Towards a Deeper Understanding of Neural Networks

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Motivation

Important questions about neural networks:

1. What functions can be expressed by neural networks?
2. When does low empirical risk imply low expected risk?
3. Why do algorithms such as SGD often find good weights?

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3. Why do algorithms such as SGD often find good weights?

Focus: Why can we find good weights for NNs?

Paper Overview

- A NN learns a higher-dimensional representation of your data.
- How does that representation change with the weights?

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"Theorem": If our neural network has:

- enough redundancy
- random weights (no training),

then with high probability the neural network will encode "the same" representation of your data.

So what?

- Gives evidence for random initialization of weights.
- No need to train the hidden layer weights!
- Reduces neural network training to a *convex* problem.

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Still...

- Empirical evidence supports some of these claims.
- Better theoretical constants in the works?

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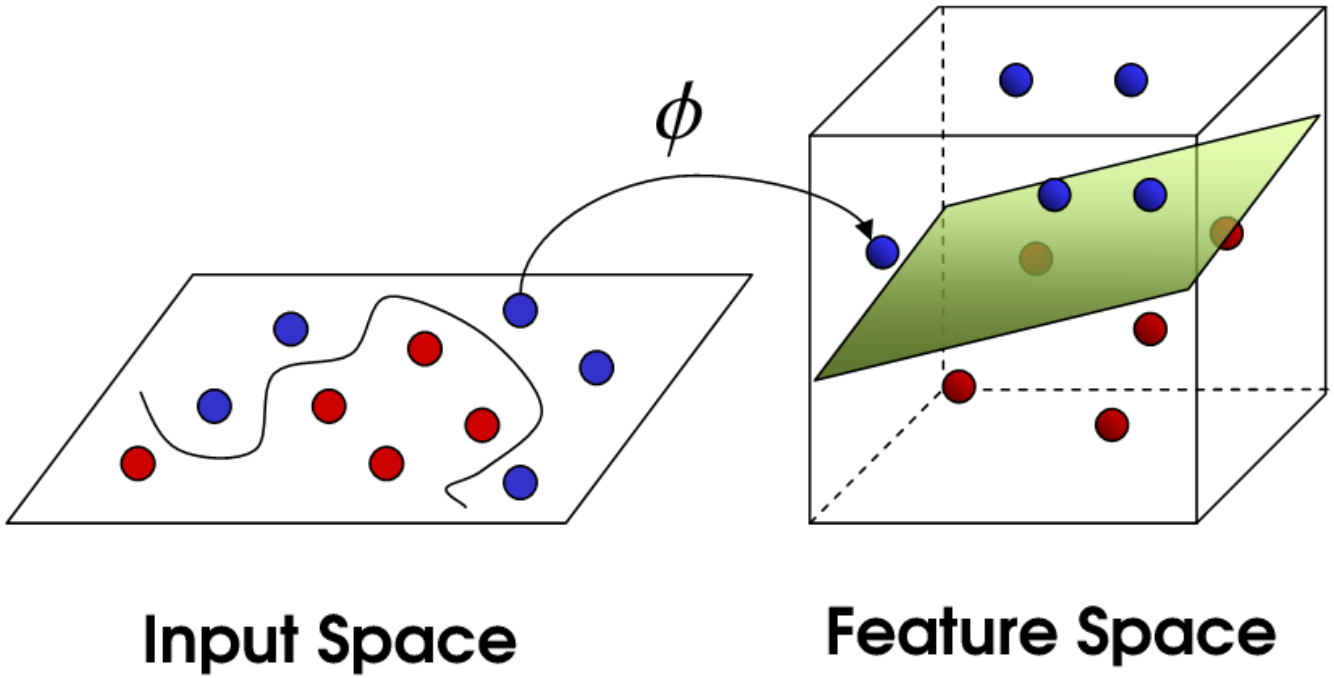

