb{R}$ and $\ell(y, y') := (y - y')^2$. Goal is to find a predictor f from

$$\mathcal{F} := \{\beta_1 x + \beta_0 \mid \beta_1, \beta_0 \in \mathbb{R}\}$$

with small risk.

Overfitting

- Since μ is unknown, we can not calculate $R(f)$ directly. In practice we estimate $R(f)$ by calculating its empirical risk with respect to our sample $S = \{(x_1, y_1), \ldots, (x_N, y_N)\}$:

$$R_S(f) := \frac{1}{N} \sum_{i=1}^{N} \ell(f(x_i), y_i)$$

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- If $\mathcal{F}$ is sufficiently expressive w.r.t. S, the problem of finding $f \in \mathcal{F}$ with small $R_S(f)$ is ill-posed: there are many predictors in $\mathcal{F}$ that have a small empirical risk, but many of them will overfit.

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  - Consider for example the case where $\mathcal{X} = \mathcal{Y} = \mathbb{R}$, $\ell(y, y') = |y - y'|$ and

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- How to find a predictor which also has a small risk?

Example: support vector machines and ℓ_2-regularization

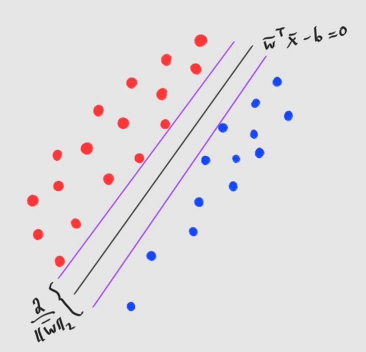
- Let $\mathcal{X} = \mathbb{R}^d, \mathcal{Y} = \{-1, 1\}$ and

$$\ell(y, y') = \begin{cases} 1 & \text{, if } y \neq y' \\ 0 & \text{, otherwise} \end{cases}$$

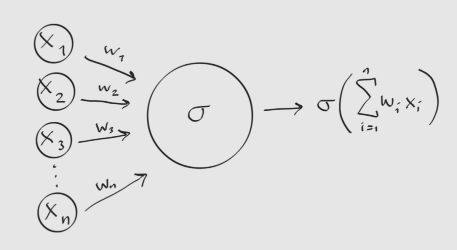
  Set

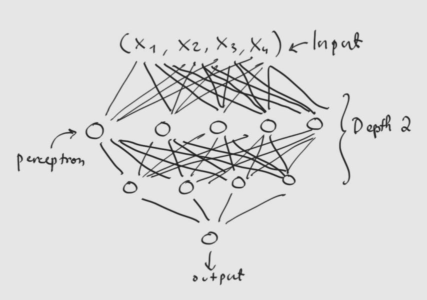
$$\mathcal{F} := \{\text{hyperplanes in } \mathbb{R}^d\}.$$

  If $S \subseteq \mathbb{R}^d \times \{-1, 1\}$ is linearly separable, then there are many predictors in $f \in \mathcal{F}$ for which $R_S(f) = 0$. The main idea in support vector machines is that we should select a hyperplane with a minimal norm.



Neural networks





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- The main optimization algorithm that is used to train modern neural networks is the stochastic gradient descent (SGD), which is a "noisy" variant of GD. At each step of the iteration the current vector of weights $\overline{w}$ are updated as follows: go through the points x in the sample S in a random order and for each of them do

$$\overline{w} \leftarrow \overline{w} - \eta \nabla R_{\{x\}}(\overline{w})$$

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Example

The CIFAR-10 image classification benchmark has 50000 training examples spread across 10 classes. The following table demonstrates the performance of a common architecture, called Inception, on CIFAR-10. Inception has more than 1.5 million parameters.

ℓ_2-regularization	Train accuracy	Test accuracy
Yes	100.0	86.03
No	100.0	85.75

Table: Inception on CIFAR-10.

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- Furthermore, architectures that have less parameters than the number of sample points seem to be more prone to overfit.

Implicit regularization

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- The nature of this regularization is not clear and it seems to depend on SGD having a good initialization. E.g. Liu et al. (2019) gave a simple way of initializing the weights in such a way that SGD does not learn a “simple” model. (This was also mentioned in Nakkiran et al. (2019).)

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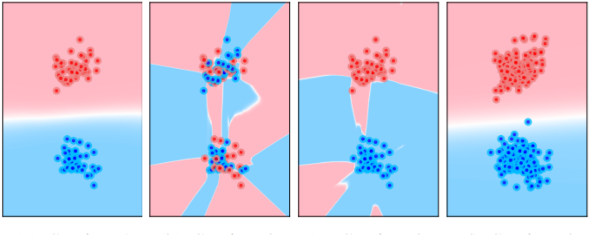

Figure: Picture from Liu et al. (2019)

Flat minimas

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- The correspondence between flat minimas and good models was emphasized already by Hochreiter and Schmidhuber (1997), who designed a learning algorithm that explicitly preferred flat minimas.
- As far as I can tell, there is no water-proof explanation for why SGD is able to find flat minimas in the overparameterized region.

Nice loss landscape

- Somewhat surprisingly, Chiang et al. (2023) demonstrated empirically that in the over-parameterized regime "most" weights that work on the sample work also outside the sample. That is, in principle one can replace SGD with a random guessing.

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Nice loss landscape

- Somewhat surprisingly, Chiang et al. (2023) demonstrated empirically that in the over-parameterized regime “most” weights that work on the sample work also outside the sample. That is, in principle one can replace SGD with a random guessing.
- More generally, they argue that the use of gradient-based optimizers is not the main source of generalization behavior of neural networks.
- The experiments were limited to the small-sample regime, so verifying them in a more realistic setting is an interesting research direction.

That's all folks!

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