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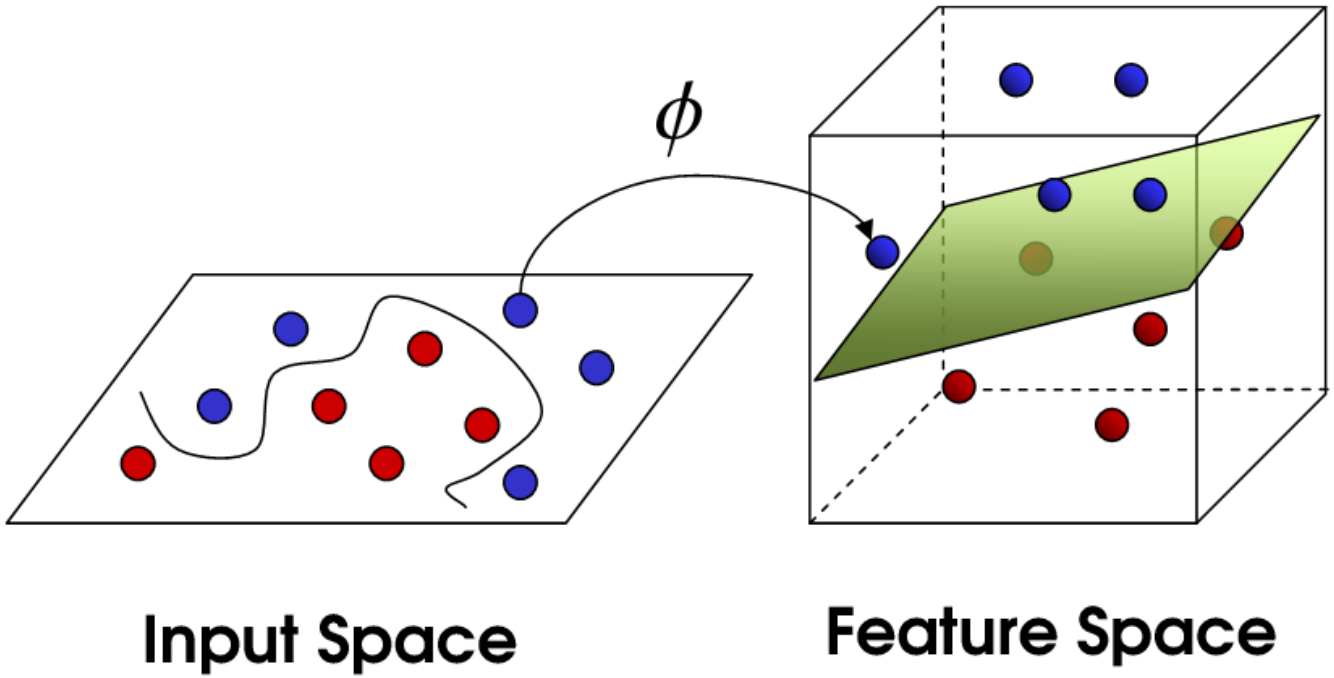

Want a map $\phi : X \to \mathcal{H}$, where $\mathcal{H}$ is a "nice" higher dimensional space.
This gives us a more rich representation of our data.

Kernels

To do machine learning on $\mathcal{H}$, we want a similarity measure.

- Mathematically, we want $\mathcal{H}$ with inner product $\langle x, y \rangle_{\mathcal{H}}$

For $x, y \in X$, define the **kernel** of $\mathcal{H}$ by:

$$K(x, y) = \langle \phi(x), \phi(y) \rangle_{\mathcal{H}}$$

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Examples:

$$K(x, y) = \langle x, y \rangle \leftrightarrow \phi(x) = x$$
$$K(x, y) = \langle x, y \rangle^p \leftrightarrow \phi(x) = (1, x, x^2, \ldots, x^p)$$
$$K(x, y) = \exp(-||x - y||) \leftrightarrow \phi(x) = e^{-x^2}(1, x, x^2, \ldots)$$

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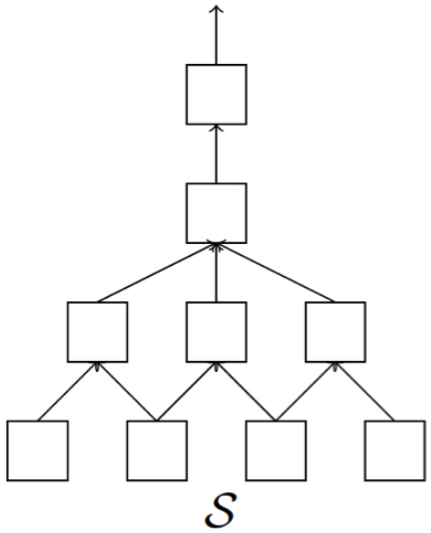
Bottom line: Kernels correspond to representations of your data.

The Computational Skeleton:



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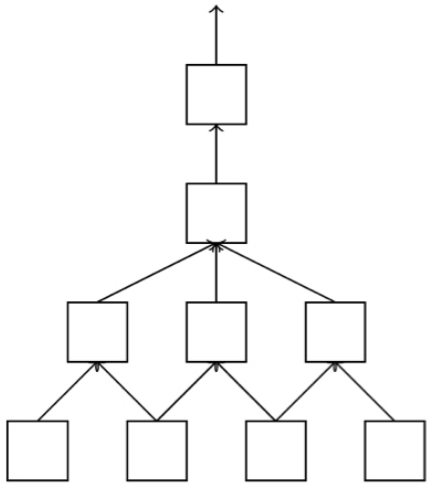

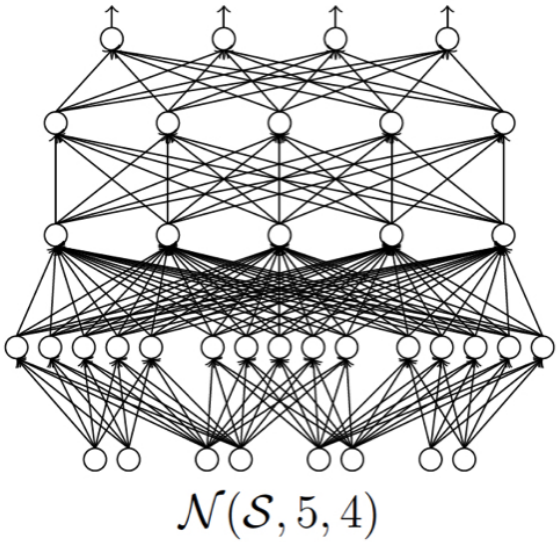

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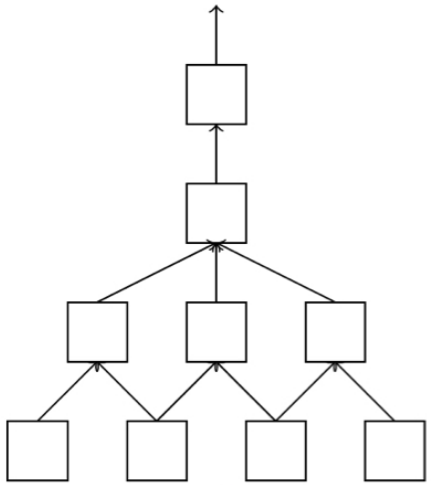
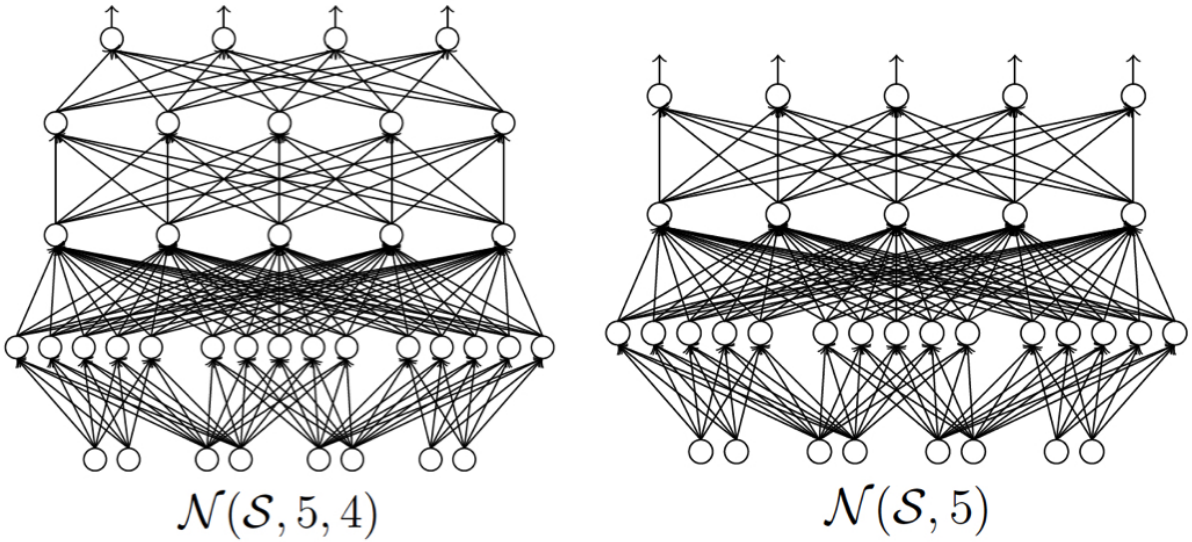
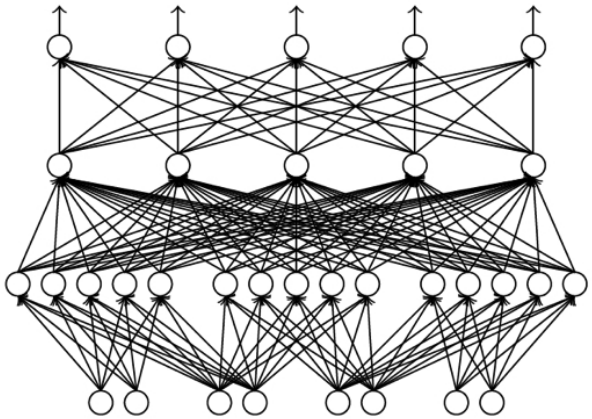




Computational Skeletons to Kernels:

w - given weights on edges of $\mathcal{N}(S, r)$

v - output node in representation



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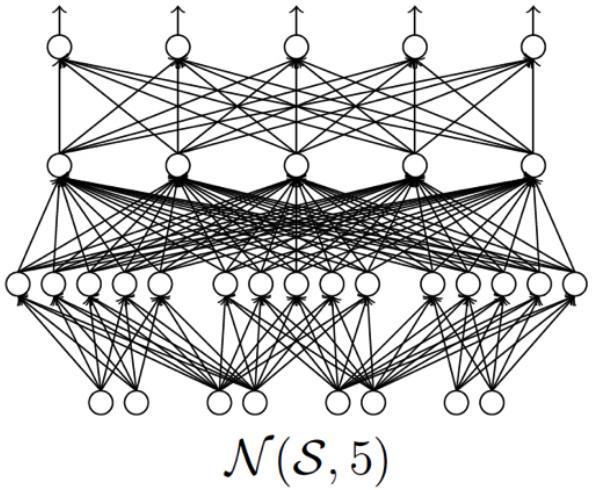

Empirical Kernel κ_w:

$$\Psi_w(x) \approx \text{ vector of (normalized) outputs indexed by } v$$

$$\kappa_w(x, x') = \langle \Psi(x), \Psi(x') \rangle$$

"Theoretical" Kernel:

Compositional Kernel κ_S:

Inductively define a kernel κ_v for each node v as follows:

- For an input node v define $\kappa_v(x, y) = \langle x, y \rangle$.
- For a non-input node v define

$$\kappa_v = \hat{\sigma}_v \left(\frac{\sum_{u \in \text{in}(v)} \kappa_u(x, y)}{|\text{in}(v)|} \right)$$

Pretend there is a single output node o, $\kappa_S = \kappa_o$

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Dual Activation $\hat{\sigma}$:

Let $\Sigma_\rho = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix}$. Given an activation σ, the dual activation $\hat{\sigma} : [-1, 1] \to \mathbb{R}$ is defined as

$$\hat{\sigma}(\rho) = \mathop{\mathbb{E}}_{X, Y \sim \mathcal{N}(0, \Sigma_\rho)} \sigma(X)\sigma(Y)$$

Main Theorem:

Theorem:
ReLU activations, a random initialization of weights $w \sim \mathcal{N}(0, 1)$.
If

$$r \geq \frac{\text{depth}^2(S) \log(|S|/\delta)}{\epsilon^2}$$

Then for all x, x', with probability at least $1 - \delta$,

$$|\kappa_w(x, x') - \kappa_S(x, x')| \leq \epsilon$$

"Proof":

- An activation σ is (α, β, γ)-**decent** if the following holds:
  - The dual activation $\hat{\sigma}$ is β - Lipschitz (in a specific sense)
  - Concentration : for X_i, Y_i $i = 1, \ldots r \sim \mathcal{N}(0, \Sigma_\rho)$

$$\Pr\left(\left|\frac{\sum_i \sigma(X_i)\sigma(Y_i)}{r} - \hat{\sigma}(\rho)\right| \geq \epsilon\right) \leq 2\exp\left(-\frac{r\epsilon^2}{2C^4}\right)$$

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- **Lemma :** ReLU is decent.
  - Measure concentration property from standard concentration bounds for sub-exponential random variables.
  - $\hat{\sigma}$ is Lipschitz - work.
- **Theorem:** For (α, β, γ)-decent activations, random weights w for

$$r \geq \frac{2\alpha^2(\sum_{i=1}^{\text{depth}} \beta_i)^2 \log(|S|/\delta)}{\epsilon^2}$$

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  - Saxe et al., 2011, *On random weights and unsupervised feature learning*
  - Metrics induced by the initial and fully trained representations are not substantially different
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  - Metrics induced by the initial and fully trained representations are not substantially different
  - Giryes et al. demonstrated for the MNIST and CIFAR-10 datasets
- Usefulness of ReLU – even for quite deep networks with ReLU activations, random initialization approximates the corresponding kernel.